## Optimal Coating Layer Thicknesses of a TRISO under the Normal Operation Conditions of a VHTS

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## 1. Introduction

A very high temperature system (VHTS) is a high temperature gas reactor (HTGR) that can supply the heat required for hydrogen production through very high temperature operation of 950 °C [1]. The operating temperature is much higher than that of the typical HTGR at 750 °C, and the operating period is longer. A tri-structural isotropic coated fuel particle (TRISO) of the VHTS consists of a fuel kernel in its innermost center and four surrounding coating layers such as a low-density pyrocarbon called buffer, an inner highdensity pyrocarbon (IPyC), a silicon carbide (SiC), and an outer high-density pyrocarbon (OPyC) from its inside part. In the VHTS, the possibility of increased fuel kernel migration, intensified chemical attack of fission products on the coating layers of a TRISO, increased thermal decomposition of the coating layers, and increased release of fission products increases compared to the conventional HTGR. The optimal design of a TRISO through a fuel performance analysis under normal operation and accident conditions of the VHTS is very necessary to secure the safety of the VHTS nuclear fuel.

This study describes the optimal design for a TRISO under normal operation conditions of the VHTS using a response surface method (RSM) [2] and suggests the optimal thicknesses of the coating layers of a TRISO with a UO<sub>2</sub> kernel of 500  $\mu$ m and a buffer of 100  $\mu$ m that can be loaded in a VHTS.

#### 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<sup>®</sup> [3] 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 fractional releases of Ag-110m, Cs-137, Sr-90, Kr-85 was chosen as the objective function to be minimized:

$$y = PF \cdot FR_{Ag} \cdot FR_{Cs} \cdot FR_{Sr} \cdot FR_{Kr}, \qquad (1)$$

where y is the objective function (dimensionless)  $\in [0, 1]$ , *PF* is the packing fraction (dimensionless)  $\in [0, 1]$ , and *FR* is the fractional release of a fission product (dimensionless)  $\in [0, 1]$ . The lower the values of the packing fraction and the fractional release, the more preferable.

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

$$PF = \frac{4\pi N_{TRISO}}{3V_{compact}} 1 \times 10^{-12} \left( r_K + t_B + t_I + t_S + t_O \right)^3, \quad (2)$$

where  $N_{TRISO}$  is the number of TRISOs in a compact,  $V_{compact}$  is the volume of a compact (cm<sup>3</sup>),  $r_K$  is the radius of a kernel ( $\mu$ m),  $t_B$  is the buffer thickness ( $\mu$ m),  $t_I$  is the IPyC thickness ( $\mu$ m),  $t_S$  is the SiC thickness ( $\mu$ m), and  $t_O$  is the OPyC thickness ( $\mu$ m).

#### 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:

$$t_{I,\min} + t_{S,\min} + t_{O,\min} + t_{O,\min} \le t_{I} + t_{S} + t_{O} \le \left(\frac{3V_{compact} \cdot PF^{\max}}{4\pi N_{TRISO} \cdot 10^{-12}}\right)^{\frac{1}{3}} - r_{K} - t_{B},$$
(3)

where  $t_{min}$  is the minimum thickness of a coating layer,  $PF^{max}$  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 IPyC, SiC, and OPyC layers. They affect the mechanical state of the coating layers and then the failure probabilities of the coating layers.

## 3.1. A VHTS

The VHTS considered in this study is assumed to have a fuel loading cycle of 1500 days. The TRISO kernel is UO<sub>2</sub> with an enrichment of 15.5 w/o and its diameter is 500 um. The densities of the kernel, buffer, IPyC, SiC and OPyC are 10.4, 1.0, 1.9, 3.2 and 1.9 g/cm<sup>3</sup>, respectively. The linear heat generation rate of the VHTS compact is 35.318 W/cm. The McCARD code [4] is used to calculate the depletion of the VHTS 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 °C. 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 20 to 60  $\mu$ m for the IPyC and OPyC layers, and 20 to 100 for the SiC layer. The compact considered is 1 cm in length and 1.245 cm in diameter whose volume is 1.217 cm<sup>3</sup>. 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., 867 particles.

When the maximum packing fraction of 40 % is applied, the constraint Eq. (3) becomes:

$$20 \le t_B + t_I + t_S + t_O \le 161.635 \,. \tag{4}$$

The fractional releases were calculated after evaluating the failure fractions of the coating layers using the COPA code [5]. The median strengths and Weibull moduli applied in the failure analysis are 350 MPa and 9.5 for the IPyC and OPyC layers, and 770 MPa and 6 for the SiC layer, respectively [6].

The 'Optimal (custom) Design' of the software Design-Expert<sup>®</sup> 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. The values of the fractional releases at 1500 days are used.

During an optimization using the 'Optimal (custom) Design', the importances of the packing fraction and the fractional releases were set to '\*\*\*' and '\*\*\*\*'. respectively. That is, the importance of the fractional releases was artificially adjusted to be higher than the importance of the packing fraction. In the Criteria menu of numerical optimization, the thicknesses of the IPyC and OPyC layers are targeted to 40 µm, and the SiC thickness, packing fraction and fractional releases are set to minimize. The optimum thicknesses produced by Design-Expert<sup>®</sup> are 35.9, 42.2, 39.0 µm, respectively. was set to produced 2 local optimums currently. Fig. 3 shows a ramp-type solution of the optimum. Fig. 4 is a three-dimensional surface of the optimum. Compared to the conventional design of a 500-µm UO2 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 are reduced by about 4 and 1 µm, respectively, and the SiC layer thickness is increased by about 2 µm. The packing fraction of the optimum TRISOs is about 30 %, which is close to that of the conventional HTGR.



Fig. 3. A ramp-type solution of the optimum.

## 4. Summary

The optimal thicknesses of the coating layers of a TRISO with a UO<sub>2</sub> kernel of 500  $\mu$ m and a buffer of 100  $\mu$ m under normal operation conditions of a VHTS have been evaluated using a computer-generated optimal design of a response surface methodology. The optimum solution is that the thicknesses of the IPyC, SiC and OPyC layers are 35.9, 42.2, 39.0  $\mu$ m, respectively. In order to get a more accurate optimum solution, it is necessary to include the influence of the VHTS accident conditions.

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Run	A:IPyC	B:SiC	C:OPyC	Packing	Fractional release (FR), dimensionless			
	thickness,	thickness,	thickness,	fraction (PF),	Ag-110m	Cs-137	Kr-85	Sr-90
	μm	μm	μm	dimensionless	- C			
1	38	36	20	0.261	6.296E-09	3.325E-11	6.831E-05	2.056E-48
2	38	20	38	0.265	1.874E-07	9.785E-10	2.085E-03	7.029E-45
3	58	56	20	0.339	7.156E-10	3.721E-12	7.513E-06	1.249E-49
4	37	45	52	0.339	1.912E-09	1.009E-11	2.015E-05	3.427E-49
5	38	36	20	0.261	6.296E-09	3.325E-11	6.831E-05	2.056E-48
6	20	57	20	0.267	2.486E-10	1.164E-12	3.536E-06	3.005E-50
7	20	37	42	0.270	3.516E-09	1.756E-11	4.355E-05	1.036E-48
8	60	41	34	0.341	4.365E-09	2.347E-11	4.550E-05	1.007E-48
9	20	37	42	0.270	3.516E-09	1.756E-11	4.355E-05	1.036E-48
10	20	90	26	0.343	1.291E-20	8.685E-24	1.151E-76	6.674E-56
11	37	45	52	0.339	1.912E-09	1.009E-11	2.015E-05	3.427E-49
12	60	20	20	0.272	2.809E-07	1.630E-09	2.860E-03	6.695E-45
13	38	20	38	0.265	1.874E-07	9.785E-10	2.085E-03	7.029E-45
14	20	20	60	0.272	1.332E-07	6.856E-10	1.581E-03	7.163E-45
15	20	20	20	0.206	1.354E-07	7.101E-10	1.526E-03	9.380E-45
16	38	20	38	0.265	1.874E-07	9.785E-10	2.085E-03	7.029E-45
17	20	56	60	0.343	3.063E-10	1.444E-12	4.188E-06	3.422E-50
18	44	71	20	0.341	1.155E-10	6.021E-13	1.232E-06	2.048E-50
19	32	65	36	0.337	1.472E-10	7.435E-13	1.758E-06	2.269E-50
20	56	20	60	0.343	2.532E-07	1.342E-09	2.802E-03	4.800E-45

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



Fig. 4. Three-dimensional surface of the optimum.