The development of TRIAC-BATAN: a triso fuel performance analysis code

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Abstract. A computer code for analyzing the safety feature of triso coated particles for high temperature reactor has been developed based on PANAMA code. This python based code were separated into several modules to perform the main TRIAC-BATAN and linear interpolation calculation, to read the input data file, and to control the sequence of all TRIAC-BATAN calculation. In this initial development phase, TRIAC-BATAN can produce similar pattern as PANAMA calculation in the case of failure fraction of triso particles, either for Depressurized Loss Of Forced Cooling (DLOFC), $100^\circ$C higher than DLOFC temperature and constant accident temperature at $1600^\circ$C. By using the euclidean distance, TRIAC-BATAN calculation and PANAMA for DLOFC condition are separated in around $3.23 \cdot 10^{-7}$.

Keywords. computer code, fuel performance, triso coated particles

1. Introduction

National Nuclear Energy Agency of Indonesia (BATAN) was mandated to utilize nuclear energy with a strict safety feature to contribute in a national development. Based on the mandate, BATAN plans to design a nuclear based experimental power reactor called RDE (Reaktor Daya Eksperimental) [1]. Due to the safety feature consideration, BATAN focuses on designing a high temperature gas cooled reactor (HTGR)-based nuclear reactor. One part of the design process is to develop an application that can be used for safety evaluation of the fuel performance. This is the background of a TRIAC-BATAN (TRIso Analysis Code) development. While the triso means tri structural isotrophic [2] particle as depicted in Figure 1.

There are several reasons why the HTGR fuel performance analysis should be conducted. One of the reason is like Sun et.al [3] explanation about the graphite dust, resulted from friction and abrasion between the fuel elements and other graphite structures. The dust can be deposited on the tube or the equipment surface and affect the reactor safety in a long time operation. The impurities in a graphite material can also be a non-negligible poison effect on the criticality as was explained by Fukaya [4]. From the system-scale perspective, the thermal conductivity characteristics of the fuel, can be something very interesting to learn, especially in deploying HTGR for other than electricity, such as in a hydrogen production process [5]. Evaluation of HTGR fuel performance is also important to be analyzed due to the fission of product release [6] which ultimately contribute to the reactor source term [7]. One of the fission product from the HTGR operation is $^{110}$Ag. The retention parameter of the triso particle to $^{110}$Ag can be affected by SiC layer grain boundary distribution [8]. From these examples, we can conclude that conducting HTGR-based fuel performance is very important.
In conducting HTGR-based fuel performance, a number of calculation methods in fuel performance analysis code have been developed. One of them was Fuel Temperature Computer Code (FTCC) developed by JAEA [9]. FTCC was developed to ensure the thermal integrity of the HTGR fuel and also to improve the user friendliness of the analysis code, especially for prismatic-type HTGR reactors. Another computer code which has been developed is BISON [10]. BISON code provides rapid solutions of 1D spherical symmetric and 2D axially symmetric models. This finite element based computer code was also capable in providing scalable parallel processing for the solutions of large and complex 3D models. Another computer code in a system level is called HCP (HTR Code Package). The HCP can be used to simulate the long term operation scenarios based on OTTO or MEDUL fuel shuffling schemes [11].

In supporting the RDE development, it is required to have a computer code for fuel performance analysis. However, there are no such computer codes available to be used. This is the main reason why TRIAC-BATAN is developed. On the other hand, it is also a good reason to increase human capacity development.

TRIAC-BATAN development was mainly developed based on PANAMA calculation [6, 12, 13] using python programming language. It consists of two different types of calculations. The first is the calculation before heating (irradiation condition) and the last is the calculation after heating (accident condition). In predicting triso particles failure fraction, PANAMA uses SiC layer (see Figure 1) tensile strength parameter. In this model, a triso particle is said to be failed if its SiC layer tensile strength is lower than the internal pressure from the underneath layer.

2. The calculation model
TRIAC-BATAN calculation model is divided into two different parts, each are irradiation and accident condition calculation. All of the calculation model applied in TRIAC-BATAN either in irradiation or accident condition was adopted from PANAMA technical document [12]. PANAMA also uses different empirical equations for different types of triso particles. Because RDE will use $UO_2$ fuel type, then TRIAC-BATAN will use all the empirical equations provided in that document.

2.1. Irradiation condition
The first calculation in irradiation condition is OPF (Oxygen Per Fission) which is the number of oxygen atoms detached along the atomic fission of $U^{235}$ or $Pu^{239}$. These oxygen atoms affect the formation
of CO compounds which can increase the internal pressure of a triso particle. From the OPF value, the average irradiation temperature \(T_B\) can be calculated.

After obtaining the value of \(T_B\), the calculation continues to obtain the value of \(DS\), which is the factor of diffusion coefficient diminished due to fission gas produced in the particle kernel. Then, the value of \(DS\) will be used to calculate the dimensionless value, denoted as \(\tau_i\). \(T_B\) is also used to calculate the tensile strength of SiC layer (denoted as \(\sigma_0\) after irradiation condition. Finally, \(T_B\) is used to calculate the value of \(m_0\), which is the Weibull parameter due to irradiation.

Besides the previous calculations, the volume of each coated particles layer, especially the two innermost layer (kernel and buffer) were also calculated. These layers will be used in the internal pressure calculation at the accident condition. Irradiation condition calculation can be depicted in Figure 2. This figure shows an interdependence relationship among the parameters. The intersection point shown in that figure means that the parameters being calculated are independence each other. In this phase, only OPF calculation that use the irradiation mesh history.

![Figure 2. Parameter interdependence relationship in irradiation condition calculation](image)

### 2.2. Accident condition

In the accident condition, several calculation will be conducted as depicted in Figure 3. This calculation phase is dependent on \(T_B\), \(\tau_i\), \(\sigma_0\) and \(m_0\) obtained from the previous phase. Differ from the previous calculation, all calculation depicted in Figure 3 are conducted in every accident mesh history. For every accident mesh history, there are two kinds of calculation will be conducted independently. The first is \(Fd\) calculation which is dependent on \(\tau_a\) and \(DS_a\). While the second is \(OPF_a\) which is the oxygen per fission occurred due to accident. Both \(Fd\) and \(OPF_a\) will be used in the calculation of \(\sigma_t\) (SiC layer tensile strength after a certain time of accident) and \(\phi_1\). Then the calculation will be continued for the next mesh.

The most important calculation is triso particle failure fraction \(\phi_1\), as defined in eq.(1), which is the target of TRIAC-BATAN calculation. The index 1 in parameter \(\phi_1\) refer to the first failure cause, that is the changes of internal pressure and SiC tensile strength. PANAMA also applied another failure caused by the weight loss. However, the weight loss will start to occur after the reactor temperature reach the 2000°C. In TRIAC-BATAN development, it was assumed that the temperature will not reach 2000°C as designed in RDE. Then, the particle failure can only caused by the changes of internal pressure and SiC tensile strength. Because of that, there is no difference between the symbol of \(\phi_1\) and \(\phi\) (written in several
Figure 3. Parameter interdependence relationship in accident condition calculation

\[
\phi_1(t, T) = 1 - e^{-\frac{\ln 2}{\sigma_0} \cdot \left(\sigma_t / \sigma_0\right)^m}
\]

PANAMA uses the scheme as shown in Figure 4 to model triso particle failure fraction changes from time to time along the accident condition. At certain time of the accident condition, PANAMA always uses the beginning of the accident condition as a reference point to the failure fraction \(\phi_1\). The model certainly contains error due to the temperature changes that are not considered in eq.(1). Then PANAMA uses the parameter of \(\Delta\phi_1\) as defined in eq.(2).

If we are concern to the mesh between \(t_1\) and \(t_2\), then \(T_M = T_{12} = \frac{T_1 + T_2}{2}\). Then, the rule is: if \(\Delta\phi_1 > 0\), then \(\phi_1(t_2) = \phi_1(t_1) + \Delta\phi_1\); otherwise, \(\phi_1(t_2) = \phi_1(t_1)\). It means that there are no further failure occurred from \(t_1\) to \(t_2\).

Figure 4. A model of triso particle failure fraction changes

\[
\Delta\phi_1 = \phi_1(t_2, T_m) - \phi_1(t_1, T_m)
\]

3. The code structure

TRIAC-BATAN was composed by four different python modules as the following items.
1) The core module is the module where all the calculation model explained in sec. 2 conducted.
2) The input file processing. This module was intended to read the triso particle data, including its geometry, physical properties and its irradiation and accident history which have the characteristics similar to Figure 5 and Figure 6 respectively, based on the PANAMA input file format [12].
3) The interpolation module is where the linear interpolation calculation is conducted. This module is used to estimate the pair value of time and temperature in more detail.
4) The execution module is where TRIAC-BATAN calculation is organized, from reading the input file to presenting the value of triso particle failure fraction.

![Figure 5. An example of irradiation history](image)

![Figure 6. An example of accident history](image)
4. Result and Discussion

The result obtained from the input data containing irradiation and accident history as depicted in Figure 5 and 6. While the dimension and material characteristics of triso particle are supplied in Table 1. In the case of dimension, each value representing the distance between the outer layer to the center. While in material characteristics, index \( \sigma_{oo} \) means the parameters are obtained from the measurement process before irradiation. Then, \( \sigma_{oo} \) representing SiC tensile strength while \( m_{oo} \) is a weibull parameter. Besides that, PANAMA also provided the simulation scenario through \( T_B = 776^\circ C, m_0 = 6.93 \) and oxygen atom per fission at the beginning of accident condition is \( 5.11 \times 10^{-2} \).

| Dimension | OPyC layer | SiC Layer | IPyC | Buffer | Kernel |
|-----------|------------|-----------|------|--------|--------|
|           | 4.60x10\(^{-4}\) | 4.20x10\(^{-4}\) | 3.85x10\(^{-4}\) | 3.45x10\(^{-4}\) | 2.50x10\(^{-4}\) |
| Material characteristics | \( \sigma_{oo} \) | \( m_{oo} \) | FIMA | \( Ff \) | \( \Gamma \) |
|           | 8.34x10\(^8\) | 8.02 | 0.08 | 0.31 | 1.4 |

4.1. TRIAC-BATAN using PANAMA scenario

In this simulation, TRIAC-BATAN uses parameters supplied by PANAMA as provided in Table 1. The value \( T_B \) also uses the value provided as 776°C. TRIAC-BATAN calculation then will be compared to PANAMA for DLOFC, DLOFC with 100°C higher and constant accident temperature at 1600°C. Because \( T_B \) is set to 776°C, then no \( T_B \) calculation will be executed. Figure 7 shows that TRIAC-BATAN produce the similar pattern compare to PANAMA for the three simulation scenarios.

Figure 7 shows how TRIAC-BATAN calculation is close enough to PANAMA. Authors then calculate how close they are by using the euclidean distance parameter, described in eq.(3). From that equation, \( i \) representing \( \phi_1 \) from TRIAC-BATAN calculation, while \( j \) representing \( \phi_1 \) from PANAMA fitting function. In this test, PANAMA result prediction for DLOFC condition were fitted which produce
Figure 8. Changes occured in $T_B$ due to interpolation parameter $dt$

$$f(x) = 2.27 \cdot 10^{-7} \ln(x) - 6.64 \cdot 10^{-7}$$ as a fitting function. In that function, $x$ representing hours from the beginning of accident condition, while $f(x)$ representing failure fraction occured at time $x$. Finally, by using eq.(3), TRIAC-BATAN and PANAMA are separated in $3.23 \cdot 10^{-7}$.

$$d(i, j) = \sqrt{(x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \cdots + (x_{ip} - x_{jp})^2}$$ (3)

4.2. Interpolation

One of parameters from irradiation condition that will be used in accident condition calculation is $T_B$. How this parameter changes on interpolation parameter changes along the irradiation condition ($dt_{irr}$) can be depicted in Figure 8. It can be shown that increasing $dt_{irr}$ will decrease $T_B$ until $dt$ reaches 10. For $dt > 10$, the value of $T_B$ will only change slightly. Figure 8 shows that the changes in $dt_{irr}$ affecting the value of $T_B$.

After knowing the characteristics of $dt_{irr}$ vs. $T_B$, the next scenario is to find out how the value of $\phi_1$ will changes as a respond to the changes in $T_B$ produced from the previous result. Figure 9(a), shows that the higher $T_B$ more triso particles will be failed. Because the higher $T_B$ comes from the lower $dt_{irr}$, then $\phi_1$ is conversely proportional to $dt_{irr}$.

On the other hand, the use of interpolation in accident condition ($dt_{acc}$) will produce $\phi_1$ as depicted in Figure 9(b) when $T_B$ equal to 776°C. In that figure, $\phi_1$ varies slightly in respond to $dt_{acc}$. This result seems supporting the eq(1) which is defined not in the iterative mode. Then we can conclude that it is not important to use interpolation scheme in accident condition. The next simulation will uses $dt_{irr} = 10$ and $dt_{acc} = 1$.

4.3. Fission products, Pressure and $\phi_1$

As already explained in the previous section, PANAMA uses a SiC layer tensile strength ($\sigma$) as a criteria for the triso particles failure fraction. The $\sigma$ itself depends on internal fission gas pressure in triso particles. Then it is interesting to show the relationship between fission gas production, either $Fd$ or $OPF_a$ to the internal pressure and finally to $\phi_1$. Figure 10 shows how the parameters behave.

$Fd$ and $OPF_a$ tend to be stable after about 10 hours from the beginning of accident. On the other hand, pressure, denoted in a yellow diamond style dot, fluctuates as accident temperature shown in
Figure 6. From the figure, pressure depends more on accident temperature than $F_d$ or $OPF_a$. Then, it is very important to keep the temperature in the operational range. Consequently, $\phi_1$ reach its peak very close to the internal pressure peak. After accident temperature decrease, represented in internal pressure decrease, $\phi_1$ tends to stable, means very small failure fraction occurred.

Figure 10. The plot data of parameter $F_d$, $p$ and $\phi_1$

5. Conclusions and further works
From section 4, TRIAC-BATAN shows similar result, either in the value of $\phi_1$ or its plot pattern. TRIAC-BATAN calculation and PANAMA for DLOFC condition are also separated in around $3.23 \cdot 10^{-7}$. From that point, this initial phase of TRIAC-BATAN development is successfully reproduce PANAMA calculation model. The next work deals with TRIAC-BATAN development is implementing uncertainty analysis by using Latin Hypercube Sampling (LHS) calculation. This implementation will be usefull for evaluating uncertainty in triso particles dimension and how this uncertainty will affecting the value of $\phi_1$. 
6. Acknowledgments
Authors thank Mr. Surip Widodo for providing PANAMA failure fraction data extracted from the data plot image in technical document [12]. This research was supported financially by PTKRN-BATAN through DIPA 2018 and Ministry of Research, Technology and Higher Education, Republic Indonesia through the FLAGSHIP INSINAS program 2018.

7. References
[1] Setiadipura T, Bakhri S, Sunaryo G R and Wisnubroto D S 2017 Cooling passive safety features of reaktor daya eksperimental AIP Proceeding of International Conference on Thermal Science and Technology
[2] Setiadipura T, Irwanto D and Zuhair 2015 Atom Indonesia 41 7–15
[3] Sun Q, Zhao G, Peng W, Wang J, Jiang Y and Yu S 2018 Annals of Nuclear Energy 115 195 – 208 ISSN 0306-4549 URL http://www.sciencedirect.com/science/article/pii/S0306454917303596
[4] Fukaya Y, Goto M and Nishihara T 2018 Nuclear Engineering and Design 326 108 – 113 ISSN 0029-5493 URL http://www.sciencedirect.com/science/article/pii/S0029549317305071
[5] Shin D H, Yoon S J, Cho H K, Park G C and Kim T 2017 International Journal of Hydrogen Energy 42 18614 – 18625 ISSN 0360-3199 special Issue on The 5th International Conference on Energy Engineering and Environmental Engineering (ICEEEE2017), 15-16 April 2017, Xiamen, China URL http://www.sciencedirect.com/science/article/pii/S0360319917315367
[6] Verfondern K, Xhonneux A, Nabielek H and Allelein H J 2014 Nuclear Engineering and Design 273 85 – 97 ISSN 0029-5493 URL http://www.sciencedirect.com/science/article/pii/S0029549314001502
[7] Hanson D L 2018 Nuclear Engineering and Design 329 60 – 72 ISSN 0029-5493 the Best of HTR 2016: International Topical Meeting on High Temperature Reactor Technology URL http://www.sciencedirect.com/science/article/pii/S0029549317305241
[8] Lillo T, van Rooyen I and Aguiar J 2018 Nuclear Engineering and Design 329 46 – 52 ISSN 0029-5493 the Best of HTR 2016: International Topical Meeting on High Temperature Reactor Technology URL http://www.sciencedirect.com/science/article/pii/S0029549317305691
[9] Inaba Y and Nishihara T 2017 Annals of Nuclear Energy 101 383 – 389 ISSN 0306-4549 URL http://www.sciencedirect.com/science/article/pii/S0306454916302900
[10] Hales J, Williamson R, Novascone S, Perez D, Spencer B and Pastore G 2013 Journal of Nuclear Materials 443 531 – 543 ISSN 0022-3115 URL http://www.sciencedirect.com/science/article/pii/S0022311513009586
[11] Kasselmann S, Xhonneux A, Tantillo F, Trabadelo A, Lambertz D and Allelein H J 2018 Nuclear Engineering and Design 329 167 – 176 ISSN 0029-5493 the Best of HTR 2016: International Topical Meeting on High Temperature Reactor Technology URL http://www.sciencedirect.com/science/article/pii/S0029549317305666
[12] Verfondern K and Nabielek H 1990 The mathematical basis of the panama-i code for modelling pressure vessel failure of triso coated particles under accident conditions Tech. rep. Julich Research Center, Germany
[13] Verfondern K, Cao J, Liu T and Allelein H J 2014 Nuclear Engineering and Design 271 84 – 91 ISSN 0029-5493 s1 : HTR 2012 URL http://www.sciencedirect.com/science/article/pii/S0029549313005992