Design of Optimal Coating Layer Thicknesses for an 800-μm UCO TRISO of a small prismatic HTR

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1. Introduction

A large number of coated fuel particles are contained in a fuel element of a high temperature reactor (HTR). A tri-structural isotropic coated fuel particle (TRISO) consists of a fuel kernel in its innermost center and four surrounding coating layers such as a low-density pyrocarbon called buffer, an inner high-density pyrocarbon (IPyC), a silicon carbide (SiC), and an outer high-density pyrocarbon (OPyC) from its inside part.

A TRISO with a large-sized UCO fuel kernel up to 800 μm is a candidate fuel for a small and long-life HTR for power supply in polar and remote areas since many fissile materials can be loaded in it. The UCO kernel produces fission gases only, but not CO and CO_2 that are major gases in the TRISO with a UO_2 kernel. For an extended fuel life, more fission gases will be generated in the TRISO with an 800-μm kernel than in the TRISO with a 500-μm kernel. The design of the TRISO with a large-sized kernel must be changed to ensure fuel safety. The optimal design for a TRISO improves the TRISO fuel economy and safety.

This study describes the optimal design for a TRISO using a response surface method (RSM) [1] and suggests the optimal thicknesses of the coating layers of a TRISO with a UCO kernel of 800 μm that can be loaded in a small prismatic HTR.

2. Optimal Design for a TRISO

The optimal design for a TRISO is to find the best combinations of its design variables that maximize its fuel performance. Numerically, the optimal design is to maximize or minimize an objective function with its constraints, where the objective function describes the TRISO fuel performance and measures the merits of different TRISO designs.

An RSM is applicable to an optimal design when its objective function is difficult to express mathematically and/or its evaluation is very time-consuming. In an RSM, an objective function becomes a product of responses that are polynomial models fitted with points (the values of design variables) in a design space. A standard RSM, such as Central Composite Design or Ben-Behnken Design, may place points in regions that are not accessible due to constraints. A computer-generated optimal design of Design-Expert® [2] places the sample points in the safe regions of a design space.

2.1 An objective function

The objective function in the optimal design for a TRISO is a function of the design variables of a TRISO. The product of the packing fraction of TRISO particles in a compact and the failure probability of the SiC layers was chosen as the objective function to be minimized:

$$y = PF \cdot FR_{Cs} \cdot FR_{Ag} \cdot FR_{Sr} \cdot P_{f,SiC}\,, \tag{1}$$

where y is the objective function (dimensionless) $\in$ [0, 1], PF is the packing fraction (dimensionless) $\in$ [0, 1], FR_{Cs} is the fractional release of cesium from a TRISO $\in$ [0, 1], FR_{Ag} is the fractional release of silver from a TRISO $\in$ [0, 1], FR_{Sr} is the fractional release of strontium from a TRISO $\in$ [0, 1], and $P_{f,SiC}$ is the failure probability of the SiC layers (dimensionless) $\in$ [0, 1]. The lower the values of the packing fraction, the fractional releases and the SiC failure probability, the more preferable.

The packing fraction of TRISO particles in a compact is given by:

$$PF = \frac{4\pi N_{TRISO}}{3V_{compact}} 1\times10^{-12}\left(r_K + t_B + t_I + t_S + t_O\right)^3, \tag{2}$$

where N_{TRISO} is the number of TRISOs in a compact, $V_{compact}$ is the volume of a compact (cm^3), r_K is the radius of a kernel (μm), t_B is the buffer thickness (μm), t_I is the IPyC thickness (μm), t_S is the SiC thickness (μm), and t_O is the OPyC thickness (μm).

The fractional release of a metallic fission product from a TRISO is defined as the ratio of the accumulated amount released that is not decayed to the accumulated amount generated that is not decayed. Classic Fickian diffusion accompanying a thermal analysis has been used as a simplified approach for the fission product transport analysis because of incomplete knowledge of the actual transport behavior in a TRISO. The temperature distribution in a TRISO is described by a heat transfer equation.

The failure probability of the SiC coating layers is given using a cumulative Weibull distribution as follows [3]:

$$P_f = 1 - e^{-\ln 2\cdot\left(\sigma_\theta/\sigma_{med}\right)^m}\,, \tag{3}$$

where σ_θ is the tangential stress acting on the inner surface of the SiC layer (MPa), σ_{med} is the median strength of the SiC layer (MPa), and m is the Weibull modulus (dimensionless). The tangential stress acting on the inner surface of the SiC layer is a function of the design variables of a TRISO.

2.2 A constraint

The packing fraction of the spherical TRISO particles in a cylindrical compact has its upper value limiting the sizes of the buffer, IPyC, SiC, and OPyC layers:

$$0 \le t_B + t_I + t_S + t_O \le \left(\frac{3V_{compact} \cdot PF^{\max}}{4\pi N_{TRISO} \cdot 10^{-12}} \right)^{1/3} - r_K , \qquad (4)$$

where PF^{max} is the maximum packing fraction of the spherical TRISO particles in a cylindrical compact, and the other variables are described in Eq. (2).

3. Evaluation of Optimal Thicknesses of Coating Layers

The design variables considered here are the thicknesses of the buffer, IPyC, SiC, and OPyC layers. They affect the mechanical state of the SiC layer and then the failure probability of the SiC layers.

3.1. A reference reactor

The small prismatic HTR considered in this study is assumed to have a fuel loading cycle of 10000 days. The TRISO kernel of the small prismatic HTR is UCO with an enrichment of 15.5 w/o and its diameter is 800 μm. The densities of the kernel, buffer, IPyC, SiC and OPyC are 10.5, 1.0, 1.9, 3.2 and 1.9 g/cm^3, respectively. The linear heat generation rate of the small prismatic HTR compact is 8.122 W/cm. The McCARD code [4] is used to calculate the depletion of the small prismatic HTR TRISO fuel of which the thicknesses of the buffer, IPyC, SiC and OPyC layers are 100, 40, 35 and 40 μm, respectively. Fig. 1 shows the variation of fuel burnup and fast fluence with irradiation time. Fig. 2 presents the variation of fission yields of the gases produced in a TRISO irradiated at the temperature of 1200 ℃. These gas yields are input data for calculating the gas pressure buildup in a TRISO.

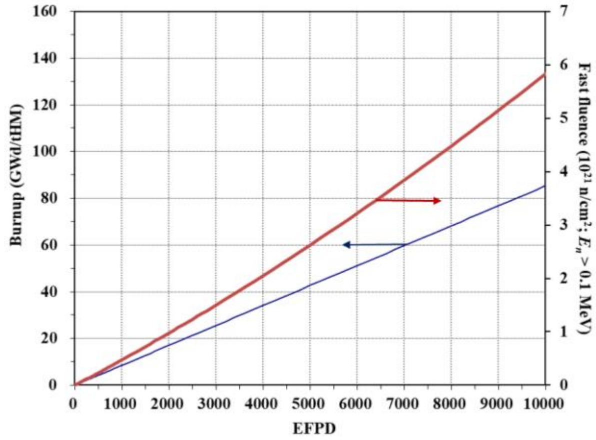

Fig. 1. Variation of fuel burnup and fast fluence.

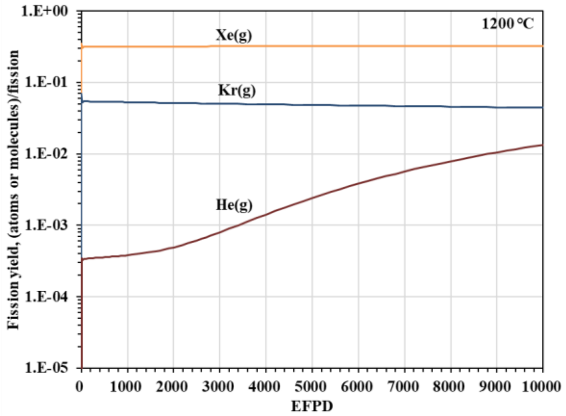

Fig. 2. Variation of the fission yields of gases produced in a TRISO.

3.2. An optimal design for the coating layer thicknesses

The thickness ranges considered are 100 to 150 μm for the buffer, 20 to 60 μm for the IPyC and OPyC layers, and 20 to 100 for the SiC layer. The compact considered is 1 cm in length and 1.162 cm in diameter whose volume is 1.060 cm^3. In order to maintain the same compact power, the number of TRISO particles should be equal to the number of the nominal TRISO particles described in Section 3.1, i.e., 381 particles.

Morris and Pappano [5] suggested the maximum packing fraction of TRISO particles in a cylindrical compact is in the neighborhood of 40-50 %. When the maximum packing fraction of 40 % is applied, the constraint Eq. (4) becomes:

$$0 \le t_B + t_I + t_S + t_O \le 242.992 . \qquad (5)$$

The calculation of the failure probability of the SiC layer using Eq. (3) requires the SiC maximum tangential stresses that can be calculated using the COPA code [6]. The median strengths and Weibull moduli are 350 MPa and 9.5 for the IPyC and OPyC layers, and 770 MPa and 6 for the SiC layer, respectively [7]. It was estimated that no SiC failure had occurred throughout the irradiation. The response 'the failure probability of the SiC layers' in Eq. (1) is excluded in this optimization.

The releases of metallic fission products such as cesium, silver, strontium from a TRISO is also calculated using the COPA code.

The 'Optimal (custom) Design' of the software Design-Expert® is used to perform the optimal design of a TRISO. In the 'Optimal (custom) Design', the search menu was set to Best, the optimality menu to I, the Lack-of-fit points to 5, the Replicate points to 5, and the rest of the menus to default values. Table I shows a design layout for the coating layers of a TRISO which is generated using the 'Optimal (custom) Design', Eq. (2) and the COPA code.

During an optimization using the 'Optimal (custom) Design', the importance of a value of 3 is assigned to the packing fraction and the importance of a value of 5 to the SiC failure probability, with a value of 5 being the highest importance. That is, the importance of the SiC failure probability was artificially adjusted to be higher than the importance of the packing fraction. In the Criteria menu of numerical optimization, the lower and upper limits of the SiC failure probability are set to 0 and 0.01, respectively. Design-Expert® was set to produce 100 local optimums currently.

Table II shows the optimal thicknesses of the coating layers of a UCO TRISO for three optimum strategies. When the thicknesses of the IPyC and OPyC layers are targeted at 35 and 40 μm, the optimum thicknesses of the buffer, IPyC, SiC, OPyC layers are 100, 35, 63, 34 μm, respectively. Compared to the conventional design of a 500-μm UCO TRISO where the thicknesses of the buffer, IPyC, SiC and OPyC layers are 100, 40, 35 and 40 μm, respectively, the thicknesses of the IPyC and OPyC layers decreased by about 5 and 6 μm, respectively, and the SiC layer thickness increased by about 28 μm. The packing fraction of the first optimum TRISOs is about 37.7 %. When the thicknesses of the IPyC and OPyC layers equal 40 μm, the optimum thicknesses of the buffer, IPyC, SiC, OPyC layers are 100, 40, 54, 40 μm, respectively. Compared to the conventional design of a 500-μm UCO TRISO where the thicknesses of the buffer, IPyC, SiC and OPyC layers are 100, 40, 35 and 40 μm, respectively, the SiC layer thickness increased by about 19 μm. The packing fraction of the first optimum TRISOs is about 38.3 %.

4. Summary

The optimal thicknesses of the coating layers of an 800-μm UCO TRISO have been evaluated using a computer-generated optimal design of a response surface methodology. The optimum solutions are that the thicknesses of the buffer, IPyC, SiC and OPyC layers are 100, 35, 63, 34 μm, or 100, 40, 54, 40 μm. The packing fraction of the optimum TRISOs is about 38 %, and it increased by 3 % compared to the conventional packing fraction 35 %. Better decisions about which one to choose requires considering the ease of making a compact and the failure due to long-term chemical attack.

ACKNOWLEDGEMENTS

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REFERENCES

[1] Myers, R.H, Montgomery, D.C., Anderson-cook, C.M., 2009. Response Surface Methodology: Process and Product Optimization Using Designed Experiments. John Wiley &Sons, Inc.

[2] Stat-Ease, Inc., 2017. Design-Expert® Version 10.

[3] Green, A.E. and Bourne, A.J., 1972. Reliability Technology. John Wiley & Sons Ltd.

[4] Shim, H.J., Han B.S., Jung J.S., Park, H.J., and Kim C.H., 2012. MCCARD: Monte Carlo Code for Advanced Reactor Design and Analysis. Nuclear Engineering and Technology 44(2), pp. 161-176.

[5] Morris, R.N. and Pappano, P.J., 2007. Estimation of maximum coated particle fuel compact packing fraction. Journal of Nuclear Materials 361, pp. 18-29.

[6] Kim, Y.M. and Jo, C.K., 2019. COPA Ver. 1.0: Theory Report. KAERI/TR-7945/2019.

[7] CEGA Corporation, 1993. NP-MHTGR Material Models of Pyrocarbon and Pyrolytic Silicon Carbide. CEGA-002820, Rev. 1.

Table I: Design layout for the coating layer thicknesses of a TRISO

Run	A:Buffer thickness, μm	B:IPyC thickness, μm	C:SiC thickness, μm	D:OPyC thickness, μm	Packing fraction, dimensionless	Fractional releases, dimensionless		
						Cs	Ag	Sr
1	150.000	20.000	36.187	36.805	0.399999461	1.830E-01	2.522E-01	3.180E-02
2	100.000	40.000	40.000	22.000	0.328270737	1.714E-01	2.401E-01	3.190E-02
3	120.000	37.482	20.000	38.400	0.351508821	3.250E-01	3.957E-01	3.400E-02
4	125.000	20.200	30.400	26.818	0.328955777	2.289E-01	3.010E-01	3.290E-02
5	126.750	39.600	52.800	23.800	0.399921082	1.142E-01	1.752E-01	2.980E-02
6	138.097	60.000	20.000	24.895	0.399999461	3.074E-01	3.787E-01	3.360E-02
7	100.000	20.000	61.200	20.000	0.326963755	9.862E-02	1.590E-01	3.000E-02
8	100.000	42.406	54.199	46.387	0.399999461	1.135E-01	1.757E-01	3.020E-02
9	150.000	20.000	20.000	20.000	0.34153263	3.227E-01	3.929E-01	3.390E-02
10	100.000	60.000	20.000	20.000	0.325009794	3.240E-01	3.945E-01	3.390E-02
11	100.000	20.000	20.000	60.000	0.325009794	3.414E-01	4.118E-01	3.430E-02
12	150.000	20.000	36.187	36.805	0.399999461	1.830E-01	2.522E-01	3.180E-02
13	150.000	42.992	30.000	20.000	0.399999461	2.154E-01	2.862E-01	3.230E-02
14	100.000	60.000	20.000	60.000	0.394441516	3.196E-01	3.915E-01	3.390E-02
15	120.000	37.482	20.000	38.400	0.351508821	3.250E-01	3.957E-01	3.400E-02
16	100.000	42.406	54.199	46.387	0.399999461	1.135E-01	1.757E-01	3.020E-02
17	114.937	60.000	27.684	40.372	0.399999461	2.368E-01	3.092E-01	3.280E-02
18	100.000	20.000	100.000	22.992	0.399999461	3.240E-02	7.716E-02	2.580E-02
19	126.750	39.600	52.800	23.800	0.399921082	1.142E-01	1.752E-01	2.980E-02
20	100.000	20.000	20.000	20.000	0.264245	3.460E-01	4.148E-01	3.430E-02
21	100.000	20.000	62.992	60.000	0.399999461	9.264E-02	1.527E-01	2.980E-02
22	142.992	20.000	20.000	60.000	0.399999461	3.213E-01	3.928E-01	3.390E-02
23	120.000	37.482	20.000	38.400	0.351508821	3.250E-01	3.957E-01	3.400E-02
24	100.000	60.000	62.992	20.000	0.399999461	8.689E-02	1.437E-01	2.870E-02
25	131.523	20.000	71.469	20.000	0.399999461	7.019E-02	1.241E-01	2.800E-02

Table II: Optimal thicknesses of the coating layers of a TRISO

Thickness range, μm				Optimal thickness, μm				Packing fraction, %
Buffer	IPyC	SiC	OPyC	Buffer	IPyC	SiC	OPyC	
100~150	20~60 Targets at 35	20~100	20~60 Targets at 35	100	35	63	34	37.7
100~150	20~60 Targets at 40	20~100	20~60 Targets at 40	100	35	63	34	37.7
100~150	20~60 Equals 40	20~100	20~60 Equals 40	100	40	54	40	38.3