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Development of a Tritium Analysis Module for COPA code

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1. Introduction

In a high-temperature gas-cooled reactor (HTGR), tritium is one of the major radionuclides that provides radiation exposure to workers and environment, so its evaluation is very important. Several computer codes have been developed to evaluate the distribution and release of tritium in/from an HTGR. Most computer codes input the tritium release fraction from core structures to a coolant as a single value without calculating it. However, the TBEC code [1] calculates the release fraction by obtaining an analytical solution for the migration of tritium in the SiC layer of a coated fuel particle (CFP) and the graphite of a fuel element. It is assumed that the PyC layer does not impede the migration of tritium. The COPA code [2] calculates the transport of fission products in all layers of a coated fuel particle and in a fuel element through numerical analysis, and presents the amount of fission products released to the coolant. This can be applied to the currently developed HTGR tritium analysis model.

This study treats the development of a COPA tritium analysis module that combines the COPA code fission product release calculation model with the TRITGO code [3] tritium analysis model.

2. Tritium Analysis Models

2.1. Tritium production and distribution

Tritium is produced in fuel or graphite and released from them into a coolant. It is also generated through the neutron reaction ^{3}He(n,p)^{3}H in a coolant, and some is recoiled into a graphite. Table I presents the tritium production rate from various sources in an HTGR.

Tritium in a coolant disappears through leak, purification, permeation and decay. The change in the number of tritium atoms in a coolant can be expressed as the following first-order ordinary differential equation:

$$\frac{dN_{T,i}^{(cool)(j)}}{dt} = \alpha_i^{(j)} Q_i^{(j)} - \lambda N_{T,i}^{(cool)(j)}, \quad (19)$$

where $N_{T,i}^{(cool)}$ is the number of tritium atoms in a coolant (atom), α is $f_{rel}/(1+\xi)$ for the tritium sources *fuel*, *Li-6, Li-7, B-10(fast), B-10(therm), C-12, Be-9* and $(1-f_{recoil})/(1+\xi)$ for the tritium source *He-3*, f_{rel} is the fraction of tritium atoms produced in a solid material and released into a coolant (dimensionless), f_{recoil} is the fraction of tritium atoms produced in a coolant and recoiled into a graphite, ξ is an sorption ratio which means the ratio of the number of hydrogen atoms sorbed on a graphite surface to the number of hydrogen atoms in the primary coolant (dimensionless), Q_i is the production rate (atom/s) (*KPY* for *fuel*, $a_1 N_{Li-6}^{(prod)}$ for *Li-6*, $a_2 N_{Li-7}^{(prod)}$ for *Li-7*, $a_3 N_{B-10}^{(prod)}$ for *B-10*(*fast*), $a_2 N_{Li-7}^{(prod)}$ for *B-10*(*therm*), $a_1 N_{Li-6}^{(prod)}$ for *C-12*, $a_1 N_{Li-6}^{(prod)}$ for *Be-9*, $a_7 N_{He-3}^{(prod)}$ for *He*-3), L is the loss rate ((leak rate + purification rate + permeation rate)/(1+ξ) + decay constant) (s^{-1}) and the subscript i means the tritium sources *fuel*, *Li-6*, *Li-7*, *B-10*(*fast*), *B-10*(*therm*), *C-12*, *Be-9*, and *He-3*.

2.2. Tritium release

A tritium transport and temperature distribution within a fuel element can be described by the following Fickian diffusion equation and steady state heat transfer equation, respectively:

$$\frac{\partial C_i(r,t)}{\partial t} = \dot{S}_i(r,t) - \lambda C_i(r,t) + \frac{1}{r^z}\frac{\partial}{\partial r}\left[r^z D_i \frac{\partial C_i(r,t)}{\partial r}\right], \quad (20)$$

$$0 = \dot{q}_i(r,t) + \frac{1}{r^z}\frac{\partial}{\partial r}\left[r^z k_i \frac{\partial T_i(r,t)}{\partial r}\right], \quad (21)$$

where r is the r coordinate (m), t is the time (s), the subscript i means a layer in a fuel element, the superscript z is 0 for a slab, 1 for a cylinder, 2 for a sphere, C is the tritium concentration (mol/m^3), $\dot{S}$ is the volumetric generation rate of tritium (mol m^{-3} s^{-1}), λ is the decay constant of tritium (s^{-1}), D is the diffusion coefficient of tritium (m^2/s), T is the temperature (K), $\dot{q}$ is the volumetric heat generation rate (W/m^3), and k is the thermal conductivity (W m^{-1} K^{-1}). The generation term is the volumetric tritium release rates from the intact, defective and broken coated fuel particles (CFPs), the volumetric birth rate due to nuclear fissions of heavy metal contamination in the solid material, and the volumetric generation rates due to the neutron capture reactions of source nuclides present in a fuel element:

$$\dot{S}_i(r,t) = n\sum_{j=0}^{NF} f_j \dot{R}_{CFP,j} + f_{HM}\dot{B}_{fission} + \dot{B}_{\mathrm{reaction}}, \quad (22)$$

where n is the CFP density (particles/m^3), the subscript j means the specific failure mode of a CFP, NF is the total number of failure modes of a CFP, f is the failure fraction, $\dot{R}_{CFP}$ is the release rate from a CFP into a fuel matrix (mol/s), f_{HM} is the heavy metal contamination fraction, $\dot{B}_{fission}$ is the volumetric birth rate due to nuclear fission (mol m^{-3} s^{-1}), and $\dot{B}_{\mathrm{reaction}}$ is the

volumetric birth rate due to neutron capture reactions (mol m^{-3} s^{-1}).

In order to calculate the tritium release from a CFP into a fuel matrix, the tritium transport and temperature distribution within a CFP must be evaluated. They can be described by the following Fickian diffusion equation and steady state heat transfer equation, respectively:

$$\frac{\partial C_i(r,t)}{\partial t} = \dot{B}_i(r,t) - \lambda C_i(r,t) + \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2 D_i \frac{\partial C_i(r,t)}{\partial r}\right], \quad (23)$$

$$0 = \dot{q}_i(r,t) + \frac{1}{r^2}\frac{\partial}{\partial r}\left[k_i r^2 \frac{\partial T_i(r,t)}{\partial r}\right], \quad (24)$$

where r is the radial coordinate (m), t is the time (s), the subscript i means a CFP layer (K for kernel, B for buffer, I for IPyC, S for SiC, O for OPyC), C is the tritium concentration (mol/m^3), $\dot{B}$ is the volumetric birth rate of tritium (mol m^{-3} s^{-1}), D is the diffusion coefficient of tritium (m^2/s), T is the temperature (K), $\dot{q}$ is the volumetric heat generation rate (W/m^3), and k is the thermal conductivity of a CFP layer (W/(m K)). The volumetric birth rate of tritium in a layer i can be given by:

$$\dot{B}_i(\mathrm{r,t}) = \left[f_{HM,i} + \pi\left(\eta r_i^2 - \eta^3/12\right)\right] Y \dot{F}/N_A, \quad (25)$$

where f_{HM} is the heavy metal contamination fraction, Y is the fission yield (atom/fission), $\dot{F}$ is the fission density rate (fissions m^{-3} s^{-1}), N_A is the Avogadro's number, η is the recoil length (m), and r_i is the radial position of outer surface of layer i (m).

The fraction of tritium released from nuclear fuel or graphite to coolant is the ratio of a cumulative release amount to a cumulative production amount:

$$f_{rel} = \frac{e^{-\lambda t}\int_0^t \dot{R}_V e^{\lambda x} dx}{e^{-\lambda t}\int_0^t \dot{S}_V e^{\lambda x} dx}, \quad (26)$$

where $\dot{R}_V$ is the tritium release rate (mol/s) and $\dot{S}_V$ is the tritium generation rate (mol/s).

3. Development of a COPA Tritium Analysis Module

Module FPRF of the COPA code calculates the temperature distribution of a CFP and a fuel element, the transport of fission products in them, and the release of fission products from a fuel to a coolant. Therefore, the fraction of tritium released to the coolant over time can be calculated. This mechanistic fractional release can be directly applied to the tritium analysis model to calculate tritium release from a solid to a coolant. A FORTRAN program was developed for the above solution procedure and the completed program was inserted into the COPA code under the module name TRIT, as shown in Fig. 1. The module TRIT can evaluate tritium release according to the tritium diffusion in a CFP and a fuel element and the failure behavior of the CFP coating layers.

4. Test Calculations

The tritium release from an HTGR was calculated using the developed module TRIT. Table II shows the design and operation parameters of an HTGR for the tritium release calculation. Table III shows the reactor regions where tritium is generated in an HTGR and the related data. Table IV shows the diffusion coefficients of tritium used in the calculation. In the case of "SiC diffusion", the value is recommended in Ref. [4], and in the case of "PyC+SiC diffusion", the diffusion coefficient of Kr was applied instead. Fig. 2 shows the failure fraction of the coating layers used in the calculation. The SiC layer started to fail at 13244 days. Fig. 3 shows the tritium release fraction. It increases over time and tends to depend on the failure mode and failure fraction. Fig. 4 shows the amount of tritium released into the environment. Calculations were performed for three cases: (1) SiC diffusion-COPA release fraction-failure fraction, (2) PyC+SiC diffusion-COPA release fraction- failure fraction, and (3) the cases of release fraction 0.05 from the nuclear fuel and release fraction 1 from the graphite. The release amount in Case (3) is about 10 times larger than those in Cases (1) and (2). The tritium release amount in the case of PyC+SiC diffusion is slightly smaller than that in the case of SiC diffusion, but the difference disappears as the CFP coating layers break.

Table II: Design and operation parameters of an HTGR

Parameter	Value
Thermal output (MW)	350
Core power density (W/cm^3)	5.9
Weight of helium in coolant (kg)	2948
Coolant pressure (MPa)	6.38
Coolant temperature (°C)	471.5
Fraction of ^{3}He in coolant	2×10^{-7}
Hydrogen content in coolant (ppmH_2)	10
Helium makeup rate (s^{-1})	3.17×10^{-9}
Coolant purification rate (s^{-1})	9.50×10^{-4}
Weight of water in steam generator (kg)	6.078×10^{4}
Makeup of water in steam generator (kg/day)	6.078×10^{3}

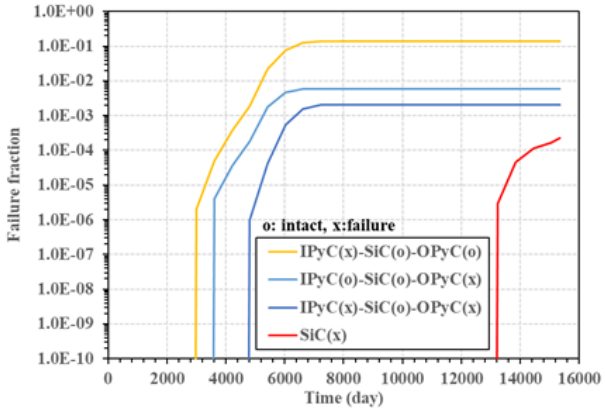

Fig. 2. Failure fraction of coating layers of coated fuel particles.

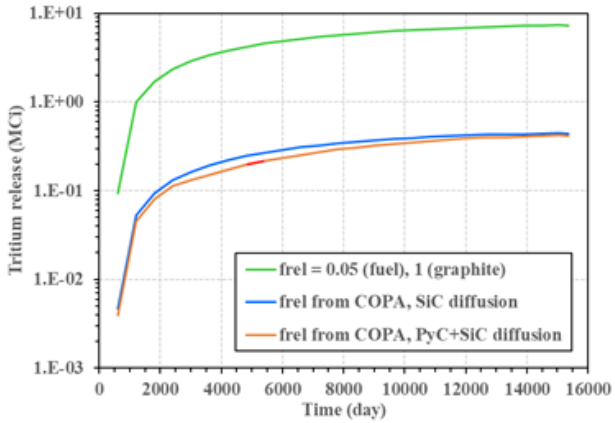

Fig. 4. Radioactivity of tritium released to environment.

5. Summary

An HTGR tritium analysis module TRIT was developed by combining the fission product analysis module FPRF of the COPA code and the tritium analysis model of the TRITGO code. The tritium release fraction from nuclear fuel and graphite can be directly calculated within TRIT. In addition, the effects of the CFP failure and the tritium diffusion in a CFP and a fuel element can be included. As a result of the test calculation, the influence of the failure behavior was well reflected in the calculated tritium release fraction. When the tritium release fraction was directly calculated in TRIT, the tritium release amount was estimated to be lower than when it was analyzed by setting it to a constant value. Currently, only the tritium diffusion data in the SiC layer are presented, and a large value (for example, 1×10^{-6} m^2/s) is assigned as the diffusion coefficient for the kernel, buffer, and PyC layer graphite, meaning that they are all released. If experimental data on these are secured, the tritium release amount can be estimated to be lower than the current value.

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Table I: Tritium sources and production rates

Source	Notation	Production rate
Ternay fission	*fuel*	$\frac{dN_{T,fuel}^{(prod)(j)}}{dt} = KP^{(j)}Y - \lambda N_{T,fuel}^{(prod)(j)}$ (1)
$^{6}Li(n,\alpha)^{3}H$	*Li-6*	$\frac{dN_{Li-6}^{(prod)(j)}}{dt} = -a_1 N_{Li-6}^{(prod)(j)}$ (2) $\frac{dN_{T,Li-6}^{(prod)(j)}}{dt} = a_1 N_{Li-6}^{(prod)(j)} - \lambda N_{T,Li-6}^{(prod)(j)}$ (3)
$^{7}Li(n,n\alpha)^{3}H$	*Li-7*	$\frac{dN_{Li-7}^{(prod)(j)}}{dt} = -a_2 N_{Li-7}^{(prod)(j)}$ (4) $\frac{dN_{T,Li-7}^{(prod)(j)}}{dt} = a_2 N_{Li-7}^{(prod)(j)} - \lambda N_{T,Li-7}^{(prod)(j)}$ (5)
$^{10}B(n,2\alpha)^{3}H$	*B-10(fast)*	$\frac{dN_{B-10}^{(prod)(j)}}{dt} = -(a_3 + a_4) N_{B-10}^{(prod)(j)}$ (6) $\frac{dN_{T,B-10(fast)}^{(prod)(j)}}{dt} = a_3 N_{B-10}^{(prod)(j)} - \lambda N_{T,B-10(fast)}^{(prod)(j)}$ (7)
$^{10}B(n,\alpha)^{7}Li(n,n\alpha)^{3}H$	*B-10(therm)*	$\frac{dN_{B-10}^{(prod)(j)}}{dt} = -(a_3 + a_4) N_{B-10}^{(prod)(j)}$ (6) $\frac{dN_{Li-7,B-10(therm)}^{(prod)(j)}}{dt} = a_4 N_{B-10}^{(prod)(j)} - a_2 N_{Li-7,B-10(therm)}^{(prod)(j)}$ (8) $\frac{dN_{T,B-10(therm)}^{(prod)(j)}}{dt} = a_2 N_{Li-7,B-10(therm)}^{(prod)(j)} - \lambda N_{T,B-10(therm)}^{(prod)(j)}$ (9)
$^{12}C(n,\alpha)^{9}Be(n,\alpha)^{6}Li(n,\alpha)^{3}H$	*C-12*	$\frac{dN_{C-12}^{(prod)(j)}}{dt} = -a_5 N_{C-12}^{(prod)(j)}$ (10) $\frac{dN_{Be-9,C-12}^{(prod)(j)}}{dt} = a_5 N_{C-12}^{(prod)(j)} - a_6 N_{Be-9,C-12}^{(prod)(j)}$ (11) $\frac{dN_{Li-6,C-12}^{(prod)(j)}}{dt} = a_6 N_{Be-9,C-12}^{(prod)(j)} - a_1 N_{Li-6,C-12}^{(prod)(j)}$ (12) $\frac{dN_{T,C-12}^{(prod)(j)}}{dt} = a_1 N_{Li-6,C-12}^{(prod)(j)} - \lambda N_{T,C-12}^{(prod)(j)}$ (13)
$^{9}Be(n,\alpha)^{6}Li(n,\alpha)^{3}H$	*Be-9*	$\frac{dN_{Be-9}^{(prod)(j)}}{dt} = -a_6 N_{Be-9}^{(prod)(j)}$ (14) $\frac{dN_{Li-6,Be-9}^{(prod)(j)}}{dt} = a_6 N_{Be-9}^{(prod)(j)} - a_1 N_{Li-6,Be-9}^{(prod)(j)}$ (15) $\frac{dN_{T,Be-9}^{(prod)(j)}}{dt} = a_1 N_{Li-6,Be-9}^{(prod)(j)} - \lambda N_{T,Be-9}^{(prod)(j)}$ (16)
$^{3}He(n,p)^{3}H$	*He-3*	$\frac{dN_{He-3}^{(prod)(j)}}{dt} = a_9 - a_8 N_{He-3}^{(prod)(j)}$ (17) $\frac{dN_{T,He-3}^{(prod)(j)}}{dt} = a_7 N_{He-3}^{(prod)(j)} - \lambda N_{T,He-3}^{(prod)(j)}$ (18)

$a_1 = \pi\phi_{therm}\sigma_{Li-6,therm}$, $a_2 = \pi\phi_{fast}\sigma_{Li-7,fast}$, $a_3 = \pi\phi_{fast}\sigma_{B-10,fast}$, $a_4 = \pi\phi_{therm}\sigma_{B-10,therm}$, $a_5 = \pi\phi_{fast}\sigma_{C-12,fast}$, $a_6 = \pi\phi_{fast}\sigma_{Be-9,fast}$, $a_7 = \pi Q_s/N_{He-4}$, $a_8 = M + \pi Q_s/N_{He-4}$, $a_9 = MX_{He-3}^{o}N_{He-4}F^{(j)}$, K = fission rate per unit power (3.121×10^{16} fissions/(MW s)), $P^{(j)}$ = the power produced in region j (MW) ($= \pi P_{tot}U^{(j)}\phi^{(j)}/\sum_{i=1}^{NOR}U^{(i)}\phi^{(i)}$), π = the fraction of full reactor power generated for the time period, P_{tot} is the full reactor power (MW), $U^{(j)}$ = the volume occupied by fuel elements in region j, (cm^3), $\phi^{(j)}$ = the neutron flux for region j (n cm^{-2} s^{-1}), NOR is the number of regions, Y = the fission yield (1.0×10^{-4} (tritium atoms)/fission), λ is the tritium decay constant (1.792×10^{-9} s^{-1}), the subscript T means tritium, the superscript (j) means region j, t = time (s), ϕ_{therm} = thermal neutron flux (n cm^{-2} s^{-1}), ϕ_{fast} = fast neutron flux (n cm^{-2} s^{-1}), $\sigma_{Li\text{-}6,therm}$ = thermal neutron cross section of ^{6}Li (cm^2), $\sigma_{Li\text{-}7,fast}$ = fast neutron cross section of ^{7}Li (cm^2), $\sigma_{B\text{-}10,fast}$ = fast neutron cross section of ^{10}B (cm^2), $\sigma_{B\text{-}10,therm}$ = thermal neutron cross section of ^{10}B (cm^2), $\sigma_{Be\text{-}9,fast}$ = fast neutron cross section of ^{9}Be (cm^2), $\sigma_{C\text{-}12,fast}$ = fast neutron cross section of ^{12}C (cm^2), M = makeup rate constant for primary coolant (s^{-1}), X_3^0 = abundance of ^{3}He in input helium (dimensionless), $N_{He\text{-}4}$ = number of ^{4}He atoms in the primary coolant (atom), $F^{(j)} = Q^{(j)}/Q_s$ (dimensionless), $Q^{(j)} = \phi^{(j)}\sigma V^{(j)}C^{(j)}$ (atom/s), σ = neutron cross section of ^{3}He for tritium production (cm^2), $V^{(j)}$ = space accessible to helium in region j (cm^3), $C^{(j)}$ = atoms of helium per unit volume in region j (atom/cm^3), $Q_s = \sum_{j=1}^{NOR}Q^{(j)}$ (atom/s).

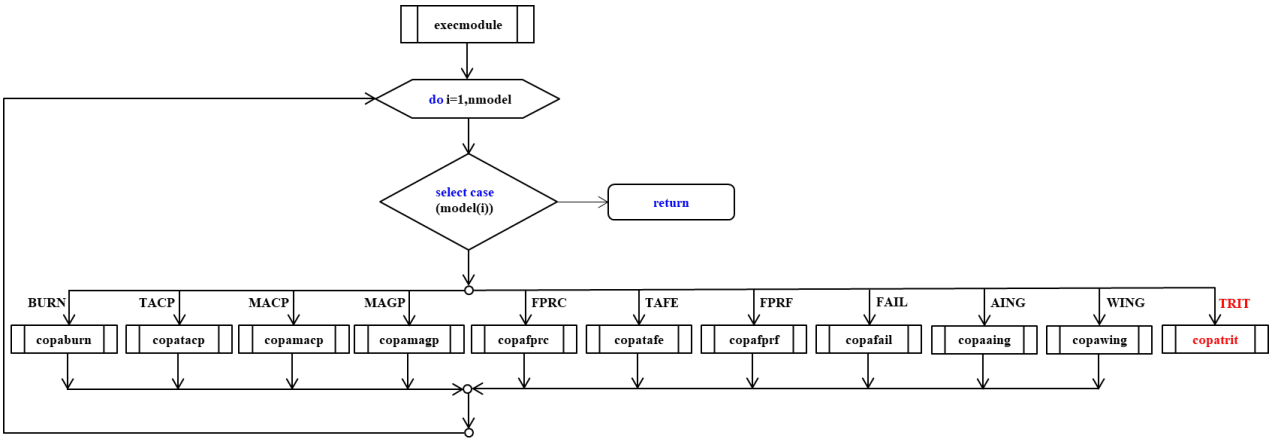

Fig. 1. Modules of COPA code.

Table III: Reactor regions and the related data for test calculation

Region	Weight (kg)	Density (g/cm^3)	BET area (m^2/g)	Temperature (°C)
Core 1	32658.624	1.74	0.2	600
Core 2	48987.936	1.74	0.2	704
Top reflector	20003.407	1.74	0.2	258
Bottom reflector	18733.350	1.74	0.2	685
Inner reflector	42637.648	1.74	0.2	477
Side reflector	385553.200	1.74	0.2	327
Control rod	125.645	1.74	0.2	400
Region	Carbon fraction	Li content (ppm)	B content (ppm)	Be content (ppm)
Core 1	1.0	0.036	41.0	0.0
Core 2	1.0	0.036	41.0	0.0
Top reflector	1.0	0.036	2.0	0.0
Bottom reflector	1.0	0.036	2.0	0.0
Inner reflector	1.0	0.036	2.0	0.0
Side reflector	1.0	0.036	2.0	0.0
Control rod	1.0	0.27	1×10^6	0.0

Table IV: Diffusion coefficient of tritium in a coated fuel particle and a fuel element

Material	Diffusion coefficient (m^2/s): $D = D_{0,1}e^{-\frac{Q_1}{RT}} + D_{0,2}e^{-\frac{Q_2}{RT}}$							
	SiC diffusion				PyC+SiC diffusion			
	$D_{0,1}$ (m^2/s)	Q_1 (J/mol)	$D_{0,2}$ (m^2/s)	Q_2 (J/mol)	$D_{0,1}$ (m^2/s)	Q_1 (J/mol)	$D_{0,2}$ (m^2/s)	Q_2 (J/mol)
Kernel	1×10^{-6}	0	0	0	1.3×10^{-12}	126000	0	0
Buffer	1×10^{-6}	0	0	0	1×10^{-6}	0	0	0
PyC	1×10^{-6}	0	0	0	2.9×10^{-8}	291000	2×10^5	923000
SiC	4.7×10^{-15}	76500	0	0	8.6×10^{-10}	326000	0	0
Graphite	1×10^{-6}	0	0	0	6×10^{-6}	0	0	0

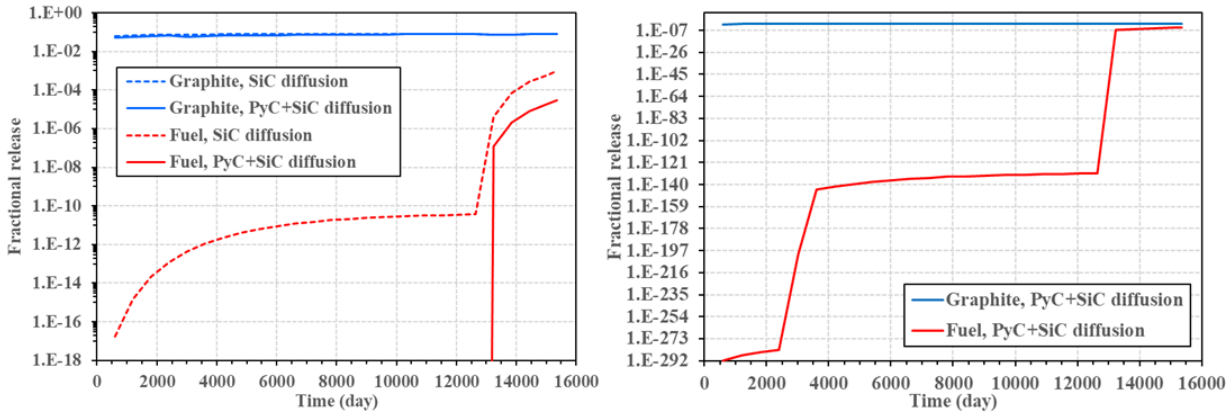

Fig. 3. Release fractions of tritium.