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## Modeling the performance of TRISO-based fully ceramic matrix (FCM) fuel in an LWR environment using BISON



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#### ABSTRACT

Fully ceramic microencapsulated (FCM) fuel is a proposed fuel type for improved accident performance in LWRs (Light Water Reactors) that involves TRISO (TRistructural-ISOtropic) particles embedded in a nano-powder sintered silicon carbide (SiC) matrix. The TRISO particles contain a spherical fuel kernel ranging from 500 to 800 µm in diameter. The kernel and buffer layer are then coated with three layers, each of which is 30–40 µm thick, composed of dense inner pyrolytic carbon (IPyC), chemically vapor deposited silicon carbide (SiC) layer, and an outer pyrolytic carbon (OPyC) layer. These TRISO particles are then embedded in a fully dense sintered SiC matrix with an expected particle packing fraction of about 35–40% by volume. As is the case for gas reactor applications, the release of radioactivity into the coolant is dependent on the integrity of the silicon carbide layer of the TRISO particles, in addition to the SiC matrix. In this work, we report on fuel performance modeling of TRISO-bearing FCM fuel using the BISON code to simulate the thermo-mechanical behavior of this fuel in a prototypic LWR environment. This paper considers the effects of embedding a TRISO particle in the SiC pellet matrix and includes a discussion of the irradiation-induced dimensional change in the pyrolytic carbon (PyC) layers of the TRISO particle. Additionally, methods were developed to simulate a FCM pellet containing a large number of discrete and independent particles. Future work will report on developing an interface debonding model, a fracture model, and a radionuclide transport model.

#### 1. Introduction

The purpose of TRistructural-ISOtropic (TRISO) based Fully Ceramic Microencapsulated (FCM) fuel is to improve the accident performance of nuclear fuel by minimizing the probability of fuel failure and radioactivity release under severe conditions. The FCM concept involves embedding spherical kernels of fuel in concentric layers of pyrolytic carbon and Chemical Vapor Deposited Silicon Carbide (CVD-SiC). The resulting TRISO particles are embedded in a cylindrical, nano-powder sintered SiC matrix, (Venneri et al., 2016) which is referred to as the pellet. The SiC pellets are contained by traditional zircaloy cladding for use in an existing conventional Light Water Reactor (LWR) (Powers et al., 2013; Snead et al., 2011; Venneri et al., 2011).

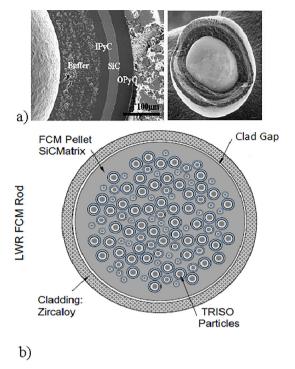
Fig. 1a (Hales et al., 2013) is a micrograph of a TRISO particle, and Fig. 1b (Terrani et al., 2012a) is a schematic showing the TRISO particles embedded in the cylindrical SiC matrix or FCM pellet, that is surrounded by the zircaloy cladding. The matrix sintering process uses cold pressing to consolidate the SiC nanopowder with aluminum and

The improvements with this fuel form are that additional barriers, which are the SiC matrix and the CVD-SiC layer within the TRISO particles, are expected to provide improved containment of fission products during accident scenarios when compared to UO2 (Terrani et al., 2015, 2012b). In addition, the thermal conductivity of the SiC matrix is higher than that of UO2 (Snead et al., 2007), and is expected to produce lower centerline temperatures for comparative rod average linear powers. The SiC matrix is expected to be very stable under irradiation for temperatures below 1000 °C, since the SiC swelling saturates at a fast neutron fluence of about  $1 \times 10^{25} \,\mathrm{n\,m^{-2}}$  and the irradiation creep rate appears to depend on the swelling rate (Terrani et al., 2015; Snead et al., 2014). Thus, it is anticipated that the SiC materials will not experience additional large displacements due to subsequent irradiation and temperature changes. As a result, this fuel form may be suitable for load following and high neutron fluence conditions in LWRs. The limitations of this fuel form are that the smear fuel volume

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yttrium oxides. This "green" pellet is then sintered to form the SiC matrix. A recent article by Terrani et al. (2015) as well as the original FCM patent (Venneri et al., 2016) discuss the process in detail.

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**Fig. 1.** a) Photomicrographs showing a TRISO particle with its individual layers of porous carbon buffer, inner pyrolytic carbon, silicon carbide, and outer pyrolytic carbon (Hales et al., 2013). b) Schematic illustration of the geometrical model for an FCM particle containing 40% packing fraction of TRISO particles (Terrani et al., 2012).

fraction of the pellet is only about 10–20% that of a traditional  $UO_2$  pellet. As a result and in comparison to traditional  $UO_2$  fuel, either higher enrichments, shorter fuel cycle durations, or lower power densities will be required.

There are several established TRISO Fuel Performance Models (FPMs) such as PARFUME, ATLAS, and Stress3 (Petti et al., 2004; IAEA, 2012). PARFUME is considered the state of the art TRISO FPM, and is a 1D model that uses ABAQUS to calculate 3D effects such as cracking, debonding, and asphericity however, PARFUME only models the particle and not the matrix (Petti et al., 2004; IAEA, 2012; Powers and Wirth, 2010; Miller et al., 2009). The BISON fuel performance code is a finite element program developed by Idaho National Laboratory. Due to its framework, BISON is highly adaptable, parallelizable, and designed for one, two, and three dimensional simulations. This structure gives BISON the ability to analyze large, complex, and highly coupled systems, which is essential for FCM fuel performance simulations (Perez et al., 2013; Hales et al., 2013). This paper will discuss the material models, the BISON fuel performance code comparison, and then the methods used to simulate a FCM pellet in a LWR environment. A followon paper will discuss the methods used to simulate interface debonding, matrix fracture, and radio nuclide transport.

#### 2. Modeling approach

Due to the random arrangement of the TRISO particles in the matrix and the resulting lack of symmetry, it is necessary to model the entire pellet and the embedded particles. Additionally, it was found that the thickness of the outer pyrolytic carbon layer can potentially have a significant impact on the stresses induced in the SiC materials, and that a substantial fraction of the heat flows through additional particles and interface gaps during its transport to the pellet surface. As a result, homogenous particles are unable to produce representative results over a wide range of conditions, and it will be necessary to discretely model the TRISO particles embedded in the SiC matrix. Thus, the BISON finite

element code was selected to simulate the resulting large and complicated systems due to its adaptability and parallel computing capabilities

The BISON code developed by Idaho National Laboratory, which is built upon the Multi-physics Object Oriented Simulation Environment (MOOSE) (Perez et al., 2013; Hales et al., 2013; Williamson et al., 2012), has been used to model the TRISO-FCM fuel in this work. MOOSE is a massively parallel, finite element computational system that uses a Preconditioned Jacobian-free Newton-Krylov (PJFNK) method with an implicit Euler solver to provide solutions to coupled systems and non-linear partial differential equations. The partial differential equations are contained in separate files stored within the BISON program. MOOSE is built on the libMesh and PETSc libraries that provide the numerical solutions (Hales et al., 2013). This configuration allows highly coupled physics to be solved simultaneously. Also, equations can be added or modified with minimal disruption to the other kernels (Gaston et al., 2009).

The material properties of interest are the thermal conductivity, swelling or irradiation-induced dimensional change, irradiation creep, and fission gas pressure, which depend on temperature, neutron irradiation conditions, and burnup in the case of the fuel kernels. It is expected that these material properties will have the dominant effect on the integrity and capability of the fuel to retain fission products and thus its performance. The following section discusses these material correlations and the assumptions inherent in their selection and use.

#### 3. Materials

There are five materials used in the FCM fuel form: uranium nitride (UN), a porous carbon buffer, pyrolytic carbon (PyC), CVD-SiC used as a particle coating layer, and a sintered SiC which is the matrix material in the FCM fuel concept. UN was selected for the fuel kernel over UO<sub>2</sub> or UCO due to its higher uranium density. The porous carbon buffer is used to accommodate the fission gas released from the kernel and the kernel swelling. The IPyC protects the kernel from chorine chemical attack during the deposition of the SiC layer, and the OPyC provides a material for adhesion with the matrix. Additionally, the inner and outer PyC layers are designed to protect the CVD-SiC layer by deflecting cracks, and to provide a barrier against fission product recoils from damaging the SiC coating layer, respectively. The CVD-SiC coating layer is the pressure vessel and provides containment of the fission products and fission gas pressure. The sintered SiC matrix protects the TRISO particles and provides additional containment in the event of a failed SiC coating layer. As this matrix is formed at near full density there is no direct path to the fuel plenum for fission products escaping a ruptured TRISO.

#### 3.1. Uranium nitride

Fig. 2a plots a parabolic curve fit to the unirradiated UN thermal conductivity from 500 to 2000 K (Kim and Hofman, 2018). The curve fit is based on experimental data using a laser flash method performed by Arai et al. (Arai et al., 1992). The curve was extrapolated to 3000 K to ensure the prediction of representative values that decrease to a value of  $17.8~\rm W~m^{-1}~K^{-1}$  at a temperature of 3000 K, which appears to be a reasonable trend given the lack of experimental data above 2000 K. We should also note that temperatures above 2000 K are not expected for simulated LWR conditions. Fig. 2b plots the predicted UN thermal conductivity trends versus burnup. These trends are based on the known thermal conductivity degradation in UO<sub>2</sub> (Lucuta et al., 1996), where the thermal conductivity degradation is inversely proportional to temperature. Eq. (1) provides the corresponding correlation for the UN thermal conductivity, where B is the burnup in MWD per kg of UN, and T is the temperature is in K.

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