# Inter-Comparison of Computer Codes for TRISO-Based Fuel Micro-Modeling and Performance Assessment

### **HTR 2010**

Brian Boer Young Min Kim Wen Wu Abderrafi M. Ougouag Donald McEachern Francesco Venneri

### October 2010

This is a preprint of a paper intended for publication in a journal or proceedings. Since changes may be made before publication, this preprint should not be cited or reproduced without permission of the author. This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, or any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for any third party's use, or the results of such use, of any information, apparatus, product or process disclosed in this report, or represents that its use by such third party would not infringe privately owned rights. The views expressed in this paper are not necessarily those of the United States Government or the sponsoring agency.

The INL is a U.S. Department of Energy National Laboratory operated by Battelle Energy Alliance



# Inter-comparison of Computer Codes for TRISO-based Fuel Micro-Modeling and Performance Assessment

Brian Boer<sup>1</sup>, Young Min Kim<sup>2</sup>, Wen Wu<sup>3</sup>, Abderrafi M. Ougouag<sup>1</sup>, Donald McEachern<sup>3</sup>, Francesco Venneri<sup>4</sup>

<sup>1</sup>Idaho National Laboratory, 2525 Fremont Avenue, Idaho Falls, ID 83415, USA, brian.boer@inl.gov

<sup>2</sup>Korea Atomic Energy Research Institute, 1045 Daedeok-daero, Yuseong-gu, Daejeon, 305-600, Republic of Korea

<sup>3</sup>General Atomics, P.O. Box 85608, San Diego, CA 92186-5608

<sup>4</sup>Logos Technologies, Inc., 3811 N. Fairfax Drive, Suite 100, Arlington, VA 22203, U.S.A.

Abstract - The Next Generation Nuclear Plant (NGNP), the Deep Burn Pebble Bed Reactor (DB-PBR) and the Deep Burn Prismatic Modular Reactor (DB-PMR) are all based on fuels that use TRISO particles as their fundamental constituent. The TRISO particle properties include very high durability in radiation environments, hence the designs reliance on TRISO to form the principal barrier to radioactive materials release. This durability forms the basis for the selection of this fuel type for applications such as Deep Burn (DB), featuring burn-up levels much higher than those expected in other gas-cooled reactors or light water reactors. It follows that the study and prediction of the durability of TRISO particles must be carried out as part of the safety and overall performance characterization of all the designs mentioned above. These evaluations have been carried out in the DB project using independently developed computer codes. The codes (PASTA, COPA and PISA) incorporate different models for stress analysis on the various layers of the TRISO particle, models for fission products release, migration and accumulation within the TRISO particle, models for free oxygen and CO formation, models for temperature field within the various layers of the TRISO particle, and models for the prediction of failure rates.

The large number of models, and the possibility of different constitutive data, formulations and solution techniques make it likely that some differences in the results of the three codes will be found in the modeling of identical situations. An inter-comparison has been carried out by the cooperating institutions within the workscope of the Deep Burn Project of the Department Of Energy (DOE), using a set of pre-defined TRISO conditions (burn-up level, temperature and power level, etc.) and the outcome is tabulated. The inter-comparion aims at identifying the areas of disagreement and their impact on the fuel performance. To this end, several sensitivity studies on the input parameters have been performed and areas for further modeling or reconciliation are shown.

#### I. INTRODUCTION

Both the Next Generation Nuclear Plant (NGNP) and the Deep-Burn (DB) concept employ the TRISO

coated particle as the fuel constituent. In DB concept the fuel kernel itself is composed of transuranics (TRU) that is extracted from used light water reactor fuel. The DB fuel is irradiated up to a fractional burn-

up of the order of 60-70% of fission events per initial metal atom (FIMA). The coated particles are either embedded in the fuel zone of graphite pebbles or in cylindrical fuel compacts that are placed in prismatic fuel blocks.

In any case, the TRISO coated particle forms the main barrier for the release of the radioactive fission products during operation of the reactor and storage of the used fuel in a repository. Its durability is therefore key in both the NGNP and DB concepts. In the framework of the DB project several codes (PASTA, COPA and PISA) have been used to analyze the durability of the coated particle fuel for different cases. The PASTA code [1, 2] has been applied to analyze the fuel performance of the coated particles in the DB pebble-bed reactor design, while the COPA code [3] was used for fuel analysis of the DB prismatic reactor design. The performance of the DB fuel during long-term storage in a repository has been evaluated with the PISA code [4, 5].

The codes (PASTA, COPA and PISA) that are described in the following section employ different models and assumptions for the analysis of the coated particle performance. These differences can be found in the models for stress analysis on the various layers of the TRISO particle, models for fission products release, migration and accumulation within the TRISO particle, models for free oxygen and CO formation and migration, models for temperature field within the various layers of the TRISO particle, and models for the prediction of failure rates. Moreover, the possibility of different constitutive data for mechanical and thermal properties make it highly unlikely that the three codes would give identical results in the modeling of identical situations.

An inter-comparison has been carried out by the cooperating institutions within the workscope of the DOE Deep-Burn Project, using a common set of predefined TRISO conditions (burn-up levels, temperature or power levels, etc.). The coated particle under investigation is a design that is currently considered within the Deep-Burn Project to be fabricated within the near future. Besides the inter-comparison of the results for the performance of this fuel design additional investigations are performed to quantify the sensitivity of the input parameters. Finally, conclusions are drawn regarding both the performance analysis methods and the performance of the envisioned DB particle design.

## II. CODES FOR DEEP-BURN FUEL PERFORMANCE ANALYSIS

The following subsections give a description of the PASTA, COPA and PISA codes, their capabilities and modeling assumptions.

I/OPyC material property	Value
Young's modulus of elasticity [MPa]	$3.96 \times 10^{4}$
Poisson's ratio [-]	0.33
Poisson's ratio of creep [-]	0.4
Creep coefficient $[10^{-25} (\text{MPa.m}^{-2})^{-1}]$	$2.0 \times 10^{-4}$
Dimensional change rate	Ref. [6]
$[10^{-25} (\text{MPa.m}^{-2})^{-1}]$	
Thermal expansion coefficient $[K^{-1}]$	Ref. [6]
BAF	1.036
Median strength [MPa]	388, Ref.[7]
Weibull modulus of strength [-]	7.9, Ref.[7]
SiC material property	Value
Young's modulus of elasticity [MPa]	$4.0 \times 10^{5}$
Poisson's ratio [-]	0.13
Thermal expansion coefficient $[K^{-1}]$	Ref. [7]
Median strength [MPa]	300
Weibull modulus of strength [-]	9.6

Table 1: Overview of material properties of the coatings assumed in the PASTA code. In the intercomparison case the PISA and COPA codes assume the same properties unless stated otherwise.

#### II.A Description of the PASTA code

The PASTA code [1, 2] describes the mechanical behavior of TRISO particles during irradiation and aims at calculating the coating stresses and the corresponding failure probabilities. In general, DB TRISO particles have a Pu/MA- $O_{2-x}$  fuel kernel of 200-350  $\mu m$  in diameter at their very center. Adjacent to the kernel is a 90-150  $\mu m$  thick porous carbon buffer, which is coated with an inner pyrolytic carbon (IPyC) layer (35  $\mu m$ ), a silicon carbide (SiC) layer (45  $\mu m$ ), and an outer pyrolytic carbon (OPyC) layer (35  $\mu m$ ). These coatings provide the primary containment of the fission products that are generated within the fuel kernel.

PASTA embodies a one-dimensional analytical and multi-layer model that takes into account the visco-elastic behavior of the coating layers and the surrounding graphite during irradiation. The main source of stress in all layers is due to the pressure build-up from the gaseous fission products in the buffer layer resulting in a radial stress on the IPyC. Moreover, the Pyrocarbon (IPyC and OPyC) layers exhibit radiation-induced dimensional changes and creep (in the radial and tangential directions). Finally, the model allows thermal expansion of all layers. PASTA solves the general stress strain equations in spherical geometry, which include the aforementioned effects [1].

The mechanical failure probability of the coated particle is determined from the magnitude of the (tensile) stress in the SiC layer, which is the main load-bearer, according to a Weibull distribution [7].

The resulting pressure (from both fission products and CO accumulation) on the IPyC layer is calculated as a function of the kernel temperature and the buffer volume with the Redlich-Kwong equation of state. In the analysis of the fission product diffusion data for  $\rm UO_2$  fuel is used [8], since diffusion coefficients for Deep-Burn fuel kernels are not yet available. The amount of CO formation from free oxygen is calculated from thermo-chemical data as a function of the burn-up level, the oxygen getter characteristics, and the temperature [9].

The PyC coating layers exhibit a dimensional change under irradiation in a fast neutron flux. The dimensional change as a function of the fast neutron fluence (E >0.18 MeV) is fitted for several temperatures and Bacon Anisotropy Factors (BAFs) [6]. Table 1 shows an overview of the data used in PASTA for the mechanical properties.

Recently, the PASTA code was coupled to the PEBBED code [10] for neutronic, thermal-hydraulic and depletion analysis of pebble-bed cores. This coupled code system [11] allows for the determination of the coated particle performance as a function of the local and time dependent core parameters (temperature, kernel power, fast fluence level, burn-up level, core residence time and fission product (Xe, Kr) concentration). This allows for determination of the stress effects caused by the power and temperature peaking that are typically found in a DB core design. The variation in the thicknesses of the coating layers that can be found in a typical batch of particles is treated by a statistical method [12]. Furthermore, stresses can be evaluated for slow transients such as a Loss Of Forced Cooling (LOFC) incident.

#### II.B Description of the COPA code

The COPA (COated PArticle) code consists of nine modules as follows [3]:

COPA-BURN: This module calculates the neutron flux and fluence with time, and then burn-up, fission rate per volume, power generation and fission product inventory throughout a fuel element and a fuel particle for a given location in the core. This is inserted into the COPA-MECH, COPA-FAIL, and COPA-FPREL modules.

COPA-TEMTR: This module calculates the temperature distribution in a coated particle by using a finite element method utilizing the Galerkin form of the weighted residuals procedure [13]. The numerical modeling is one-dimensional. The geometric elements for the numerical modeling are the fuel kernel, a gap between the kernel and the buffer, the buffer, a gap between the buffer and the IPyC, the IPyC layer, the SiC layer and the OPyC layer.

COPA-TEMPEB: This module calculates the temperature distribution in a pebble by using the finite element method. This model is one-dimensional for a pebble. The geometric elements are a fuel region and a matrix graphite region. The fuel region is assumed to be a homogeneous mixture of matrix graphite and coated particles.

COPA-TEMBL: This module calculates the temperature distribution in an equivalent slab or an equivalent cylinder for a fuel block in the prismatic modular reactor by using the finite element method. The fuel compact is assumed to be a homogeneous mixture of matrix graphite and coated fuel particles.

COPA-MECH: This module performs mechanical analyses on an intact coated fuel particle by using the finite element method [14]. The models are one-dimensional. The geometric elements for a numerical modeling are a fuel kernel, a buffer, and three coating layers. This calculates the contact forces or pressures acting on interfaces between the layers of a coated particle. This is inserted into the COPA-FAIL module to calculate the failure fraction of the coated fuel particles during a reactor operation.

COPA-FAIL: This module calculates the failure fractions of coated fuel particles under reactor operational conditions. It uses a Monte Carlo method for a random particle sampling in which a sample is equivalent to a coated fuel particle. The particle has different dimensional sizes, material properties, and frac-

ture strengths of the coating layers through the Monte Carlo sampling. It is assumed that the variations in the kernel diameter, the thicknesses of the buffer and the other coating layers and the densities of the kernel and coatings follow a normal distribution. The strengths of the SiC and PyC layers are expressed in the Weibull distribution. In order to calculate the stresses of the coating layers of a coated particle and check the particle integrity, the COPA-FAIL uses the COPA-MECH for an intact coated fuel particle and the statistical correlations obtained in the COPA-ABAQ for a particle with de-bonded or cracked layers.

COPA-FPREL: This module analyzes the fission product migration in the fuel during the irradiation using a finite element method [15]. Both coated particle fuel embedded in pebbles and prismatic block type fuel can be modeled. Besides normal operating conditions, specific conditions such as a heat-up of the fuel or irradiation tests can be simulated. For a fuel block, an equivalent slab or equivalent cylinder is assumed. The migration mechanism is assumed to be diffusion only.

COPA-ABAQ: This module analyzes the crack and de-bonding of the coating layers using ABAQUS. These models are two-dimensional. This produces the maximum SiC stresses in the cracked or de-bonded particles according to several parameters such as particle sizes, material properties and irradiation temperature. A statistical correlation can be developed through a statistical method which correlates the maximum SiC stress to the particle parameters. The correlation is inserted into the COPA-FAIL to calculate the maximum SiC stress for particles with de-bonded or cracked layers.

COPA-MPRO: This module calculates or provides (1) the material properties of the kernel material, buffer, high-density pyrocarbon, silicon carbide, matrix graphite, and structural graphite, (2) the conductivity over a gap, (3) the partition factors at the layer interfaces of a coated fuel particle, (4) the diffusion coefficients of the fission products, (5) the sorption isotherm data of the fission products on the surfaces of a pebble, a compact, or a fuel block, (6) heat and mass transfer coefficients of fission products in helium.

Each module is a stand-alone program. It is inserted into other modules or is used to generate the input data for other modules.

#### II.C Description of the PISA code

The PISA code [4, 5] is a stand-alone onedimensional Finite Element Analysis (FEA) program developed by General Atomics, Inc. It uses a spherically symmetric formulation designed to perform thermal-stress history analysis of irradiated fuel particles. PISA has been widely utilized for estimating the performance of the multi-layered coated fuel particle designs. PISA performs a coupled thermal-stress time-history analysis. A list of capabilities currently available in the PISA code is provided below [4, 5]:

The thermal model solves the radial steady-state heat transfer equilibrium equations. Volumetric heat generation rates and prescribed temperature at the outer surface are used as the boundary conditions.

The stress model solves the radial equilibrium equations using a Finite Element Method (FEM) formulation based on one-dimensional quadratic elements (3 nodes per element). The boundary conditions for this model are a prescribed pressure at the material interfaces and/or the outer surface. It can adopt linear-elastic and visco-elastic material models. Irradiation-induced strains as a function of fluence and temperature can be treated. The model computes thermal strain based on a given reference temperature. Irradiation strains take into account the coupling of preferred orientation to apparent creep strain (Kaae model [16]). The stress model has an option for large deformation analysis: true stresses, true strains.

The kernel pressure is either adopted from the (manual) input or is calculated internally using the fuel burn-up level and temperature, the particle geometry, the kernel type and the buffer density.

The determination of the failure probabilities for each coating layer of the particle is based on Weibull distribution for each particular material. Material parameters and the boundary conditions may be functions of the temperature and the fluence level.

The code has a Monte Carlo driver for statistical analysis, which can generate random variables for normal or Weibull distributions. The PISA-Wrapper is capable of treating variations in the coating layer thickness as a function of time or fluence, which are fed into PISA.

PISA has been used recently in the performance modeling of Deep-Burn TRISO fuel particle that used ZrC both as the main load-bearer and as an oxygen getter [17].

### III. DESCRIPTION OF THE COATED PARTICLE DESIGN

The coated particle design specifications used for the inter-comparison are derived from the particle design that is considered to be fabricated in the near future within the Deep-Burn Project. The fuel kernel consists of transuranics (TRUs) and a SiC 'getter' that reduces the CO production in the particle. The mole ratio of TRU:SiC in the kernel is 1:0.6 having an average density of 7.6 g/cm<sup>3</sup>. The Minor Actinide oxide (MAO<sub>2-x</sub>) fuel is sub-stoichiometric having 1.8 oxygen atoms per MA atom on average. The isotopic compositions of the transuranics are shown in Table 2. Table 3 shows the dimensions of the kernel and coating layers and their statistical variation in size.

Isotope	Fraction (wt. %)
<sup>237</sup> Np	6.8
<sup>238</sup> Pu	2.9
<sup>239</sup> Pu	49.38
<sup>240</sup> Pu	23
<sup>241</sup> Pu	8.8
<sup>242</sup> Pu	4.9
$^{241}$ Am	2.8
$^{242m}$ Am	0.02
$^{243}\mathrm{Am}$	1.4

Table 2: Isotopic composition of Deep-Burn fuel.

Layer	Thickness	Density
	$(\mu m)$	$(g/cm^3)$
Kernel	350*± 10	7.6
$(MAO_{1.8}(SiC)_{0.6})$		
Buffer	$100 \pm 5$	1.0
IPyC	$35 \pm 5$	1.9
SiC	$45 \pm 5$	3.2
OPyC	$35 \pm 5$	1.9

<sup>\*</sup> Kernel diameter.

Table 3: Dimensions of the coating layers and its statistical variation for the DB coated particle design.

### IV. CASE DEFINITION FOR CODE INTER-COMPARISON

To compare the fuel performance codes predefined boundary conditions (Table 4) are adopted instead of using core analysis tools. It is assumed that

the fuel particle has a fixed (outer surface) temperature of 1200 K at a power level of  $2.0 \times 10^{-2}$  W for 1120 days of irradiation in the core. The temperature within the kernel and in the coating layers is calculated by the fuel performance codes from the particle surface temperature and kernel power. At the end of the irradiation the particle reaches a burn-up level of 560 MWd per kilogram of Initial Heavy Metal (IHM) loading. The adopted parameters are taken from a PEBBED analysis of a Pebble Bed Modular Reactor design (400 MW<sub>th</sub>) loaded with Deep-Burn fuel (Table 2) [11]. In the inter-comparison case, the fuel burn-up and the fast neutron fleunce level attained, are linear functions of the irradiation time, since the kernel power level is assumed to be constant. It is noted that the boundary conditions presented above are intended to represent the typical environment of a Deep-Burn reactor core without making any specific assumptions about the type of reactor (pebble bed or prismatic).

Final burn-up level	560 MWd/kg IHM
Final fast fluence (E>0.1 MeV)	$5.0 \times 10^{21} \text{ cm}^{-2}$
Particle surface temperature	1200 K
Kernel power	$2.0 \times 10^{-2} \text{ W}$
Irradiation time	1120 d

Table 4: Assumptions and boundary conditions adopted in the fuel performance analysis.

#### V. RESULTS

In the following section (Section V.A) the results of the fuel performance analysis of the three codes are compared and analyzed. In Section V.B the sensitivity of several input parameters on the results is investigated.

#### V.A Analysis of the reference coated particle

During the irradiation of the coated particle fuel gaseous fission products that are formed in the kernel diffuse to the porous carbon buffer layer. Figure 1 shows the amount of fission products released from the kernel to the buffer layer as a function of the fast neutron fluence attained. The PASTA and COPA codes assume the release according to the Kidson and Booth models [18]. In these models the diffusion of the fission products is a function of the time and the

temperature (diffusion coefficients adopted from [8] and [19], respectively), while PISA assumes a fixed value of 60 % release fraction. As a result the PISA code gives a linear build-up of the fission products in the buffer layer, while in the PASTA and COPA codes the release is somewhat delayed (see Figure 2). It is noted that no formation of CO by free oxygen is expected, since the kernel contains a SiC getter [9]. Furthermore, the contribution to the internal pressure by the formation of He is in general one order of magnitude smaller than the contribution of Xe. Although its contribution can be significant for certain DB fuel types [20], it is not considered in the current intercomparison.

The calculation results for the available (void) volume for the gaseous fission products is shown in Figure 3. In the PASTA and PISA codes the initial void volume in the buffer is calculated according to:

$$V_{void} = 1 - \frac{\rho_{buf}}{\rho_{graphite}},\tag{1}$$

in which,  $\rho_{buf}$  is the buffer density and  $\rho_{graphite}$  is the theoretical maximum value of the density of graphite. The COPA code assumes that the kernel volume also has some void space (0.5 % of the kernel pore volume). Furthermore, the PISA and COPA codes assume that the void space in the buffer reduces with increasing radiation due to kernel swelling, which is caused by build-up of solid and gaseous fission products.

The build-up of gaseous fission products in the buffer results in a pressure (see Figure 4) on the IPyC layer, which is calculated by all three codes by the Redlich-Kwong equation of state. The pressure is directly dependent on the buffer void volume. Therefore the PISA code calculates the highest pressure and the PASTA code the lowest, resulting from the low and high values for the void volume, respectively.

In principle, the buffer pressure results in a tangential tensile stress on the SiC layer, which is the main load-bearer of the particle. However, the PyC layers shrink (see Figure 5) and thereby put the SiC under compression. The following references and assumptions were used by the codes to determine the PyC dimensional change as a function of the fast fluence level:

• COPA: Ref. [6], with  $\rho_{PyC} = 1.9 \text{ g/cm}^3$ , T = 1200 K, BAF<sub>0</sub>=1.0

- PASTA: Ref. [6], with  $\rho_{PyC}$  = 1.9 g/cm<sup>3</sup>, T = 1200 K, BAF<sub>0</sub>=1.036
- PISA: Ref. [21] page 30, with T = 1473 K, BAF<sub>0</sub>=1.036

The shrinkage and swelling behavior of the PyC layers is a function of the Bacon Anisotropy Factor (BAF), which is determined by the fabrication process of the layers. For a PyC layer that is isotropic (BAF=1) the dimensional change in the radial and tangential dimension are equal, which is assumed in the COPA code. The PASTA and PISA codes assumed that the PyC is slightly anisotropic (BAF=1.036), which results in less shrinkage of the PyC in the radial direction in the beginning of the irradiation. Furthermore, there exists a turnaround point where the shrinkage in the radial direction turns into swelling. It is noted that the effective length of the PyC layers is significantly larger in the tangential direction than in the radial direction. The dimensional change behavior of the first is therefore more impor-

In the beginning of the irradiation of the particle, the dimensional change of the PyC determines the stress state of all three layers (IPyC, SiC, and OPyC) entirely (see Figures 6-8). Since the three codes use similar dimensional change rates of the PyC in the tangential direction there is good agreement between the codes for the calculated stresses for low fluence levels. With increasing fluence level some differences can be identified, which can be explained as follows. The PASTA code has a lower buffer pressure than the COPA code, resulting in a lower stress on the SiC layer at the end of the irradiation. The PISA code has a higher buffer pressure than PASTA, but this seems to be compensated by the higher shrinkage (tangential) rate of the PyC. Therefore the PASTA and PISA codes show a similar result for the final SiC stress at the end of the irradiation.

There is a relatively good agreement between the failure probabilities of the three codes (see Figure 9), because the maximum IPyC and OPyC stresses are similar. Although the failure probability of the IPyC layer is relatively high, no significant failure probability was found for the SiC layer. While the PASTA and PISA codes calculated the failure probabilities from the maximum stress during the irradiation, the COPA code performed a Monte-Carlo calculation to the determine the failure probability.

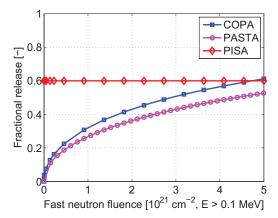


Fig. 1: Fractional release of gaseous fission products from the fuel kernel to the buffer layer, calculated by the COPA, PASTA and PISA codes.

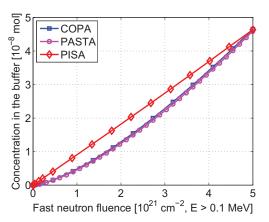


Fig. 2: Concentration of Xe and Kr in the buffer layer calculated by the COPA, PASTA and PISA codes.

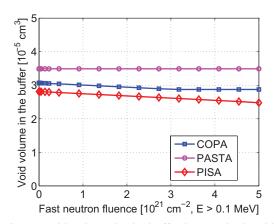


Fig. 3: Void volume in the buffer layer calculated by the COPA, PASTA and PISA codes.

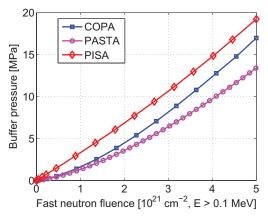


Fig. 4: Buffer pressure calculated by the COPA, PASTA and PISA codes.

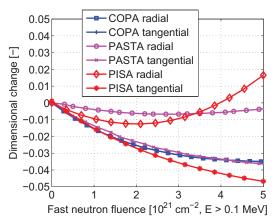


Fig. 5: Correlations for the PyC dimensional change used by the fuel performance codes.

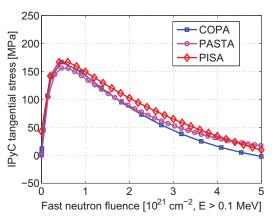


Fig. 6: Tangential stress in the IPyC layer calculated by the COPA, PASTA and PISA codes.

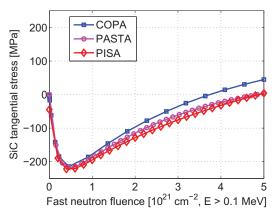


Fig. 7: Tangential stress in the SiC layer calculated by the COPA, PASTA and PISA codes.

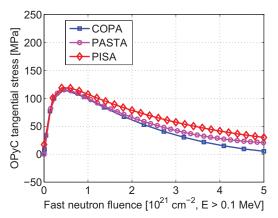


Fig. 8: Tangential stress in the SiC layer calculated by the COPA, PASTA and PISA codes.

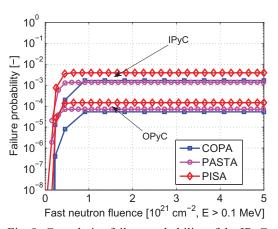


Fig. 9: Cumulative failure probability of the IPyC and OPyC coating layers as a function of the fast fluence calculated by the COPA, PASTA and PISA codes.

### V.B Sensitivity of input parameters on fuel performance

In the previous section some differences in the results were found resulting from the various assumptions made in the codes. Especially, the buffer void volume and the dimensional change of the PyC layers were modeled differently, which led to a small spread in the results of the coating stresses and the failure probability. In order to quantify the sensitivity of several input parameters on the coating stress and failure probability of the layers additional studies have been performed. The following parameters have been investigated:

- The particle coating dimensions.
- The dimensional change of the PyC layers.
- The creep coefficient of the PyC layers.
- The available volume (void) for the fission products in the buffer and kernel.

#### V.B.I Particle coating dimension sensitivity

The effect of the variation in the thickness of the SiC and buffer layer has been investigated with the PASTA code. The two layers were allowed to vary around their average value, assuming a normal distribution with a standard deviation of 5  $\mu m$ , according to Table 3. The failure probability for a given set of coating dimensions was weighted with its probability of occurrence. It was found that the variation in coating size did not have a large impact on the average failure probability of the SiC layer.

The failure probability of this 'batch' of particles was found to be  $< 1.0 \times 10^{-9}$ .

#### V.B.II PyC dimensional change sensitivity

An analysis was made with the PASTA code using three different BAF values, which correspond with three different PyC irradiation induced dimensional change rates for the radial and tangential directions (see Figure 10). It can be seen from Figure 11 that especially the final stress level of the SiC layer is sensitive to the dimensional change of the PyC, while the maximum stress of the IPyC and OPyC is relatively insensitive. This conclusion appears to be at variance with observations during irradiations and to the importance usually assigned to the BAF $_0$  of pyrocarbon coatings.

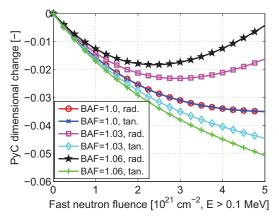


Fig. 10: Irradiation induced dimensional change as a function of the fast fluence level (E > 0.1 MeV) for three BAF values (1.00, 1.03, 1.06).

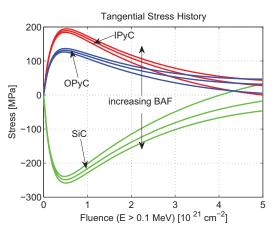


Fig. 11: Effect of the BAF value (1.00, 1.03, 1.06) on the stresses in the coating layers (IPyC, SiC, OPyC) during irradiation.

#### V.B.III PyC creep coefficient sensitivity

From the analysis in Section V.A it was found that the maximum stress in the PyC layers ( $\sim$ 170 MPa) is relatively close to its median strength (300 MPa). This is expected to be the result of a relatively low value of the creep coefficient for radiation induced creep. An additional case was investigated with the PISA code in which the creep coefficient was doubled. The results for the coating stresses are shown in Figure 12. It can be seen that the increased creep coefficient reduces the effect of the dimensional change of the PyC layers. The tangential stresses are lower in all three layers for the increased creep coefficient

case, while the SiC stress at the end of the irradiation is higher.

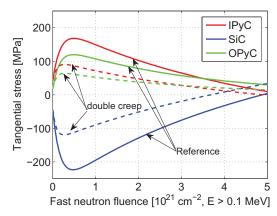


Fig. 12: Tangential stress as a function of the fast fluence calculated by the PISA code, assuming either the reference value for the creep coefficient  $(2.0 \times 10^{-29} (\text{MPa.m}^{-2})^{-1})$  or double this value.

#### V.B.IV Void volume sensitivity

The PASTA code has been used to investigate the sensitivity of the void volume in the buffer on the SiC stress. Results are shown in Figure 13. It can be seen that a reduction of the void volume significantly increases the SiC, while an increase of the void volume only results in a moderate reduction of the stress.

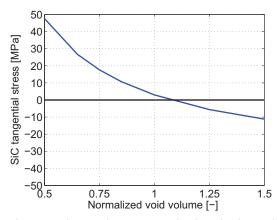


Fig. 13: The maximum stress in the SiC layer during the irradiation as a function of the void volume in the buffer calculated with the PASTA code (reference volume =  $3.5 \times 10^{-6}$  cm<sup>3</sup>).

#### VI. CONCLUSION

## VI.A Conclusions regarding fuel performance modeling of Deep-Burn coated particles

An inter-comparison of the fuel performance modeling of Deep-Burn coated particle fuel has been performed. It was found that there are several differences in the modeling approach between the COPA, PASTA and PISA codes.

- The models for the void volume in the kernel and buffer layer to which the fission products diffuse differ slightly between the codes. In the PISA and COPA models, the kernel is assumed to expand as a function of the irradiation level, thereby reducing the buffer void volume. Therefore, the buffer pressure in these models is higher, which results in a higher SiC stress.
- The dimensional change of the PyC layers has a large impact on the stress state of the coating layers. For a coated particle design that has a sufficient buffer volume to accommodate the fission products, the dimensional change determines the stress state of the coatings almost entirely.
- The effect of the dimensional change of the PyC layer is reduced in case the layers exhibit significant radiation induced creep. Proper experimental data on PyC radiation induced strain creep is key to accurate prediction of coated particle performance.
- VI.B Conclusions regarding the design and performance of the Deep-Burn coated particle
- The particle design in this paper adopts a SiC oxygen getter in the fuel kernel. This particle design was found to perform well, since CO formation in the buffer layer from free oxygen is avoided. All three codes used in the analyses (COPA, PASTA and PISA) indicate that there will be no significant through coating failure in the current DB coated particle design.
- In the presented analysis normal operating conditions were assumed. Further analysis for core transient conditions have to be analyzed in the future.

#### **ACKNOWLEDGEMENTS**

Work supported by the U.S. Department of Energy, Office of Nuclear Energy (NE), under DOE Idaho Operations Office Contract DE-AC07-05ID14517.

#### REFERENCES

- [1] B. Boer, A. M. Ougouag, J. L. Kloosterman, G. K. Miller. Stress analysis of coated particle fuel in graphite of High-Temperature Reactors. Nuclear Technology, 162, p. 276–292, 2008.
- [2] J. Jonnet, J. L. Kloosterman, B. Boer. Development of a stress analysis code for TRISO particles in HTRs. In Proceedings of the International Conference on the Physics of Reactors (PHYSOR-2008), Nuclear Power: A Sustainable Resource. Switzerland, 2008.
- [3] Y. M. Kim, M. S. Cho, Y. W. Lee, W. J. Lee. Development of a Fuel Performance Analysis Code COPA. In Proceedings of the 4th International Topical Meeting on High Temperature Reactor Technology (HTR-2008). Washington D.C., USA, Sep.-Oct. 2008.
- [4] CEGA-002549. PISA Software Requirement Specifications for Code to Perform Mechanical Analysis of Irradiated Fuel Particles. Technical report, CEGA Corporation, 1993.
- [5] CEGA-002550. PISA: A Coupled Thermal-Stress Code for the Mechanical Analysis of Irradiated Fuel Particles - User's Manual. Technical report, CEGA Corporation, 1993.
- [6] F. Ho. Material Models of Pyrocarbon and Pyrolytic Silicon Carbide. Technical Report CEGA-002820, CEGA Corporation, San Diego, CA, 1993.
- [7] L. L. Snead, T. Nozawa, Y. Katoh, T.-S. Byun, S. Kondo, D. Petti. Handbook of SiC properties for fuel performance modeling. Journal of Nuclear Materials, 371, p. 329–377, 2007.
- [8] H. Nabielek, K. Verfondern, H. Werner. "Can we predict coated particle failure?" A conversation on CONVOL, PANAMA and other codes. In Technical Meeting on: "Current Status and

- Future Prospects of Gas Cooled Reactor Fuels". IAEA, 2004.
- [9] T. M. Besmann. Thermochemical assessment of oxygen gettering by SiC or ZrC in  $PuO_{2-x}$  TRISO fuel. Journal of Nuclear Materials, 397, p. 69–73, 2010.
- [10] W. K. Terry, H. D. Gougar, A. M. Ougouag. Direct Deterministic Method for Neutronics Analysis and Computation of Asymptotic Burnup Distribution in a Recirculating Pebble-Bed Reactor. Annals of Nuclear Energy, 29, p. 1345–1364, 2002.
- [11] B. Boer, A. M. Ougouag. Core Analysis, Design and Optimization of a Deep-Burn Pebble Bed Reactor. In Proceedings of the PHYSOR 2010 Advances in Reactor Physics to Power the Nuclear Renaissance. American Nuclear Society, Pittsburgh, USA, May 2010.
- [12] B. Boer, A. M. Ougouag. Stress Analysis of Coated Particle Fuel in the Deep-Burn Pebble Bed Reactor Design. In Proceedings of the PHYSOR 2010 - Advances in Reactor Physics to Power the Nuclear Renaissance. American Nuclear Society, Pittsburgh, USA, May 2010.
- [13] D. W. Pepper, J. C. Heinrich. The Finite Element Method. Hemisphere Publishing Corp., USA, 1992.
- [14] Y. M. Kim, M. S. Cho. A Stress Analysis for a Coated Fuel Particle of a HTGR using a Finite Element Method. Nuclear Engineering and Technology, 41, 8, p. 1087–1100, Oct. 2009.
- [15] Y. M. Kim, M. S. Cho. Development of the Fission Product Release Analysis Code COPA-FPREL. Nuclear Technology, 170, p. 231–243, 2010.
- [16] J. Kaae. The Mechanical Behavior of Bisocoated Fuel Particles during Irradiation. Part I: Analysis of Stresses and Strains Generated in the Coating of a Biso Fuel Particle during Irradiation. Nuclear Technology, 35, p. 359–367, 1977.
- [17] D. Wongsawaeng. Performance modeling of Deep-Burn fuel using ZrC as a load-bearing

- layer and an oxygen getter. Journal of Nuclear Materials, 396, p. 149–158, 2010.
- [18] G. Kidson. A generalized analysis of the cumulative delusional release of fission product gases from an equivalent sphere of UO<sub>2</sub>. Journal of Nuclear Materials, 88, p. 299–308, 1980.
- [19] IAEA. Fuel performance and fission product behaviour in gas cooled reactors. Technical report, International Atomic Energy Agency, Vienna, 1997.
- [20] J. Jonnet, J. Kloosterman, B. Boer. Performance of TRISO particles fueled with plutonium and minor actinides in a PBMR-400 core design. Nuclear Engineering and Design, 240, p. 1320– 1331, 2010.
- [21] INERI. Development of improved models and designs for coated-particle gas reactor fuels. Technical Report INEL/EXT-05-02615, Final report under the international nuclear energy research initiative, December 2004.