Procedure for Evaluating Tritium Source Term in VHTR using McCARD

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1. Introduction

In the hydrogen production process by high-temperature steam electrolysis with the very high-temperature gas-cooled reactor (VHTR), tritium can be permeated as an impurity in the produced hydrogen. The concentration evaluation of such tritium is one of the key technical issues in the licensing of nuclear hydrogen production systems. In VHTRs, helium gas coolant circulates through the entire system and can transport tritium mixed with it, so an accurate assessment of tritium behavior is required. Previously, when evaluating the behavior of tritium, a conservative view was taken to predict and evaluate the tritium source term. In order to improve the accuracy of the analysis, KAERI is conducting research to accurately predict the tritium source term in the reactor core through Monte Carlo particle transport analysis.

In this paper, we developed a procedure to evaluate the tritium source term using McCARD [1], a Monte Carlo neutron transport analysis code developed by Seoul National University. Based on the evaluation procedure, tritium production is evaluated for the VHTR benchmark core [2] being developed at KAERI and compared with the results and trends in the existing literature [3].

2. Methodology

In this section some of the techniques used to model the detector channel are described.

2.1 Generation and Loss of Tritium

The main reactions that generate tritium in VHTR are as follows:

- Ternary fission
- Li-6 (n,α) H-3 or Li-6 (n,t) He-4
- Li-7 (n,nα) H-3
- He-3 (n,p) H-3
- B-10 (n,2α) H-3 or B-10 (n,t) Be-8
- B-10 (n,α) Li-7 (chain reaction)

Table I is a survey of the nuclear reaction cross section libraries provided for the tritium production model in the major widely used cross section libraries.

2.2 Calculations in McCARD

McCARD has a built-in depletion module based on the ORIGEN2 code. It allows you to measure nuclide abundance changes due to (n,γ), (n,α), (n,p), (n,2n), (n,3n), (n,fission) reactions and decay. However, there are several issues that need to be addressed in the evaluation of tritium source terms using the McCARD depletion module.

First, the depletion module does not handle the some tritium-producing reactions such as (n,2α), (n,nα), and (n,t) mentioned in section 2.1; a special exception is made for the (n,t) reaction of Li-6, which is treated as an (n,α) reaction. Therefore, it is necessary to handle (n,t) reactions and add exceptions for specific reactions.

Second, in order to evaluate the tritium source term through the depletion module, a depletion analysis must be performed on every cell including coolant and cladding cells, which requires excessive computing time and memory usage.

Therefore, it is a realistic alternative to estimate the reaction rates for the generation and loss of tritium and thus evaluate the net tritium production rate. For this purpose, a module which estimates the macroscopic and microscopic reaction rates for all nuclear reactions was added to the McCARD.

Table I: Tritium-generating Reaction Forms from Various Evaluated Nuclear Cross-section Data Libraries [4]

	ENDF/B -VII.1	**ENDF/B -VIII.0**	**JEFF -3.3**	**JENDL -5.0**	**CENDL -3.2**	**BROND -3.1**
Nation, Year	USA, 2011	USA, 2018	Europe, 2017	Japan, 2021	China, 2020	Russia, 2016
(n,t) reactions*	182	243	434	676	242	200
Li-6(n,α)H-3	(n,t)	(n,t)	(n,t)	(n,t)	(n,α)	(n,t)
He-3(n,p)H-3	(n,p)	(n,p)	(n,p)	(n,p)	(n,p)	(n,p)
B-10(n,2α)H-3	(n,t+2α)	(n,t+2α), (n,t')	(n,t+2α)	(n,t)	(n,t+2α)	(n,t+2α)
Li-7(n,nα)H-3	None	None	None	(n,Xt)	(n,n+α)	None

* Number of nuclides containing a cross-section data of (n,t) reaction

The number density of tritium generated in each cell is calculated using Eq. (1).

$$\frac{\partial N_T}{\partial t} = \underbrace{\sum_i \int \left(y_T^i \Sigma_f^i + \Sigma_{T,P}^i \right) \phi d\boldsymbol{P}}_{\equiv R} - N_T \underbrace{\left(\lambda^T + \int \sigma_{(n,Xn)}^T \phi d\boldsymbol{P} \right)}_{\equiv \ell} \qquad (1)$$

N_T : tritium number density

y_T^i : tritium yield per fission of isotope i

Σ_f^i : macroscopic fission cross-section of isotope i

$\Sigma_{T,P}^i$: macroscopic cross-section for the tritium production reaction of isotope i

ϕ : neutron flux

$\mathbf{P}$: phase space $(\mathbf{r}, E, \mathbf{\Omega})$

λ^T : tritium decay constant

$\sigma_{(n,Xn)}^T$: microscopic cross-section for the (n, Xn) reactions of tritium

The reaction rate calculations are performed at each burnup step, and linear interpolation is used between the steps. The $(n,2n)$ reaction of tritium is a high-energy reaction, so it has very little ratio in the thermal neutron reactor VHTR and the loss term of tritium is dominated by decay ($\ell \equiv \lambda^T + \int \sigma_{(n,Xn)}^T \phi d\boldsymbol{P} \simeq \lambda^T$).

Therefore, $N_T^{(n+1)}$ can be calculated from $N_T^{(n)}$, $R^{(n)}$, and $R^{(n+1)}$ as shown in Equation (2). The superscript (i) denotes the i-th burnup step and $T^{(i)}$ denotes the time at the i-th step.

$$N_T^{(n+1)} = \left[N_T^{(n)} - \frac{R^{(n)} - a^{(n)}}{\ell} \right] exp\,[-\tau] + \frac{R^{(n+1)} - a^{(n)}}{\ell}; \quad (2)$$
$$\left(a^{(n)} \equiv \frac{R^{(n+1)} - R^{(n)}}{\tau},\ \tau \equiv \ell \left(T^{(n+1)} - T^{(n)} \right) \right).$$

3. Numerical Results

KAERI is developing a VHTR-350 benchmark core [3] to verify VHTR performance evaluation technology. The VHTR-350 is a 950°C benchmark core based on the MHTGR-350 benchmark core [5]. The radial and axial cross-sectional views of the VHTR-350 core are shown in Fig. 1. To test the tritium production evaluation procedure, VHTR-350 benchmark calculations were performed with impurity data as shown in Table II. McCARD calculations are performed using ENDF/B-VIII.0 libraries [6].

Table II. Impurity data [ppm] for VHTR-350

Region		B	Li	He-3
Coolant		-	-	0.2
Graphite Block	Active Core	41.0	0.036	-
	Reflector	2.0	0.036	-
Control Rod		-	0.27	-

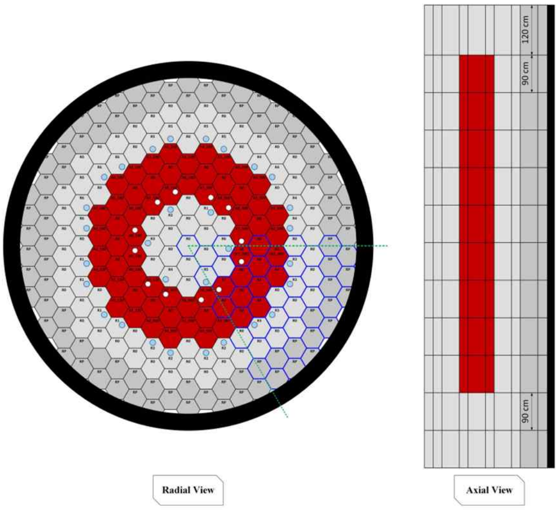

Fig. 1. Cross Sectional Views of the VHTR-350 core

Table III summarize the computed results. The results were obtained after performing the rod-wise fuel and block-wise graphite burnup analysis for 1500 Effective Full Power Days (EFPD) with a thermal power of 350 MW$_{th}$. The maximum relative standard deviation of the calculated reaction rate is about 0.4%.

Reference 3 lists the results of tritium birth rate calculations for several high temperature gas-cooled reactors. It shows that "the tritium birth rate per unit power (MW$_{th}$) ranges from 2.14×10^{11} to 4.28×10^{11} Bq/yr/MW$_{th}$". The VHTR-350 results of 3.81×10^{11} Bq/yr/MW$_{th}$ calculated with McCARD shows a similar trend with the reference results. Since tritium birth is strongly influenced by impurity (He-3, Li-6, B-10), it is necessary to use the same impurity data for future calculations for accurate comparisons.

4. Conclusions

In this study, we reviewed the methodology for evaluating the tritium source term for high-precision tritium analysis in VHTRs for hydrogen production, developed the necessary modules for the calculation, and summarized the evaluation procedure. The nuclear reactions that produce tritium were investigated, and the methods provided by various nuclear reaction cross-section libraries were investigated. We also explored how to calculate the tritium source term using McCARD, and adopted the method of calculating the tritium source term through reaction rate calculation. The procedure was applied to the VHTR-350 benchmark and a reactor-wide tritium production rate calculations were performed. The results of the analysis were found to be similar to those of the commonly known sources of tritium in VHTRs.

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Table III. Evaluation results for the tritium activity [Bq/yr/MW$_{th}$] in the VHTR-350 benchmark core with the impurity data

Region		**fission**	**He-3**	**Li-6**	**B-10**	**B-11**	**Other**	**Total**
Reflector	Top	-	1.45E+09	5.44E+09	2.01E+06	1.08E+02	1.07E+00	6.90E+09
	Bottom	-	3.56E+09	1.05E+10	2.92E+06	1.77E+02	2.94E+00	1.40E+10
	Inner	-	2.29E+09	7.59E+09	1.56E+06	1.04E+03	7.98E+01	9.88E+09
	Outer	-	6.93E+09	3.09E+10	6.14E+06	2.30E+03	1.38E+02	3.79E+10
	Permanent	-	2.19E+09	2.14E+10	5.17E+06	4.27E+00	2.87E-04	2.35E+10
Control Rod		-	1.64E+06	2.36E+05	7.24E+09	2.27E+04	4.84E+02	7.24E+09
Active Core Top	Inner	1.82E+10	1.67E+09	1.44E+09	1.63E+09	2.79E+05	2.66E+04	2.29E+10
	Middle	2.91E+10	1.39E+09	1.63E+09	3.18E+09	5.24E+05	4.05E+04	3.53E+10
	Outer	2.66E+10	2.01E+09	1.87E+09	2.35E+09	3.55E+05	3.12E+04	3.29E+10
Active Core Middle	Inner	1.99E+10	1.79E+09	1.47E+09	1.78E+09	2.79E+05	3.14E+04	2.49E+10
	Middle	3.13E+10	1.45E+09	1.66E+09	3.43E+09	5.60E+05	4.84E+04	3.78E+10
	Outer	2.88E+10	2.15E+09	1.92E+09	2.55E+09	3.91E+05	3.59E+04	3.54E+10
Active Core Bottom	Inner	1.87E+10	1.57E+09	1.43E+09	1.73E+09	2.76E+05	2.35E+04	2.34E+10
	Middle	2.92E+10	1.30E+09	1.60E+09	3.31E+09	5.61E+05	4.45E+04	3.54E+10
	Outer	2.68E+10	1.87E+09	1.85E+09	2.47E+09	3.72E+05	3.64E+04	3.30E+10
Total		**2.29E+11**	**3.16E+10**	**9.07E+10**	**2.97E+10**	**3.62E+06**	**3.19E+05**	**3.81E+11**
Ratio		60.06%	8.31%	23.83%	7.80%	0.00%	0.00%	100.00%