

## Design of Optimal Coating Layer Thicknesses for an 800- $\mu\text{m}$ $\text{UO}_2$ TRISO of a small prismatic HTR

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### 1. Introduction

A large number of coated fuel particles (CFPs) are contained in a fuel element of a high temperature reactor (HTR). A tri-structural CFP (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  $\text{UO}_2$  fuel kernel up to 800  $\mu\text{m}$  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. For an extended fuel life, more CO,  $\text{CO}_2$ , fission gases will be generated in the TRISO with a  $\text{UO}_2$  kernel of 800  $\mu\text{m}$  than in the conventional TRISO with a  $\text{UO}_2$  kernel of about 500  $\mu\text{m}$ . 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  $\text{UO}_2$  kernel of 800  $\mu\text{m}$  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<sup>®</sup> [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:

$$y = PF \cdot P_{f,SiC}, \quad (1)$$

where  $y$  is the objective function (dimensionless)  $\in [0, 1]$ ,  $PF$  is the packing fraction (dimensionless)  $\in [0, 1]$ , and  $P_{f,SiC}$  is the failure probability of the SiC layers (dimensionless)  $\in [0, 1]$ . The lower the values of the packing fraction and the SiC failure probability, the more preferable.

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

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

where  $N_{TRISO}$  is the number of TRISOs in a compact,  $V_{compact}$  is the volume of a compact ( $\text{cm}^3$ ),  $r_K$  is the radius of a kernel ( $\mu\text{m}$ ),  $t_B$  is the buffer thickness ( $\mu\text{m}$ ),  $t_I$  is the IPyC thickness ( $\mu\text{m}$ ),  $t_S$  is the SiC thickness ( $\mu\text{m}$ ), and  $t_O$  is the OPyC thickness ( $\mu\text{m}$ ). The failure probability of the SiC coating layers is given using a cumulative Weibull distribution as follows:

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

where  $\sigma_\theta$  is the tangential stress acting on the inner surface of the SiC layer (MPa),  $\sigma_{med}$  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:

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

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  $UO_2$  with an enrichment of 15.5 w/o and its diameter is 800  $\mu m$ . 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 [3] 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  $\mu m$ , 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.

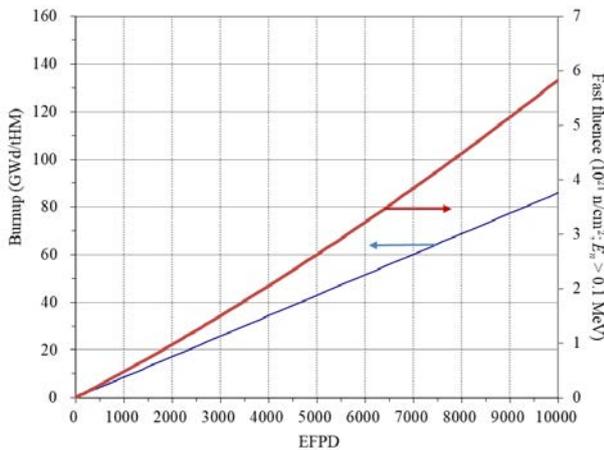


Fig. 1. Variation of fuel burnup and fast fluence.

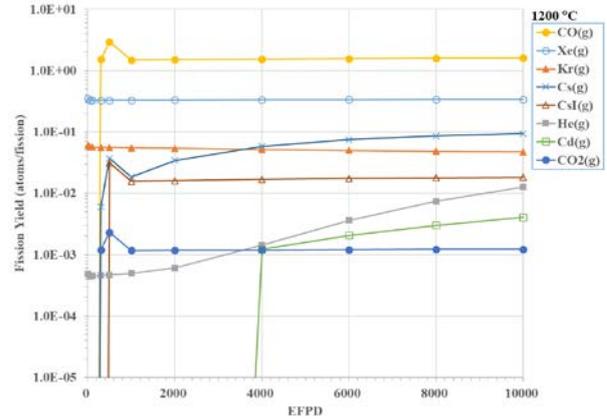


Fig. 2. Variation of the fission yields of gases produced in a TRISO.

#### 3.2. An optimal design for the coating layer thicknesses

The thickness ranges considered are 100 to 150  $\mu m$  for the buffer, 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 1.162 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 [4] 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:

$$0 \leq t_b + t_l + t_s + t_o \leq 242.992 . \quad (5)$$

The calculation of the failure probability of the SiC layer requires the SiC maximum tangential stresses that can be calculated using the COPA code [5]. 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 [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 SiC failure probability at 10000 days are used.

During an optimization using the ‘Optimal (custom) Design’, the importances of the packing fraction and the SiC failure probability were set to ‘\*\*\*’ and ‘\*\*\*\*\*’, respectively. 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<sup>®</sup> was set to produce 100 local optimums currently. Table II shows ten local optimums in the order of desirability [7]. Fig. 3 shows a ramp-type solution of the first optimum whose desirability is the best. Compared to the conventional design of a 500- $\mu\text{m}$  UO<sub>2</sub> TRISO where the thicknesses of the buffer, IPyC, SiC and OPyC layers are 100, 40, 35 and 40  $\mu\text{m}$ , respectively, the thicknesses of the IPyC and OPyC layers are reduced by about 20 and 13  $\mu\text{m}$ , respectively, and the SiC layer thickness is increased by about 32  $\mu\text{m}$ . The packing fraction of the first optimum TRISOs is about 35 %, which is equal to that of the conventional TRISOs. The SiC failure probability is near zero at 10000 days.

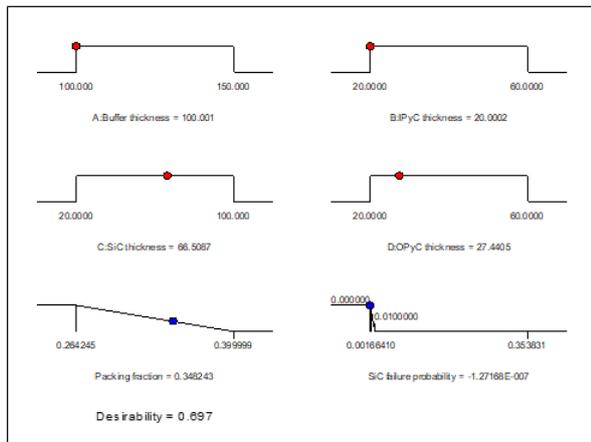


Fig. 3. A ramp-type solution of the first optimum in Table II.

#### 4. Summary

The optimal thicknesses of the coating layers of an 800- $\mu\text{m}$  UO<sub>2</sub> TRISO have been evaluated using a computer-generated optimal design of a response surface methodology. One of the optimum solutions is that the thicknesses of the buffer, IPyC, SiC and OPyC layers are 100, 20, 67 and 27  $\mu\text{m}$ , respectively. In order to get a more accurate optimum solution, it is necessary to consider all failure and fission product release mechanisms related to a TRISO in the calculation of the objective functions and to add more design variables such as density, Bacon Anisotropy Factor, and particle asphericity.

#### ACKNOWLEDGEMENTS

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

Point	A:Buffer thickness, $\mu\text{m}$	B:IPyC thickness, $\mu\text{m}$	C:SiC thickness, $\mu\text{m}$	D:OPyC thickness, $\mu\text{m}$	Packing fraction ( $PF$ ), dimensionless	SiC failure probability ( $P_{f,siC}$ ), dimensionless
1	150	20	36.18681034	36.80518966	0.399999461	0.0133981
2	100	40	40	22	0.328270737	0.197482
3	120	37.48247092	20	38.4	0.351508821	0.338994
4	125	20.2	30.4	26.81846298	0.328955777	0.259409
5	126.75	39.6	52.8	23.8	0.399921082	0.00535012
6	138.0967737	60	20	24.8952263	0.399999461	0.196018
7	100	20	61.2	20	0.326963755	0.0329327
8	100	42.40623314	54.19864279	46.38712408	0.399999461	0.0143969
9	150	20	20	20	0.34153263	0.328581
10	100	60	20	20	0.325009794	0.333998
11	100	20	20	60	0.325009794	0.31725
12	150	20	36.18681034	36.80518966	0.399999461	0.0133981
13	150	42.992	30	20	0.399999461	0.030734
14	100	60	20	60	0.394441516	0.353831
15	120	37.48247092	20	38.4	0.351508821	0.338994
16	100	42.40623314	54.19864279	46.38712408	0.399999461	0.0143969
17	114.9365738	60	27.68350456	40.37192166	0.399999461	0.107717
18	100	20	100	22.992	0.399999461	0.00170742
19	126.75	39.6	52.8	23.8	0.399921082	0.00535012
20	100	20	20	20	0.264245	0.305642
21	100	20	62.992	60	0.399999461	0.00766457
22	142.992	20	20	60	0.399999461	0.18671
23	120	37.48247092	20	38.4	0.351508821	0.338994
24	100	60	62.992	20	0.399999461	0.00845913
25	131.5230806	20	71.46891942	20	0.399999461	0.0016641

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

No	Optimal thickness ( $\mu\text{m}$ )				Packing fraction	SiC failure probability	Desirability
	Buffer	IPyC	SiC	OPyC			
1	100.001	20.0002	66.5087	27.4405	0.348243	-1.27168E-007	0.696552
2	100.000	20.0001	64.0607	29.9688	0.348379	-2.65027E-007	0.695864
3	100.102	20.0000	64.4943	29.5788	0.348626	-3.70865E-007	0.694613
4	100.001	20.0000	63.1431	31.1687	0.348861	-2.18772E-007	0.693421
5	100.000	20.0000	62.9402	31.4581	0.349008	-2.20778E-007	0.692675
6	100.000	20.0000	68.9385	25.5832	0.349218	-3.11967E-007	0.691601
7	100.000	20.0015	62.3825	32.3130	0.349517	-2.18904E-007	0.690072
8	100.000	20.0000	69.8905	24.9856	0.349823	-1.31380E-008	0.688501
9	100.003	20.0000	61.9416	33.0595	0.350042	-2.99944E-007	0.687374
10	100.365	20.0000	68.5199	26.2134	0.350203	-1.83479E-008	0.686542