

# FAST-TRISO

## Version 1.1 Code Description Document

January 2022

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Prepared for the U.S. Nuclear Regulatory Commission  
Office of Nuclear Regulatory Research  
Under Contract DE-AC05-76RL01830  
Interagency Agreement: 31310019N0001  
Task Order Number: 31310019F0047

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Pacific Northwest National Laboratory  
Richland, Washington 99354

## Revision History

Date	Rev.	General Overview of Revision Changes
June 2021	0	First release of FAST-TRISO-1.0. This version describes the code for a single TRISO particle and limited assessment
January 2022	1	Second release of FAST-TRISO-1.1. This version adds stochastic capability to model multiple TRISO particles and use results from multiple realizations to provide a probability of particle failure

## Abstract

Fuel Analysis under Steady-state and Transients (FAST) is the U.S. Nuclear Regulatory Commission (NRC)'s computer code that calculates the steady-state and transient response of nuclear reactor fuel rods during long-term in-reactor burnup, anticipated operational occurrences (AOOs), and dry storage conditions. FAST-TRISO is a variant of the FAST code that is used to model the steady-state response of individual TRISO particles. The code calculates the temperature, pressure, and deformation within a TRISO particle as functions of time-dependent fuel kernel power and outer surface temperature boundary conditions. The phenomena modeled by the code include:

- heat conduction through the fuel and other materials
- deformation within the various layers, including thermal expansion and irradiation swelling
- fission gas release from the fuel
- internal pressure and void volume
- stress distribution within the outer layers of the particle
- failure probability of the outer layers
- production and release of radioactive fission products from the particle

The code contains necessary material properties for normal operation and AOOs for anticipated TRISO-fueled reactors. FAST-TRISO has been developed for use on Windows operating systems.

This document describes FAST-TRISO-1.1, which is the second official version of this code. This document describes the structure and models within FAST-TRISO, the material property correlations, as well as its integral assessment to experiments and commercial data.

## Acronyms and Abbreviations

ANS	American Nuclear Society
AOO	Anticipated Operational Occurrence
BAF	Bacon Anisotropy Factor
FAST	Fuel Analysis under Steady-state and Transient
IPyC	Inner Pyrolytic Carbon
LOCA	Loss-of-Coolant Accident
LWR	Light Water Reactor
NRC	Nuclear Regulatory Commission
OPyC	Outer Pyrolytic Carbon
PNNL	Pacific Northwest National Laboratory
PyC	Pyrolytic Carbon
RIA	Reactivity Initiated Accident
SiC	Silicon Carbide
TRISO	TRi-structural ISOtropic particle fuel
UO <sub>2</sub>	Uranium Dioxide
UCO	Mixture of Uranium Dioxide and Uranium Carbide

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## 1.0 Introduction

### 1.1 Objective of the FAST-TRISO Code

The ability to accurately calculate the performance of TRISO particles under long-term burnup conditions and overheating scenarios is a major objective of the reactor safety research program being conducted by the U.S. Nuclear Regulatory Commission (NRC) to prepare for the licensing of advanced reactors. To achieve this objective for current reactors, the NRC has sponsored an extensive program of analytical computer code development, as well as both in-pile and out-of-pile experiments to benchmark and assess the analytical code capabilities. The computer code, FAST is the most recent LWR fuel performance code developed to calculate the long-term burnup response of a single fuel rod. FAST is not applicable to TRISO particles, but the NRC leveraged the experience developing FAST and the material property correlations and performance models in FAST to develop FAST-TRISO. This report describes FAST-TRISO-1.1, the second release of this code.

FAST (Fuel Analysis under Steady-State and Transients) is an analytical tool that calculates the thermal-mechanical behavior of nuclear fuel when given power and boundary conditions. There are two conditions that are commonly referred to as “steady-state” and “transient”. For the term “steady-state” to apply (i.e., time-independent), changes must be sufficiently slow. This includes situations such as long periods at constant power and slow power ramps that are typical of normal power reactor operations. “Transient” means rapid power and/or boundary condition changes (time-dependent) such as an anticipated operational occurrence (AOO), reactivity-initiated accident (RIA), or loss-of-coolant accident (LOCA) events. FAST-TRISO-1.1 does not include any transient heat transfer correlations, but there are not currently any anticipated events where a transient temperature solution would be necessary for TRISO fuel.

The FAST-TRISO code calculates the variation with time of all significant particle values. The main objective of FAST-TRISO are:

- Calculate component temperature<sup>1</sup> to compare with melting limits and drive other models,
- Assess protection against fuel kernel swelling afforded by the buffer to the PyC and SiC layers.
- Predict gross failure (component melting and mechanical loading due to excessive kernel swelling on the PyC and SiC layers)
- Predict fission gas production and release to void space and the resulting pressure in the void space
- Predict probability of outer layer (IPyC, SiC, OPyC) failure due to internal gas pressure
- Predict production and release of radionuclides from the TRISO particle during normal operation and overheating scenarios

---

<sup>1</sup> For TRISO, the component temperatures are the temperatures across the fuel kernel and the various layers

FAST-TRISO-1.1 Includes the option to perform a stochastic calculation of particle failure probability. After calculating a nominal case, the input parameters can be perturbed in a user-set number of realizations according to user-set distributions and the failure predictions from these realizations are combined in a statistical manner to calculate a global set of failure probabilities for particles that have the set distributions in geometric and operational parameters.

## 1.2 Limitations of FAST-TRISO

The FAST-TRISO-1.1 code has inherent limitations. The major limitations are as follows:

- FAST-TRISO is applicable to TRISO particles with a UO<sub>2</sub> or UCO fuel kernel surrounded by a porous carbon buffer layer, inner pyrolytic carbon, silicon carbide, and outer pyrolytic carbon layers. In this version it is not possible to change the order of the layers or introduce new layer materials.
- FAST-TRISO uses the same fuel material properties and models as FAST which is assessed up to a peak burnup of around 100 GWd/MTU. Based on this assessment there is a reasonable expectation that FAST-TRISO will provide adequate predictions of kernel and layer temperature and mechanical deformation up to a kernel burnup of 100 GWd/MTU.
- FAST-TRISO uses a temperature solution for a perfect sphere composed of shells some of which produce heat (fuel) and other that do not produce heat (buffer, IPyC, SiC, OPyC). Deviations from this ideal geometry due to manufacturing defects are not modeled.
- The assessment of FAST for LWR fuel was made possible by a large database of in- and ex-reactor test data. For TRISO particles, there is no in-reactor temperature data to assess the code predictions against. Additionally, it is not possible to measure stress in various layers. These code predictions can only be assessed against other code predictions. Stable fission gas release could be assessed against end of life destructive testing but there is no known data for this. There is a significant database of radioactive fission product release from TRISO under normal operating conditions and ex-reactor heating tests, that FAST-TRISO has been assessed against. There is no known data on failure fraction to assess the FAST-TRISO predictions of failure probability.

## 1.3 Report Outline

This report provides a full documentation of this fuel performance code. A review of available literature to support modeling decisions made in FAST-TRISO are provided elsewhere (Wells, Phillips, & KJ, 2021). The code structure and behavioral models are described Section 2.0. This section also includes instructions for creating an input file. Section 3.0 describes the basic material properties used in FAST-TRISO. Section 4.0 describes the code assessment that has been performed on FAST-TRISO.

## 2.0 Model Description

FAST-TRISO is a thermal-mechanical model to calculate a single TRISO particle throughout irradiation. FAST-TRISO calculates the temperature and deformation within a particle for given time steps with provided power levels and a fixed outer surface temperature.

Figure 1 shows the flowchart that FAST-TRISO uses to perform these calculations. It can be seen that the temperature and the dimensions affect each other, so an iterative approach is used to perform these calculations. Once the component temperatures and dimensions have converged, FAST-TRISO calculates void volume, fission gas release, gas pressure, and outer shell stress distribution. FAST-TRISO also calculates failure probability and diffusional release of specific radionuclides.

FAST-TRISO-1.1 can calculate numerous realizations with inputs perturbed from the nominal values according to set distributions. Following the calculation of these realizations, FAST-TRISO-1.1 calculates global failure probabilities for TRISO particles irradiated under these conditions.

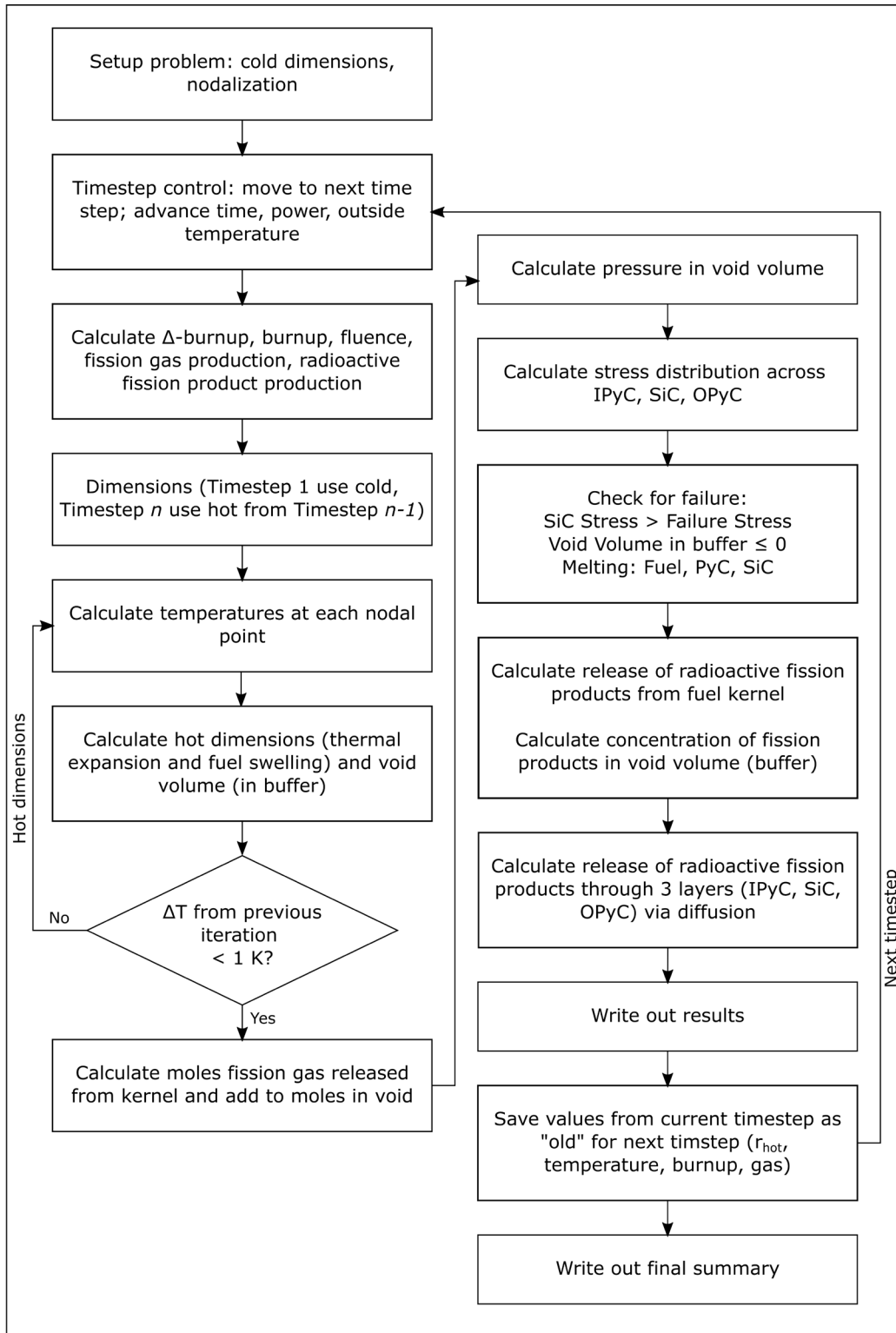


Figure 1. FAST-TRISO Flowchart

## 2.1 Running the code

FAST-TRISO should be run from the command prompt. The code is run similarly to FAST. The input file should be located in the same folder as the executable. At the command prompt, the user should type the executable name followed by the name of the input file with a space between these two names. The output file and the plot file (if requested) will have the same name as the input file with a “.out” and “.plot” file extension, respectively.

## 2.2 Input Values

Input is provided to FAST-TRISO via a text file containing namelist input. There are two required namelist input blocks. The first block is \$control and the second block is \$triso. Each block should contain the correct variables and their values and end with \$end. A sample input is shown in Figure 2.

```

$control
it=5
nr=17
$end
$triso
kernel_rad= 0.0425 , buffer_thick=0.005, IPyC_thick=0.0035
SiC_thick=0.0035, OpyC_thick=0.0035, fuel_den = 10.5, buffer_porosity = 50
ProblemTime(1) = 30, 60, 100, 200, 250
Heat_Rate(1) = 2*1.19e10, 1.4e10, 2*1.19e10
Surface_Temp(1) = 5*800.0
$end
    
```

Figure 2. FAST-TRISO Sample input file

Additionally, there is a third optional namelist input block, \$stoch that can be activated by setting *i\_stoch* = 1 in \$control. This third block contains the distribution parameters that will be used if a stochastic calculation of failure is requested.

The inputs that are required for modeling a TRISO particle are described in Table 1.

Table 1. FAST-TRISO Input Values

Variable Name (type)	Description	Units	Default values/notes
<b>Namelist \$control</b>			
it (I)	Number of time steps	-	Required input
nr (I)	Number of radial nodes in fuel kernel	-	Default=17
i_unit (I)	Flag to run unit tests. i_unit=0: do not run unit tests. i_unit=1: run unit tests	-	Default=0
i_plot (I)	Flag to create a .plot file. i_plot=0: do not create plot file. i_plot=1: create plot file	-	Default=1

Variable Name (type)	Description	Units	Default values/notes
i_stoch (I)	Flag to run a stochastic calculation of global failure probability. i_stoch=0: do not run stochastic calculation. i_stoch=1: run stochastic calculation and create .stoch file	-	Default=0
<b>Namelist \$triso</b>			
kernel_rad (R)	Fuel kernel radius	cm	Required input
buffer_thick (R)	Buffer layer thickness	cm	Required input
IPyC_thick (R)	Inner pyrolytic carbon (IPyC) layer thickness	cm	Required input
SiC_thick (R)	Silicon carbide (SiC) layer thickness	cm	Required input
OPyC_thick (R)	Outer pyrolytic carbon (IPyC) layer thickness	cm	Required input
fuel_den (R)	Density of fuel kernel	g/cm <sup>3</sup>	Required input
fuel_type (I)	Flag for fuel type. fuel_type = 1, UCO, fuel_type = 2, UO <sub>2</sub> <i>Impacts CO gas release</i>	-	Default=1
buffer_porosity (R)	Porosity of buffer layer	%	Default=50%
BAF (R)	Bacon anisotropy factor for pyrolytic carbon	-	Default=1.0
PowerToFlux (R)	Convert heat rate in W/m <sup>3</sup> to fast neutron flux in n/m <sup>2</sup> /s	n/m <sup>2</sup> /s per W/m <sup>3</sup>	Default=4.0e8
ProblemTime(IT) (R)	Cumulative time/burnup at the end of each time step. <i>See itime</i>	days, GWd/MTU, atom %	Required input
itime (I)	Flag for units on time, itime=1, days, itime=2, GWd/MTU, itime=3, atom%	-	Default=1
Heat_Rate(IT) (R)	Volumetric heat rate in kernel for each time step	W/m <sup>3</sup>	Required input <i>Heat in kernel volume</i>
Surface_Temp(IT) (R)	Surface temperature of particle for each time step	K	Required input
<b>Namelist \$stoch</b>			
total_realizations (I)	Total number of realizations to be run after the nominal case	-	Default=0
seed (I)	Seed to used for distributions 0 = get random seed from system clock Enter another value to use a set seed if it is desired to repeat exact calculation	-	Default=0
kernel_rad_dist (I)	Distribution on kernel_rad 0 = no distribution	-	Default=0

Variable Name (type)	Description	Units	Default values/notes
	1 = normal distribution 2 = uniform distribution		
kernel_rad_p1 (R)	Parameter 1 for kernel_rad_dist Standard deviation for normal Lower bias for uniform	cm	Default=0.0
kernel_rad_p2 (R)	Parameter 2 for kernel_rad_dist N/A for normal Upper bias for uniform	cm	Default=0.0
buffer_thick_dist (I)	Distribution on buffer_thick 0 = no distribution 1 = normal distribution 2 = uniform distribution	-	Default=0
buffer_thick_p1 (R)	Parameter 1 for buffer_thick_dist Standard deviation for normal Lower bias for uniform	cm	Default=0.0
buffer_thick_p2 (R)	Parameter 2 for buffer_thick_dist N/A for normal Upper bias for uniform	cm	Default=0.0
IPyC_thick_dist (I)	Distribution on IPyC_thick 0 = no distribution 1 = normal distribution 2 = uniform distribution	-	Default=0
IPyC_thick_p1 (R)	Parameter 1 for IPyC_thick_dist Standard deviation for normal Lower bias for uniform	cm	Default=0.0
IPyC_thick_p2 (R)	Parameter 2 for IPyC_thick_dist N/A for normal Upper bias for uniform	cm	Default=0.0
SiC_thick_dist (I)	Distribution on SiC_thick 0 = no distribution 1 = normal distribution 2 = uniform distribution	-	Default=0
SiC_thick_p1 (R)	Parameter 1 for SiC_thick_dist Standard deviation for normal Lower bias for uniform	cm	Default=0.0
SiC_thick_p2 (R)	Parameter 2 for SiC_thick_dist N/A for normal Upper bias for uniform	cm	Default=0.0
OPyC_thick_dist (I)	Distribution on OPyC_thick 0 = no distribution 1 = normal distribution 2 = uniform distribution	-	Default=0
OPyC_thick_p1 (R)	Parameter 1 for OPyC_thick_dist Standard deviation for normal Lower bias for uniform	cm	Default=0.0
OPyC_thick_p2 (R)	Parameter 2 for OPyC_thick_dist N/A for normal Upper bias for uniform	cm	Default=0.0
fuel_den_dist	Distribution on fuel_den	-	Default=0

Variable Name (type)	Description	Units	Default values/notes
(I)	0 = no distribution 1 = normal distribution 2 = uniform distribution		
fuel_den_p1 (R)	Parameter 1 for fuel_den_dist Standard deviation for normal Lower bias for uniform	g/cm <sup>3</sup>	Default=0.0
fuel_den_p2 (R)	Parameter 2 for fuel_den_dist N/A for normal Upper bias for uniform	g/cm <sup>3</sup>	Default=0.0
buffer_porosity_dist (I)	Distribution on buffer_porosity 0 = no distribution 1 = normal distribution 2 = uniform distribution	-	Default=0
buffer_porosity_p1 (R)	Parameter 1 for buffer_porosity_dist Standard deviation for normal Lower bias for uniform	%	Default=0.0
buffer_porosity_p2 (R)	Parameter 2 for buffer_porosity_dist N/A for normal Upper bias for uniform	%	Default=0.0
BAF_dist (I)	Distribution on BAF 0 = no distribution 1 = normal distribution 2 = uniform distribution	-	Default=0
BAF_p1 (R)	Parameter 1 for BAF_dist Standard deviation for normal Lower bias for uniform	-	Default=0.0
BAF_p2 (R)	Parameter 2 for BAF_dist N/A for normal Upper bias for uniform	-	Default=0.0
Heat_Rate_dist (I)	Distribution on multiplier on Heat_Rate array <i>Nominal multiplier=1.0</i> 0 = no distribution 1 = normal distribution 2 = uniform distribution	-	Default=0
Heat_Rate_p1 (R)	Parameter 1 for Heat_Rate_dist Standard deviation for normal Lower bias for uniform	-	Default=0.0
Heat_Rate_p2 (R)	Parameter 2 for Heat_Rate_dist N/A for normal Upper bias for uniform	-	Default=0.0
Surface_Temp_dist (I)	Distribution on adder on Surface_Temp array <i>Nominal adder=0.0</i> 0 = no distribution 1 = normal distribution 2 = uniform distribution	-	Default=0
Surface_Temp_p1 (R)	Parameter 1 for Surface_Temp_dist Standard deviation for normal Lower bias for uniform	K	Default=0.0

Variable Name (type)	Description	Units	Default values/notes
Surface_Temp_p2 (R)	Parameter 2 for Surface_Temp_dist N/A for normal Upper bias for uniform	K	Default=0.0

(R) Real  
(I) Integer  
IT = time step index

### 2.3 Nodalization

The TRISO particle is modeled as a sphere with a number of points along the radius of the sphere. The fuel kernel is divided into a number of equal thickness shells. The temperature may be determined at discrete points at the boundary of these shells. The temperature for the fuel in each shell is assumed to be the average of the temperature calculated on each side of the shell. The other layers in the TRISO particle (buffer carbon, IPyC, SiC, OPyC) are thin and are modeled as a single shell with points on each side of the shell. As with the shells in the fuel kernel, the temperature for the material in each shell is assumed to be the average of the temperature calculated on each side of the shell. The FAST-TRISO nodalization is shown in Figure 3.

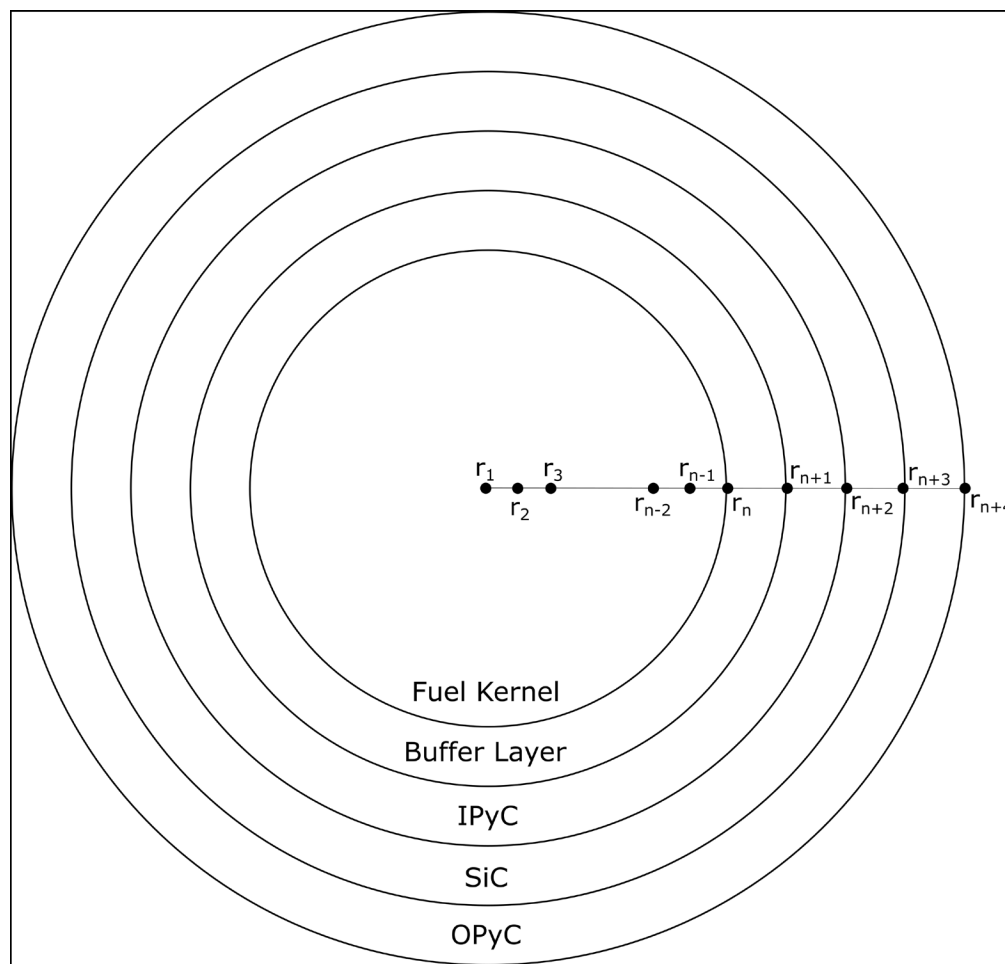


Figure 3. FAST-TRISO Nodalization

## 2.4 Temperature solution

FAST-TRISO calculates the temperature at each of the points described in the previous section starting at the outer surface where the temperature is set for the time step by an input value. FAST-TRISO assumes that no heat is produced in the outer layers (OPyC, SiC, IPyC, and buffer carbon) and that heat is produced uniformly in the fuel kernel at a rate set by an input value.

The temperature change across each of the outer layers is calculated using the equation (Jayanta, 2021):

$$T_i = T_o + \frac{Q(r_o - r_i)}{4\pi \cdot k \cdot r_o \cdot r_i}$$

Where:

$T_i$  = temperature of inner surface of shell (K)

$T_o$  = temperature of outer surface of shell (K)

$Q$  = heat rate produced within the shell (W)

$k$  = thermal conductivity of shell material (W/m-K)

$r_o$  = radius of outer surface of shell (m)

$r_i$  = radius of inner surface of shell (m)

The heat rate produced within the shell is the input volumetric heat rate multiplied by the volume of the fuel kernel. For the OPyC, the temperature of the outer surface of the shell is the input value of the surface temperature and the temperature of the inner surface can be calculated. For the other layers, the outer surface temperature will be the calculated inner surface temperature from the previous shell and the temperature of the inner surface can be calculated.

The temperature change at each radial location,  $r$ , within the fuel kernel is calculated using the equation (Jayanta, 2021):

$$T_r = T_o + \frac{q}{6 \cdot k} (r_o^2 - r^2)$$

Where:

$T_r$  = temperature at a given radius within sphere (K)

$T_o$  = temperature of outer surface of sphere (K)

$q$  = volumetric heat rate produced within the sphere (W/m<sup>3</sup>)

$k$  = thermal conductivity of sphere material (W/m-K)

$r_o$  = radius of outer surface of sphere (m)

$r$  = radius inside sphere (m)

The temperature of the outer surface of the kernel is the inner surface of the carbon buffer layer previously calculated and the temperature at each preset radial location within the fuel kernel can be calculated.

For the first time step the cold dimensions (radial locations) will be used, and then the thermal expansion will be calculated to determine hot dimensions, and the code will iterate to find a consistent set of hot dimensions and temperature values. For subsequent time steps, the hot dimensions from the previous time step will be used as the starting point for the current time step. The code will use a convergence criteria for this iteration of <1K between temperature values relative to the previous iteration.

The volumetric average temperature for the entire fuel kernel is used in several calculations within FAST-TRISO. Because FAST-TRISO uses equally spaced radial nodes, the volume of each shell is not constant. Therefore, the following formula is used to calculate the volume average temperature

$$T_{ave} = \left( \sum_{i=1}^{N-1} \frac{(T_i + T_{i+1})}{2} (r_{i+1}^3 - r_i^3) \right) / r_{kernel}^3$$

Where:

$T_{ave}$  = Volumetric average temperature of fuel kernel (K)

$N$  = Number of radial points in kernel

$T_i, T_{i+1}$  = Temperature at radial point

$r_i, r_{i+1}$  = radius at radial point

$r_{kernel}$  = kernel outer radius

## 2.5 Burnup Calculations

Burnup is the integral of the power history over time. Because FAST-TRISO assumes a constant power level the burnup for each step is just the power level multiplied by the time step size.

$$\Delta Bu = q \frac{W}{m^3} \times \Delta t \frac{days}{-} \times \frac{1 GW}{10^9 W} \times \frac{(1m)^3}{(100 cm)^3} \times \frac{1 cm^3}{\rho g fuel} \times \frac{1 g fuel}{x g U} \times \frac{10^6 gU}{1 MTU}$$

Where:

$\Delta Bu$  = burnup increment (GWd/MTU)

$q$  = volumetric heat generation (W/m<sup>3</sup>)

$\Delta t$  = time step length (days)

$\rho$  = density of fuel (g/cm<sup>3</sup>)

$x$  = ratio of U in fuel (for UO<sub>2</sub> = 238/(238+16+16) = 0.88 for UCO = 238/(238+12+16)) = 0.89

The total burnup in a given step is the previous step burnup added to the burnup increment from the current step

$$Bu_n = \Delta Bu_n + Bu_{n-1}$$

Some of the correlations in FAST-TRISO need fission rate such as the fission product production and release models. The fission rate may be calculated from the volumetric heat rate using conversion of 1 J = 6.242x10<sup>12</sup> MeV and 1 fission = 200MeV, as follows

$$\dot{f} = q \frac{W}{m^3} \times \frac{1J}{1W \cdot s} \times \frac{6.242 \times 10^{12} MeV}{1J} \times \frac{1fission}{200 MeV}$$

$\dot{f}$  = fission rate (fissions/m<sup>3</sup>-s)

FAST-TRISO assumes that power is proportional to fast neutron flux, and therefore burnup is proportional to fast neutron fluence. Because different reactors have different neutron spectrums, FAST-TRISO allows for a user input conversion factor to convert power level to fast neutron flux. The default value in FAST-TRISO for this conversion is 4.0x10<sup>8</sup> n/m<sup>2</sup>/s per W/m<sup>3</sup> based on TRISO irradiations from (IAEA, 2012). The fast neutron fluence is calculated incrementally similarly to burnup based on the fast neutron flux and time step size for each time step. The user input time and power and if a target fluence is know at a particular burnup, this parameter may be adjusted to get that fluence.

## 2.6 Thermal Expansion and Swelling

The thermal expansion and swelling of the materials in a TRISO particle are described in Section 3.0.

FAST-TRISO considers the fuel kernel and the IPyC/SiC/OPyC shell to behave independently mechanically such that the porous buffer layer imposes no stress on either part when the other part expands. This is because the porous buffer layer is typically around 50% dense and likely offers no significant mechanical connection between the fuel kernel and the outer three layers.

### 2.6.1 Deformation of fuel kernel

The radial locations defined within the fuel kernel will change based on the thermal expansion strain and the swelling calculated for the material between each radial location.

Node 1 is defined at the center of the fuel kernel, and its cold and hot radius is always assumed to be 0.

The hot radius of each successive node is defined as

$$r_{hot}(n) = (r_{cold}(n) - r_{cold}(n - 1))(1 + \varepsilon_{th} + \varepsilon_{swell}) + r_{hot}(n - 1)$$

Where:

$n$  = radial node number

$r_{hot}$  = hot radius (m)

$r_{cold}$  = room temperature radius (m)

$\epsilon_{th}$  = thermal expansion strain (m/m)

$\epsilon_{swell}$  = solid fission product swelling (m/m)

The thermal expansion strain,  $\epsilon_{th}$ , should be evaluated at the average temperature at node  $n$  and  $n-1$ . The solid fission product swelling is uniform within the kernel since power is assumed to be uniform within the kernel. Solid fission product swelling is typically given in terms of volumetric swelling,  $\Delta V/V$ , and can be converted to linear swelling by the following equation.

$$\epsilon_{swell} = \sqrt[3]{1 + \frac{\Delta V}{V}} - 1$$

## 2.6.2 Deformation of the IPyC, SiC, OPyC Shell

The radial locations defined within the IPyC, SiC, OPyC shell will change based on the thermal expansion strain for the material between each radial location.

The radius at the inner surface of the IPyC will expand based on the temperature at that inner surface.

$$r_{hot}(IPyC_i) = r_{cold}(IPyC_i)(1 + \epsilon_{th})$$

The hot radius of each successive node is defined by the expansion of the material between each node

$$r_{hot}(IPyC_o) = r_{hot}(SiC_i) = (r_{cold}(IPyC_o) - r_{cold}(IPyC_i))(1 + \epsilon_{th}(IPyC)) + r_{hot}(IPyC_i)$$

$$r_{hot}(SiC_o) = r_{hot}(OPyC_i) = (r_{cold}(SiC_o) - r_{cold}(SiC_i))(1 + \epsilon_{th}(SiC)) + r_{hot}(SiC_i)$$

$$r_{hot}(OPyC_o) = (r_{cold}(OPyC_o) - r_{cold}(OPyC_i))(1 + \epsilon_{th}(OPyC)) + r_{hot}(OPyC_i)$$

Where:

$r_{hot}$  = hot radius (m)

$r_{cold}$  = room temperature radius (m)

$\epsilon_{th}$  = thermal expansion strain (m/m)

$\epsilon_{th}(IPyC)$ ,  $\epsilon_{th}(SiC)$ , and  $\epsilon_{th}(OPyC)$  are evaluated at the average of the temperatures of each side of the layer.

## 2.7 Treatment of the Buffer Layer

The only void space within a TRISO particle is in the porous buffer layer. In FAST-TRISO, the default value is that this buffer layer is 50% open porosity and 50% carbon but this can be adjusted by changing the input value for buffer density. It is assumed that this buffer layer offers no mechanical connection between the fuel kernel and the outer shells (IPyC, SiC, and OPyC). Therefore, the fuel kernel and the outer shells can expand or contract independently of each other. Additionally, this open porosity is treated as void volume that will be filled with any stable fission gas release from the fuel kernel. The quantity of gas in this void space, along with the temperature of the buffer layer and the open porosity volume will dictate the pressure in this void space. This pressure will act against the outer shells and will result in stress in these various layers.

The initial cold void volume is calculated by determining the volume of the porous buffer layer at cold conditions

$$V_{buffer} = \frac{4}{3}\pi(r_o^3 - r_i^3)$$

Where:

$V_{buffer}$  = Volume of buffer layer (m<sup>3</sup>)

$r_o, r_i$  = Outer and inner radii at room temperature, respectively (m)

$$V_{solid} = \frac{1}{2}V_{buffer} \quad V_{void} = \frac{1}{2}V_{buffer}$$

Where:

$V_{solid}, V_{void}$  = Volume of solid material and void space in buffer (m<sup>3</sup>)

To determine the void volume at hot conditions, the volume of the buffer is calculated at hot conditions and the volume of solid material at hot conditions is subtracted

$$V_{void} = \frac{4}{3}\pi(r_o^3 - r_i^3) - V_{solid}(1 + \varepsilon_{th})^3$$

Where:

$V_{void}$  = Void space in buffer at hot conditions (m<sup>3</sup>)

$r_o, r_i$  = Outer and inner radii at hot condition, respectively (m)

$V_{solid}$  = Volume of solid material in buffer at cold conditions (m<sup>3</sup>)

$\varepsilon_{th}$  = thermal expansion of buffer material evaluated at the average of the temperature of each side of the buffer layer.

## 2.8 Stable Fission Gas Production, Release, and Pressure in the Void Volume

Stable fission gas (Xe and Kr) is assumed to be produced at a rate of 0.31 atoms per fission (Geelhood, et al., 2021) from U<sup>235</sup> fission. This rate is not observed to change significantly at high burnup where a majority of the fissions are from Pu<sup>239</sup>. Therefore, the gas produced in a given time step can be determined from the volumetric heat rate and the time step size by

$$\Delta Prod = q \frac{W}{m^3} \times \Delta t \frac{days}{-} \times \frac{86400 s}{1day} \times \frac{(1m)^3}{(100 cm)^3} \times \frac{1J}{1W \cdot s} \times \frac{6.242 \times 10^{12} MeV}{1J} \times \frac{1 fission}{200 MeV} \\ \times \frac{0.31 atoms}{1 fission} \times \frac{1 mol}{6.02 \times 10^{23} atoms}$$

Where:

$\Delta Prod$  = stable fission gas production in current time step (moles/m<sup>3</sup>)

$q$  = volumetric heat generation (W/m<sup>3</sup>)

$\Delta t$  = time step length (days)

The gas production rate is determined by dividing the production in the current time step by the time step length.

Fission gas release from the fuel kernel to the void volume in the buffer layer is calculated using the Booth diffusion model (Booth, 1957) as modified by C.S. Rim and described in (ANS Working Group 5.4, 1982) for use in a routine with time steps with various production rates and temperatures such as FAST-TRISO. This model is intended to calculate the diffusional release of fission products from a sphere. Historically this approach was used to model release from the individual grains within a fuel pellet, and once gas was released from these grains, it is released to the void space. In FAST-TRISO, this model is used to calculate the diffusional release from the spherical fuel to the void space in the buffer layer.

This model is described below:

$$f_k = 1 - \frac{1}{prod} \left[ \frac{P_1}{D'_1} \{ \tau_1 g(\tau_1) - \tau_2 g(\tau_2) \} \right. \\ \left. + \frac{P_2}{D'_2} \{ \tau_2 g(\tau_2) - \tau_3 g(\tau_3) \} \right. \\ \vdots \quad \quad \quad \vdots \\ \left. + P_k \Delta t_k g(\tau_k) \right]$$

Where:

$f_k$  = fractional release of fission gas at time step, k (fraction of produced)

$k$  = current time step number

prod = total gas production at current time step (moles/cm<sup>3</sup>)

P<sub>n</sub> = gas production rate at specified time step

$$D' = \frac{D}{a^2}$$

a = radius of fuel kernel (cm)

D = diffusion coefficient (cm<sup>2</sup>/s)

$$D = 7.6 \times 10^{-7} \exp\left(\frac{-35000}{T}\right) + 1.41 \times 10^{-21} \cdot \dot{f} \cdot \exp\left(\frac{-13800}{T}\right) + 2 \times 10^{-36} \cdot \dot{f}$$

$\dot{f}$  = fission rate (fissions/m<sup>3</sup>-s)

T = kernel volume average temperature (K)

$$\tau_n = \sum_{i=n}^k D'_i \cdot \Delta t_i$$

For  $\tau \leq 0.1$ ,  $g(\tau) = 1 - 6 \sqrt{\frac{\tau}{\pi}} + 3\tau$

For  $\tau > 0.1$ ,  $g(\tau) = \frac{1}{15\tau} - \frac{6}{\tau} \sum_{n=1}^3 \frac{e^{-n^2\pi^2\tau}}{n^4\pi^4}$

For the first time step, the first two terms in the square brackets are excluded and only the third term is included. For the second time step, the first and third terms in square brackets are used, and for the third time step and following, appropriate terms are added. It can be seen that in order to apply this equation, the values of P, D', and Δt from all previous time steps must be retained by the code in order to calculate τ<sub>n</sub>, and g(τ<sub>n</sub>) for the current time step.

At each time step the total fission gas within the void space in the buffer is given by

$$n = f_k \cdot prod \cdot V_{kernel}$$

Where:

n = moles of gas in void space in buffer (moles)

f<sub>k</sub> = fractional release of fission gas at time step, k (fraction of produced)

k = current time step number

prod = total gas production at current time step (moles/cm<sup>3</sup>)

V<sub>kernel</sub> = volume of fuel kernel (cm<sup>3</sup>)

In addition to the fission gas release,  $\text{UO}_2$  fuel kernels have been observed to release oxygen which reacts with the buffer carbon to create CO. To model this release, (Proksch & Strigl, 1982) recommends the following model.

$$\log \left[ \left( \frac{O}{f} \right) / t^2 \right] = -0.21 - \frac{8500}{T}$$

Where:

$O/f$  = oxygen release (atoms per fission)

$t$  = irradiation time (days)

$T$  = time-averaged particle surface temperature during irradiation (K)

At the end of each time step a new time-average particle surface temperature is calculated, and the total fissions up to that time step are calculated to determine the moles of O released from the fuel kernel which corresponds to the moles of CO in the void volume. This is added to the moles of fission gas in the void volume to calculate the pressure in the void volume.

For UCO fuel kernels there is negligible CO formation (Skerjanc, 2019) so FAST-TRISO assumes there will not be any CO in the void volume.

The pressure applied on the outer shells by the fission gas in the void space in the buffer is given by the ideal gas law

$$P = \frac{nR \frac{T_i + T_o}{2}}{V_{\text{void}}}$$

Where:

$P$  = pressure in the buffer void space (Pa)

$n$  = moles of gas in void space in buffer (moles)

$R$  = gas constant (8.3145 J/mol-K)

$T_i, T_o$  = Temperature at inner and outer surface of buffer layer, respectively (K)

$V_{\text{void}}$  = Void space in buffer at hot conditions ( $\text{m}^3$ )

## 2.9 Stress in IPyC, SiC, and OPyC

In FAST-TRISO, the three outer layers of IPyC, SiC, and OPyC are treated as a single pressure vessel with three layers. A correlation for stress in the radial direction and in the hoop direction as a function of radius across these three layers has been derived by (Akis & Azad, 2019). These equations are:

For the inner layer (IPyC):

$$\sigma_r = E_1 \left[ -\frac{2C_1}{r^3(1 + \nu_1)} + \frac{C_2}{1 - 2\nu_1} \right]$$

$$\sigma_\theta = E_1 \left[ \frac{C_1}{r^3(1 + \nu_1)} + \frac{C_2}{1 - 2\nu_1} \right]$$

For the middle layer (SiC):

$$\sigma_r = E_2 \left[ -\frac{2C_3}{r^3(1 + \nu_2)} + \frac{C_4}{1 - 2\nu_2} \right]$$

$$\sigma_\theta = E_2 \left[ \frac{C_3}{r^3(1 + \nu_2)} + \frac{C_4}{1 - 2\nu_2} \right]$$

For the outer layer (OPyC):

$$\sigma_r = E_3 \left[ -\frac{2C_5}{r^3(1 + \nu_3)} + \frac{C_6}{1 - 2\nu_3} \right]$$

$$\sigma_\theta = E_3 \left[ \frac{C_5}{r^3(1 + \nu_3)} + \frac{C_6}{1 - 2\nu_3} \right]$$

Where:

$\sigma_r$  and  $\sigma_\theta$  = stress in the radial direction and hoop direction, respectively (Pa, negative is compression, positive is tension)

$E_{1,2,3}$  and  $\nu_{1,2,3}$  = Young's Modulus (Pa) and Poisson's Ratio for inner(1), middle(2), and outer(3) layer materials

$r$  = radius within the three layers (m)

The model parameters are:

$$C_1 = \frac{\alpha^3 N_1 P r_1^3 (b^3 D_{11} + 2D_2 D_4 r_1^3 r_2^3 - 2D_3 D_8 r_2^6)}{2E_1 (b^3 D_5 D_9 r_1^3 + D_{12} r_2^3 - 2D_8 D_{10} r_2^6)}$$

$$C_2 = \frac{\alpha^3 N_2 P (b^3 D_{13} - 2D_1 D_4 r_1^3 r_2^3 + 2D_7 D_8 r_2^6)}{E_1 (b^3 D_5 D_9 r_1^3 + D_{12} r_2^3 - 2D_8 D_{10} r_2^6)}$$

$$C_3 = \frac{\alpha^3 D_{14} N_3 P r_1^3 r_2^3 (N_1 + 2N_2)}{2(2D_8 D_{10} r_2^6 - b^3 D_5 D_9 r_1^3 - D_{12} r_2^3)}$$

$$C_4 = \frac{\alpha^3 D_{15} N_4 P r_1^3 (N_1 + 2N_2)}{2D_8 D_{10} r_2^6 - b^3 D_5 D_9 r_1^3 - D_{12} r_2^3}$$

$$C_5 = \frac{a^3 b^3 E_2 N_5 P r_1^3 r_2^3 (N_1 + 2N_2)(N_3 + 2N_4)}{2(2D_8 D_{10} r_2^6 - b^3 D_5 D_9 r_1^3 - D_{12} r_2^3)}$$

$$C_6 = \frac{a^3 E_2 N_6 P r_1^3 r_2^3 (N_1 + 2N_2)(N_3 + 2N_4)}{2D_8 D_{10} r_2^6 - b^3 D_5 D_9 r_1^3 - D_{12} r_2^3}$$

$$N_1 = 1 + v_1$$

$$N_2 = 1 - 2v_1$$

$$N_3 = 1 + v_2$$

$$N_4 = 1 - 2v_2$$

$$N_5 = 1 + v_3$$

$$N_6 = 1 - 2v_3$$

$$D_1 = E_2 N_1 + 2E_1 N_4$$

$$D_2 = E_2 N_2 - E_1 N_4$$

$$D_3 = 2E_2 N_2 + E_1 N_3$$

$$D_4 = E_3 N_3 + 2E_2 N_6$$

$$D_5 = E_2 N_5 - E_3 N_3$$

$$D_6 = 2E_3 N_4 + E_2 N_5$$

$$D_7 = E_2 N_1 - E_1 N_3$$

$$D_8 = E_2 N_6 - E_3 N_4$$

$$D_9 = a^3 D_1 + 2D_2 r_1^3$$

$$D_{10} = a^3 D_7 + D_3 r_1^3$$

$$D_{11} = 2D_2 D_5 r_1^3 - D_3 D_6 r_2^3$$

$$D_{12} = 2D_2 D_4 r_1^6 - b^3 D_6 D_{10} + a^3 D_1 D_4 r_1^3$$

$$D_{13} = D_6 D_7 r_2^3 - D_1 D_5 r_1^3$$

$$D_{14} = b^3 D_6 + 2D_8 r_2^3$$

$$D_{15} = b^3 D_5 + D_4 r_2^3$$

Where:

b = radius to outer surface (m)

a = radius to inner surface (m)

$r_1$  = radius to boundary of inner and middle layers (m)

$r_2$  = radius to boundary of middle and outer layers (m)

P = internal pressure (Pa)

Once the stress in the hoop and radial directions are calculated, the von Mises stress ( $\sigma_{VM}$ ) may be calculated using:

$$\sigma_{VM} = |\sigma_r - \sigma_\theta|$$

The von Mises stress will be used for comparison against the failure stress in the layers.

With regard to the stress in these layers, FAST-TRISO only includes the effect of gas pressure loading. FAST-TRISO does not include the effect of PyC irradiation swelling and creep. This mechanism has been proposed to cause a compressive stress in the SiC layer, which protects it from failure due to internal overpressure. These calculations are highly dependent on the models selected for both creep and swelling. Additionally, all the PyC swelling data are from un-restrained samples. Swelling of the magnitude observed in unrestrained samples are not observed in TRISO particles and a creep term is necessary to reduce the stress predictions. The validation of this creep term is unknown. Because such calculations predict reduction in the SiC stress due to negative swelling in the PyC, they could result in a non-conservative evaluation of failure in the SiC layer if the magnitude of this swelling is overestimated. It is acknowledged that if the PyC does in fact produce a compressive stress in the SiC, then FAST-TRISO will result in a slightly conservative prediction of failure fraction.

## 2.10 Failure Limits

A number of failure limits have been identified for TRISO fuel. These include, failure of SiC layer due to internal overpressure, failure of SiC layer due to fuel kernel swelling, and component melting. Each of these is described below. At the end of each time step, FAST-TRISO performs a check to see if any of these limits has been exceeded.

### 2.10.1 Internal overpressure

Accumulation of fission gas in the buffer void space will create stress in the outer three layers of the TRISO particle.

Ceramic materials such as PyC and SiC loaded in tension often exhibit a variation in failure strengths. For this reason, in FAST-TRISO, a Weibull distribution is used to calculate the probability of failure of each layer at the calculated stress value using the mean failure strength and the Weibull modulus. The probability of failure is given by (IAEA, 2012):

$$P = 1 - \exp\left(-\ln 2 \left(\frac{\sigma}{\bar{\sigma}}\right)^m\right)$$

Where:

$P$  = probability of failure (unitless)

$\sigma$  = stress (Pa)

$\bar{\sigma}$  = mean failure stress (Pa)

$m$  = Weibull modulus (unitless)

The failure probability in each layer is calculated using the maximum VonMises stress calculated in Section 2.9. The overall probability of particle failure is then given by the product of the probability that each layer will fail. This failure probably could also be assumed to be the failure fraction in a simulation of a large number of particles.

$$P_{particle} = P_{IPyC} \times P_{SiC} \times P_{OPyC}$$

Where:

$P_{particle}$  = probability of particle failure (unitless)

$P_{IPyC}$  = probability of IPyC failure (unitless)

$P_{SiC}$  = probability of SiC failure (unitless)

$P_{OPyC}$  = probability of OPyC failure (unitless)

### 2.10.2 Fuel kernel swelling

SiC is a ceramic material and is known to have little to no ductility. In the case that the fuel kernel swells due to thermal expansion and solid fission product swelling to a level that the void space in the carbon buffer layer is completely removed, continued swelling in the fuel kernel will result in strain to the SiC layer. This strain will likely result in failure of the SiC layer. For this reason, if at the end of the time step, the hot void volume is calculated to be equal to or less than zero, FAST-TRISO will assume that the SiC layer has failed.

### 2.10.3 Component Melting

The melting temperature of each of the materials within the TRISO particle is given in Section 3.4. At the end of each time step the temperature predicted for each layer will be compared to its melting temperature and if any component is predicted to melt, FAST-TRISO will assume that the TRISO particle has failed.

## 2.11 Production and Release of Radioactive Fission Products

The release of various radionuclides from a TRISO particle are of interest from a radiological perspective. It has been identified that radioactive isotopes of silver, cesium, strontium, krypton, xenon, and iodine are of interest. Table 2 shows the radionuclides that are considered in FAST-TRISO (Japan Atomic Energy Agency, 2021). This table also include the decay constant for each of these nuclides and the relative production of each nuclide per fission. The production values shown in Table 2 are the cumulative yields taken from both direct fission yield and from precursor isotopes that decay to these isotopes.

Table 2. Radioactive fission products considered in FAST-TRISO

Isotope	Half Life	$\lambda$ (1/s)	Production (atoms/fission)
<sup>110m</sup> Ag	249.8 days	3.2109x10 <sup>-8</sup>	1.60x10 <sup>-14</sup>
<sup>134</sup> Cs	2.065 years	1.06416x10 <sup>-8</sup>	7.73x10 <sup>-8</sup>
<sup>137</sup> Cs	30.07 years	7.30791x10 <sup>-10</sup>	6.18x10 <sup>-2</sup>
<sup>90</sup> Sr	28.8 years	7.60377x10 <sup>-10</sup>	5.80x10 <sup>-2</sup>
<sup>85</sup> Kr	10.76 years	2.04228x10 <sup>-9</sup>	2.83x10 <sup>-3</sup>

(Japan Atomic Energy Agency, 2021)

In addition to the production of these radionuclides, it is important to know the diffusion coefficients of each relevant element in the various TRISO layers. Table 3 shows the diffusion coefficients for each element in each TRISO material (Collin, 2016).

Table 3. Diffusion coefficients for select elements in TRISO materials

Element	D <sub>1</sub> (m <sup>2</sup> /s)	Q <sub>1</sub> J/mol	D <sub>2</sub> (m <sup>2</sup> /s)	Q <sub>2</sub> J/mol	Notes
<b>Kernel</b>					
Ag	6.7x10 <sup>-9</sup>	165000	-	-	
Cs	5.6x10 <sup>-8</sup>	209000	5.2x10 <sup>-4</sup>	362000	
Sr	2.2x10 <sup>-3</sup>	488000	-	-	
Kr, Xe, I	8.8x10 <sup>-15</sup>	54000	6.0x10 <sup>-1</sup>	480000	1500°C-2400°C
	1.3x10 <sup>-12</sup>	126000	-	-	700°C-1500°C
<b>PyC</b>					
Ag	5.3x10 <sup>-9</sup>	154000	-	-	
Cs	6.3x10 <sup>-8</sup>	222000	-	-	
Sr	2.3x10 <sup>-6</sup>	197000	-	-	
Kr, Xe, I	2.9x10 <sup>-8</sup>	291000	2.0x10 <sup>+5</sup>	923000	
<b>SiC</b>					
Ag	3.6x10 <sup>-9</sup>	213000	-	-	
Cs	5.5x10 <sup>-14</sup>	125000	1.6x10 <sup>-2</sup>	514000	
Sr	1.2x10 <sup>-9</sup>	205000	1.8x10 <sup>+6</sup>	791000	
Kr, Xe, I	8.6x10 <sup>-10</sup>	326000			1200°C-1400°C
	3.7x10 <sup>+1</sup>	657000			1400°C-1750°C

$$D = D_1 \exp\left(\frac{-Q_1}{RT}\right) + D_2 \exp\left(\frac{-Q_2}{RT}\right)$$

Radioactive fission products are assumed to be produced at a rate of given in Table 2. Therefore, the production rate for a given time step can be determined from the fission rate by

$$B = \dot{f} \frac{\text{fission}}{\text{cm}^3 - \text{s}} \times \text{fract} \frac{\text{atoms}}{\text{fission}}$$

Where:

B = radioactive fission product production AKA “birth rate” (atoms/cm<sup>3</sup>-s)

$\dot{f}$  = fission rate (fissions/cm<sup>3</sup>-s)

fract = fission yield for nuclide (atoms/fission)

Because the radionuclides of interest in FAST-TRISO are relatively long-lived ( $t_{1/2} > 1$  year), the Booth model for release of stable fission products is most applicable (ANS5.4 Working Group, 1981). Although <sup>110m</sup>Ag has a half-life slightly less than 1 year, the typical time steps in FAST-TRISO (10-50 days) are sufficiently smaller than the half-life, and the stable fission product release model is also used for this nuclide. The Booth model applied is described in Section 2.8, but the production rates and diffusion constants from Table 2 and Table 3 are used for each nuclide.

If short-lived radionuclides were considered in FAST-TRISO it would be recommended to use the Original ANS-5.4 (Turnbull & Beyer, 2010) model for release of radioactive fission products from a sphere. In the context of TRISO, this sphere is the fuel kernel.

$$\frac{R}{B} = 3 \left[ \frac{1}{\sqrt{\mu}} \coth(\sqrt{\mu}) - \frac{1}{\mu} \right]$$

Where:

$$\mu = \frac{\lambda a^2}{D}$$

R = release rate (atoms/cm<sup>3</sup>-s)

B = production rate (atoms/cm<sup>3</sup>-s)

a = radius of fuel kernel (cm)

D = diffusion coefficient (cm<sup>2</sup>/s)

$\lambda$  = decay constant (1/s)

Regardless of the approach used, the volumetric release rate can be calculated, and then the total release rate from the kernel can be calculated by multiplying by the volume of the kernel.

These fission products diffuse into the void space in the buffer and in a given time step, if atoms are coming into this void space at a constant rate, and radioactive decay is occurring at a known rate, the concentration will reach a steady-state value when the rate of atoms entering the void space equals the rate of atoms decaying within the void space. However, for the nuclides of interest, the half-lives are considerably longer than a time step. Therefore FAST-TRISO will calculate the inventory in the void space at the beginning of the step based on the inventory at the end of the previous step (or 0 for step 1). Next the inventory at the end of the time step will be calculated based on a constant release rate from the kernel and radioactive decay over the time step. The atoms released from the kernel are uniformly released over the time step so they are decayed over half the time step length.

$$N_{BOS}(1) = 0$$

$$N_{BOS}(i) = N_{EOS}(i - 1)$$

$$N_{EOS}(i) = N_{BOS}(i) \exp\left(-\lambda(t(i) - t(i - 1))\right) + \text{relrate}(t(i) - t(i - 1)) \exp\left(-\lambda \frac{(t(i) - t(i - 1))}{2}\right)$$

Where:

N = inventory in the void space at beginning of step(BOS) and end of step(EOS) (atoms)

i = time step index

t = time (s)

$\lambda$  = decay constant (1/s)

relrate = release rate from kernel (atoms/s)

Because the concentration in the void space is not constant over the time step, the average of the BOS and EOS concentrations will be used to calculate diffusion through the shell. Once the concentration inside the void space is known, the diffusion of radionuclides through the three outer layers is calculated. The diffusion of material through a spherical shell is:

$$Q = 4\pi Dt \frac{ab}{b - a} (C_2 - C_1)$$

Where:

Q = quantity of atoms diffusing through the shell. *Negative is diffusion out of the shell and positive is diffusion into the shell* (atoms)

D = diffusion coefficient (cm<sup>2</sup>/s)

T = time (sec)

a = inner radius of shell (cm)

b = outer radius of shell (cm)

C<sub>1</sub> = concentration on the outer surface of the shell (atoms/cm<sup>3</sup>)

C<sub>2</sub> = concentration on the inner surface of the shell (atoms/cm<sup>3</sup>)

For the condition with three layers within the shell, an effective diffusion coefficient is defined using the following equation (Crank, 1975)

$$\frac{l}{D_{eff}} = \frac{l_1}{D_1} + \frac{l_2}{D_2} + \frac{l_3}{D_3}$$

Where:

$D_{1,2,3}$  = diffusion coefficient of atoms in IPyC, SiC, and OPyC (cm<sup>2</sup>/s)

$l_{1,2,3}$  = thickness of IPyC, SiC, and OPyC (cm)

$D_{eff}$  = effective diffusion coefficient for shell (cm<sup>2</sup>/s)

$l$  = thickness of shell

Additionally, for this case, it is assumed that any material that diffuses out of the TRISO is swept away so  $C_1$  is set to zero. Therefore, the rate of atoms arriving at the outer surface of the TRISO particle can be given by:

$$\dot{Q} = 4\pi D_{eff} \frac{ab}{b-a} (C_2)$$

Where:

$\dot{Q}$  = rate of atoms arriving at surface of the shell (atoms/sec)

The quantity of atoms that are released during a time step is determined by multiplying the release rate by the time step size and taking the minimum of either this value or the sum of the quantity of atoms released during the time step and the quantity previously determined as the end-of step void quantity ( $N_{EOS}$ ) such that the code will not predict a greater release from the void volume than is predicted to be in the void volume.

$$Q = \min(\dot{Q}\Delta t, N_{EOS})$$

Where:

$Q$  = atoms released from TRISO particle during time step (atoms)

$\Delta t$  = time (s)

$N_{EOS}$  = inventory in the void space at and end of step (EOS) previously determined (atoms)

The quantity of atoms in the buffer void space for the beginning of the next step is determined by subtracting the atoms released during the current time step from  $N_{EOS}$

$$N_{BOS}(i+1) = N_{EOS}(i) - Q$$

## 2.12 Stochastic Calculations

When a stochastic calculation is requested the user should enter the number of realizations that are requested as well as distributions that should be applied for each input parameter. For each input parameter that allows a distribution, the default value is 0 (no distribution is applied).

Allowed distributions are normal or uniform distributions and are shown in Figure 4. For each distribution, one or more parameters must be entered. For the normal distribution, parameter 1

is the standard deviation and parameter 2 is not used. For the uniform distribution parameter 1 is the lower bias and parameter 2 is the upper bias. (note: for a bias below the nominal enter a negative value for parameter 1)

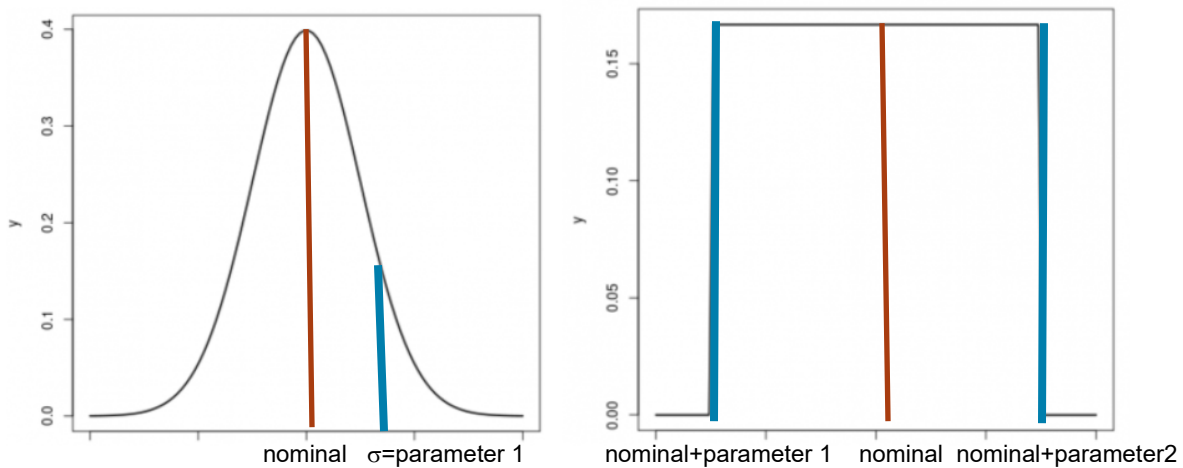


Figure 4. FAST-TRISO distribution parameters for normal and uniform distributions

To prevent the use of non-physical values in realizations, limits have been placed on most of the distributions. If a value above or below these limits are selected by the input distribution, the limit value will be used for that realization. These limits are shown in Table 4.

Table 4. Limits for stochastic calculations

Variable	Limit
kernel_rad	Lower value = 0.0001 cm
buffer_thick	Lower value = 0.00001 cm
IPyC_thick	Lower value = 0.00001 cm
SiC_thick	Lower value = 0.00001 cm
OPyC_thick	Lower value = 0.00001 cm
fuel_den	Lower value = 5 g/cm <sup>3</sup> Upper value = 10.96 g/cm <sup>3</sup>
buffer_porosity	Lower value = 0% Upper value = 100%
BAF	Lower value = 1.0
Heat_Rate multiplier	Lower value = 0.0

Following the running of a set number of realizations, FAST-TRISO will output the probability of the gross failure (due to contact of fuel and IPyC or due to melting) as well as the probability of stress failure in IPyC, SiC, and OPyC. To determine the overall probability of gross failure, FAST-TRISO divides the number of realizations where gross failure was predicted by the total number of realizations. To determine the probability of stress failure in IPyC, SiC, and OPyC, FAST-TRISO calculates the average probability predicted from each realization.

When a stochastic calculation is requested, FAST-TRISO creates a .stoch file that includes the overall probability of failure from all the realizations, the probability of failure from each realization, and the input parameters that were used for each realization.

## 3.0 Material Properties

This section shows the material property correlations that are used in FAST-TRISO. The data comparisons and justification for selecting each correlation is described elsewhere. The materials covered in this section are: fuel (UO<sub>2</sub> and UCO), buffer carbon, pyrolytic carbon, and silicon carbide.

### 3.1 Thermal Conductivity

Thermal conductivity is needed for all the materials within a TRISO particle in order to calculate the temperature distribution within the particle.

#### 3.1.1 Fuel (UO<sub>2</sub> and UCO)

FAST-TRISO uses the correlation for fuel thermal conductivity from FAST (Geelhood, Goodson, Luscher, Corson, & Kyriazidis, 2021). This correlation is a function of burnup, temperature, and density.

$$k_{95} = \left( \frac{1}{A + \alpha \cdot gad + BT + f(Bu) + (1 - 0.9 \exp(-0.04Bu) g(Bu)h(T))} \right) + \frac{C}{T^2} \exp\left(-\frac{D}{T}\right)$$

Where:

$k_{95}$  = Thermal conductivity of 95% TD fuel (W/m-K)

T = Temperature (K)

Bu = Burnup (GWd/MTU)

f(Bu) = Effect of fission products in crystal matrix (solution) = 0.00187\*Bu

g(Bu) = Effect of irradiation defects = 0.038Bu<sup>0.28</sup>

h(T) = Temperature dependence of annealing on irradiation defects

$$h(T) = \frac{1}{1 + 396 \exp\left(-\frac{Q}{T}\right)}$$

Q = Temperature-dependent parameter ("Q/R") = 6380 (K)

A = 0.0452 (m - K/W)

B = 2.46 × 10<sup>-4</sup> (m - K/W/K)

C = 3.5 × 10<sup>9</sup> (W - K/m)

D = 16361 (K)

α = Constant = 1.1599

gad = Weight fraction of gadolinia (unitless)

The above model is adjusted for the fuel density (in fraction of TD)

$$k_d = 1.0789k_{95} \frac{d}{1 + 0.5(1 - d)}$$

Where:

$k_d$  = Thermal conductivity adjusted for density (W/m-K)

$d$  = Fraction of fuel theoretical density (unitless)

### 3.1.2 Buffer Carbon

FAST-TRISO uses a constant value of 0.5 W/m-K for buffer carbon thermal conductivity (Miller, Petti, Maki, & Skerjanc, 2018).

### 3.1.3 Pyrolytic Carbon

FAST-TRISO uses a constant value of 4 W/m-K for pyrolytic carbon thermal conductivity (Miller, Petti, Maki, & Skerjanc, 2018).

### 3.1.4 Silicon Carbide

FAST-TRISO uses a correlation for silicon carbide thermal conductivity that is a function of temperature (Hales, Juang, Toptan, & Gamble, 2020).

$$k = \frac{17885}{T} + 2$$

Where:

$k$  = Thermal conductivity of silicon carbide (W/m-K)

$T$  = Temperature (K)

## 3.2 Thermal Expansion

Thermal expansion is needed for all the materials within a TRISO particle in order to calculate the hot dimensions within the particle.

### 3.2.1 Fuel (UO<sub>2</sub> and UCO)

FAST-TRISO uses the correlation for fuel thermal expansion from FAST (Geelhood, Goodson, Luscher, Corson, & Kyriazidis, 2021). This correlation is a function of temperature.

$$\varepsilon_{th} = K_1 T - K_2 + K_3 \exp\left(-\frac{E_D}{kT}\right)$$

Where:

$\varepsilon_{th}$  = linear strain caused by thermal expansion (293K reference) (unitless)

T = Temperature (K)

$$K_1 = 9.80 \times 10^{-6} \text{ (1/K)}$$

$$K_2 = 2.61 \times 10^{-3} \text{ (unitless)}$$

$$K_3 = 3.16 \times 10^{-1} \text{ (unitless)}$$

$$E_D = 1.32 \times 10^{-19} \text{ (J)}$$

k = Boltzmann's constant =  $1.38 \times 10^{-23}$  (J/K)

### 3.2.2 Buffer Carbon

FAST-TRISO uses a correlation for buffer carbon thermal expansion that is a function of temperature (Hales, Juang, Toptan, & Gamble, 2020)

$$\varepsilon_{th} = 3.92857 \times 10^{-10} T^2 + 4.4711 \times 10^{-6} T - 1.343758 \times 10^{-3}$$

Where:

$\varepsilon_{th}$  = linear strain caused by thermal expansion (293K reference) (unitless)

T = Temperature (K)

### 3.2.3 Pyrolytic Carbon

Pyrolytic carbon exhibits anisotropic thermal expansion. This anisotropy can be described by a Bacon anisotropy factor which is input to FAST TRISO. FAST-TRISO uses a correlation for pyrolytic carbon thermal expansion that is a function of temperature and BAF (CEGA Corporation, 1993).

$$\varepsilon_{th}(r) = (7.85714 \times 10^{-11} T^2 + 8.94243 \times 10^{-7} T - 2.68758 \times 10^{-4}) R$$

$$\varepsilon_{th}(h) = (7.85714 \times 10^{-11} T^2 + 8.94243 \times 10^{-7} T - 2.68758 \times 10^{-4}) H$$

Where:

$\varepsilon_{th}$  = linear strain caused by thermal expansion (293K reference) in the radial (r) and hoop (h) directions (unitless)

T = Temperature (K)

$$R = -37.5 \left[ \frac{2}{2+BAF} \right] + 30$$

$$H = 36 \left[ \frac{BAF}{2} - 1 \right]^2 + 1$$

BAF = Bacon anisotropy factor

### 3.2.4 Silicon Carbide

FAST-TRISO uses a correlation for silicon carbide thermal expansion that is a function of temperature (Snead, et al., 2007).

If  $T < 1273\text{K}$

$$\varepsilon_{th} = 1.13115 \times 10^{-15}T^4 - 5.18133 \times 10^{-12}T^3 + 8.9 \times 10^{-9}T^2 - 1.8276 \times 10^{-6}T - 1.06575 \times 10^{-4}$$

If  $T \geq 1273\text{K}$

$$\varepsilon_{th} = 5 \times 10^{-6}T - 2.09362 \times 10^{-3}$$

Where:

$\varepsilon_{th}$  = linear strain caused by thermal expansion (293K reference) (unitless)

T = Temperature (K)

## 3.3 Swelling

Irradiation swelling is needed for the fuel in order to calculate the hot dimensions within the particle as the particle is irradiated. FAST-TRISO currently assumes no swelling in the pyrolytic carbon or silicon carbide layers.

### 3.3.1 Fuel (UO<sub>2</sub> and UCO)

FAST-TRISO uses the correlation for fuel irradiation swelling from FAST (Geelhood, Goodson, Luscher, Corson, & Kyriazidis, 2021). This correlation is a function of burnup.

$$\frac{\Delta V}{V} = \begin{cases} 0 & \text{for } Bu \leq 6 \text{ GWd/MTU} \\ 0.00062(Bu - 6) & \text{for } 6 < Bu \leq 80 \text{ GWd/MTU} \\ 0.00062(74) + 0.00086(Bu - 80) & \text{for } Bu > 80 \text{ GWd/MTU} \end{cases}$$

Where:

$\Delta V/V$  = fuel volumetric swelling (unitless)

Bu = burnup (GWd/MTU)

Volumetric swelling, is related to linear swelling by:

$$\frac{\Delta l}{l} = \sqrt[3]{1 + \frac{\Delta V}{V}} - 1$$

Where:

$\Delta l/l$  = fuel linear swelling (unitless)

### 3.4 Melting Temperature

Melting temperature is needed for all the materials within a TRISO particle in order to calculate failure due to melting of any component.

#### 3.4.1 Fuel (UO<sub>2</sub> and UCO)

FAST-TRISO uses the correlation for fuel melting from FAST. This correlation is a function of burnup (Geelhood, Goodson, Luscher, Corson, & Kyriazidis, 2021).

$$T_{melt} = 3113.15 - 0.5Bu$$

Where:

$T_{melt}$  = melting temperature (K)

Bu = burnup (GWd/MTU)

#### 3.4.2 Buffer Carbon

FAST-TRISO uses a constant value of 3773K for buffer carbon melting temperature (Haynes, 2011).

#### 3.4.3 Pyrolytic Carbon

FAST-TRISO uses a constant value of 3773K for pyrolytic carbon melting temperature (Haynes, 2011).

#### 3.4.4 Silicon Carbide

FAST-TRISO uses a constant value of 3103K for silicon carbide melting temperature (Haynes, 2011).

### 3.5 Elastic Modulus and Poisson's Ratio

Elastic modulus and Poisson's Ratio are needed for the pyrolytic carbon and silicon carbide to calculate the stress in these layers.

#### 3.5.1 Pyrolytic Carbon

FAST-TRISO uses a constant value of  $2.54898 \times 10^{10}$  Pa for pyrolytic carbon elastic modulus (Miller, Petti, Maki, & Skerjanc, 2018).

FAST-TRISO uses a constant value of 0.33 for pyrolytic carbon Poisson's Ratio (Miller, Petti, Maki, & Skerjanc, 2018).

### 3.5.2 Silicon Carbide

FAST-TRISO uses a correlation for silicon carbide elastic modulus that is a function of temperature (Snead, et al., 2007).

$$E = \left( 460 - 0.04T \exp\left(\frac{962}{T}\right) \right) \cdot 10^9$$

FAST-TRISO uses a constant value of 0.21 for silicon carbide Poisson's Ratio. (Snead, et al., 2007)

## 3.6 Strength and Weibull Modulus

### 3.6.1 Pyrolytic Carbon

FAST-TRISO uses a constant value of  $218 \times 10^6$  Pa for pyrolytic carbon mean failure stress (IAEA, 2012).

FAST-TRISO uses a constant value of 9.5 for pyrolytic carbon Weibull Modulus (IAEA, 2012).

### 3.6.2 Silicon Carbide

FAST-TRISO uses a constant value of  $572 \times 10^6$  Pa for silicon carbide mean failure stress (IAEA, 2012).

FAST-TRISO uses a constant value of 6 for silicon carbide Weibull Modulus (IAEA, 2012).

## 3.7 Density

### 3.7.1 Fuel (UO<sub>2</sub> and UCO)

FAST-TRISO uses a constant value of 10.96 g/cm<sup>3</sup> for UO<sub>2</sub> theoretical density (Geelhood, Goodson, Luscher, Corson, & Kyriazidis, 2021).

FAST-TRISO uses a constant value of 11.26 g/cm<sup>3</sup> for UCO theoretical density.

### 3.7.2 Buffer Carbon

FAST-TRISO uses a constant value of 1.05 g/cm<sup>3</sup> for buffer carbon density.

### 3.7.3 Pyrolytic Carbon

FAST-TRISO uses a constant value of 1.9 g/cm<sup>3</sup> for pyrolytic carbon density.

### 3.7.4 Silicon Carbide

FAST-TRISO uses a constant value of 3.2 g/cm<sup>3</sup> for silicon carbide density.

## 4.0 Code Assessment

The code assessment consists of two portions: verification and validation. Verification confirms that the code was programmed correctly and is done by comparing various code predictions to hand calculated independently performed. Validation confirms that the code can predict measured data and although measured data on TRISO is rather limited, will be performed on what data are available. The following sections describe the verification and validation that has been performed for FAST-TRISO.

### 4.1 Verification

FAST-TRISO has built-in verification tests to confirm that the material property functions and the individual model subroutines are performing as expected. Independent calculations have been performed in Excel and the results of these calculations are compared to code calculations for these parameters.

To run the verification test suite, the input variable, *i\_unit*, should be set to 1 (See Table 1). Additionally, FAST-TRISO should be run using the input file, *unit\_test.in*. FAST-TRISO will produce an output file, *Unit-Test-Results.out*, that states if each test is passed or failed. The following is a description of what each of these unit tests is designed to confirm.

#### 4.1.1 Material Property Tests

The FAST-TRISO material property unit tests are listed in Table 5. The spreadsheet containing the independent calculations is saved with the FAST-TRISO source code.

Table 5. FAST-TRISO material property unit tests.

Test	Description	Inputs
TC_fuel_1	Fuel thermal conductivity	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K Burnup = 0 GWd/MTU Density = 0.95% T.D.
TC_fuel_2	Fuel thermal conductivity	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K Burnup = 30 GWd/MTU Density = 0.95% T.D.
TC_fuel_3	Fuel thermal conductivity	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K Burnup = 60 GWd/MTU Density = 0.94% T.D.
TC_fuel_4	Fuel thermal conductivity	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K Burnup = 100 GWd/MTU Density = 0.96% T.D.
TC_buffer	Buffer thermal conductivity	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K
TC_PyC	Pyrocarbon thermal conductivity	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K

Test	Description	Inputs
TC_SiC	Silicon carbide thermal conductivity	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K
Texp_fuel	Fuel thermal expansion	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K
Texp_buffer	Buffer thermal expansion	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K
Texp_PyC_1	Pyrocarbon thermal expansion (radial)	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K BAF = 1.05
Texp_PyC_2	Pyrocarbon thermal expansion (radial)	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K BAF = 1.0
Texp_SiC	Silicon carbide thermal expansion	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K
Swell_fuel	Fuel swelling	Burnup = 0, 10, 20, 40, 60, 80, 100 GWd/MTU
Melting	Fuel, buffer, PyC, and SiC melting temperature	Fuel Burnup = 0, 50, 100 GWd/MTU
E & v	PyC and SiC elastic modulus and Poisson's Ratio	Temperature (SiC) = 300, 800, 1000, 2000, 3000 K
Strength	PyC and SiC mean failure stress and Weibull Modulus	-
D-Kernel-Ag	Ag diffusivity in fuel	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K
D-Kernel-Cs	Cs diffusivity in fuel	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K
D-Kernel-Sr	Sr diffusivity in fuel	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K
D-Kernel-Kr	Kr diffusivity in fuel	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K
D-PyC-Ag	Ag diffusivity in PyC	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K
D-PyC-Cs	Cs diffusivity in PyC	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K
D-PyC-Sr	Sr diffusivity in PyC	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K
D-PyC-Kr	Kr diffusivity in PyC	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K
D-SiC-Ag	Ag diffusivity in SiC	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K
D-SiC-Cs	Cs diffusivity in SiC	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K
D-SiC-Sr	Sr diffusivity in SiC	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K
D-SiC-Kr	Kr diffusivity in SiC	Temperature = 300, 500, 800, 1500, 2000, 2500, 3000 K

### 4.1.2 Subroutine Tests

The FAST-TRISO subroutine unit tests are listed in Table 6. The spreadsheet containing the independent calculations is saved with the FAST-TRISO source code.

Table 6. FAST-TRISO subroutine unit tests.

Test	Description	Values Compared
Read Input I	Confirms that integers in the input file is read correctly	All input integers
Read Input R	Confirms that reals in the input file is read correctly	All input reals
Setup_Mesh	Confirms that the radial mesh is setup correctly	Each cold radial location in fuel, buffer, IPyC, SiC, and OPyC
Temperature	Confirms that temperature is calculated correctly for fixed dimensions	Temperature in fuel, buffer, IPyC, SiC, and OPyC
Expansion	Confirms that hot radial locations are calculated correctly for fixed temperatures and set burnup	Each hot radial location in fuel, buffer, IPyC, SiC, and OPyC
Buffer Vol	Confirms that the buffer volume and partition between solid and void are calculated correctly	Hot and cold buffer volume and void fraction
Burnup	Confirms that burnup is calculated correctly	Burnup at each time step in <i>unit_test.in</i>
Fission Rate	Confirms that fission rate is calculated correctly	Burnup at each time step in <i>unit_test.in</i>
FGR	Confirms that fission gas release fraction is calculated correctly	Fission gas release fraction at each time step in <i>unit_test.in</i>
FGR_moles	Confirms that fission gas release moles are calculated correctly	Fission gas release moles at each time step in <i>unit_test.in</i>
Pressure	Confirms that pressure in void space is calculated correctly	Pressure after first time step in <i>unit_test.in</i>
Radial Stress	Confirms that radial stress in IPyC, SiC, and OPyC are calculated correctly	Radial stress across IPyC, SiC, and OPyC during first time step in <i>unit_test.in</i>
Hoop Stress	Confirms that hoop stress in IPyC, SiC, and OPyC are calculated correctly	Hoop stress across IPyC, SiC, and OPyC during first time step in <i>unit_test.in</i>
VonMisses Stress	Confirms that Von Misses stress in IPyC, SiC, and OPyC are calculated correctly	VonMisses stress across IPyC, SiC, and OPyC during first time step in <i>unit_test.in</i>

Test	Description	Values Compared
Rad. release	Confirms that the release of radioactive fission products from TRISO particle are calculated correctly	Atoms of each isotope in void, released, and release fraction at end of first time step in <i>unit_test.in</i>

## 4.2 Validation

Work to validate the FAST-TRISO code predictions is currently underway. Most of the data available following irradiation is radionuclide release from post-test annealing tests at temperatures between 1400° to 1800°C. Additionally, there are even more limited data regarding particle failure fraction.

Both of these data sets are problematic to validate the FAST-TRISO predictions for in-reactor conditions. The release data are all taken at significantly higher temperatures than the fuel will be subjected to. For the failure fraction measurements, although FAST-TRISO includes some failure mechanisms, it cannot predict failure from manufacturing defects or chemical interactions that are likely the dominant failure mechanism. Nevertheless, initial validation against specific TRISO irradiations was performed for FAST-TRISO for the limited release data that exists for TRISO. Further work is underway to identify more release data and to better understand the experiments that produced these data.

IAEA describes a number of benchmarks that have been used to compare code predictions for a number of TRISO performance models (IAEA, 2012). These benchmarks include comparisons of code predictions of stress in the outer layers of a TRISO particle as well as failure fraction predictions. They also include fission product release benchmarks.

With regard to the stress benchmarks, it is noted that for the cases of gas loading only, FAST-TRISO is in good agreement with the other codes. However, FAST-TRISO does not include the effect of PyC irradiation swelling and creep. This mechanism has been proposed to cause a compressive stress in the SiC layer, which protects it from failure due to internal overpressure. These calculations are highly dependent on the models selected for both creep and swelling, and therefore may result in a non-conservative evaluation of failure in the SiC layer. It is acknowledged that if the PyC does in fact produce a compressive stress in the SiC, then FAST-TRISO will result in a slightly conservative prediction of failure fraction.

With regard to the fission product release benchmarks, there are data from specific heating tests. Initial comparisons have been made using FAST-TRISO to compare to these data. The results show that FAST-TRISO is generally in reasonable agreement with the other codes included in the IAEA study and that all of the codes including FAST-TRISO provide a conservative result (overpredict) relative to the data. Some level of overprediction is expected as FAST-TRISO does not model holdup by the graphite matrix, but only release from TRISO particles. Also, the data could be biased low as some of the radionuclides are expected to be lost prior to making it to the detector in the experimental apparatus. Further work is underway to better understand the experiment setup for these tests.

The validation of FAST-TRISO against the data in the IAEA (IAEA, 2012) report and more recent data (Demkowicz, Hunn, Petti, & Morris, 2106) (Hunn, JD; Gerczak, TJ; Montgomery,

FC; Skitt, DJ; Baldwin, CA; Helmreich, GW; Eckhart, BD; Dyer, JA, 2018) will be shown in a future document.

## 5.0 References

- Akis, T., & Azad, S. (2019). Structural Design Optimization of Multi-layer Spherical Pressure Vessels: A Metaheuristic Approach. *Iran J Sd Technol Trans Mech Eng*, 575-590.
- ANS Working Group 5.4. (1982). *Background and Derivation of ANS-5.4 Standard Fission Product Release Model, NUREG/CR-2507*. Washington DC: U.S. Nuclear Regulatory Commission.
- ANS5.4 Working Group. (1981). *Background and Derivation of ANS-5.4 Standard Fission Product Release Model, NUREG/CR-2507*. Washington DC: US Nuclear Regulatory Commission.
- Booth, A. (1957). *A Method of Calculating Fission Gas Diffusion from UO<sub>2</sub> Fuel and its Application to the X-2 Loop Test, CRDC-721*. Chalk River, Ontario: Atomic Energy of Canada Limited.
- CEGA Corporation. (1993). *NP-MHTGR Material Models of Pyrocarbon and Pyrolytic Silicon Carbide, CEGA-002820, Rev. 1*. CEGA Corporation.
- Collin, B. (2016). *Diffusivities of Ag, Cs, Sr, and Kr in TRISO Fuel Particles and Graphite, INL/EXT-16-39548*. Idaho Falls, ID: Idaho National Laboratory.
- Crank, J. (1975). *The Mathematics of Diffusion*. Oxford: Clarendon Press.
- Demkowicz, P., Hunn, J., Petti, D., & Morris, R. (2106). Key Results from Irradiation and Post-Irradiation Examination of AGR-1 UCO TRISO Fuel. *2016 Internation Topical Meeting on High Temperature Reactor Technology*.
- Geelhood, K., Goodson, C., Luscher, W., Corson, J., & Kyriazidis, L. (2021). *MatLib-1.0: Nuclear Material Properties Library, PNNL-31158*. Richland, WA: Pacific Northwest National Laboratory.
- Geelhood, K., Kyriazidis, L., Colameco, D., Goodson, C., Luscher, W., & Corson, J. (2021). *FAST-1.0.1: A Computer Code for Thermal-Mechanical Nuclear Fuel Analysis under Steady-state and Transients, PNNL-31160*. Richland, WA: Pacific Northwest National Laboratory.
- Hales, J., Juang, W., Toptan, A., & Gamble, K. (2020). *BISON TRISO Modeling Advancements and Validation to AGR-1 Data, INL/EXT-20-59368*. Idaho Falls, ID: Idaho National Laboratory.
- Haynes, W. (2011). *CRC Handbook of Chemistry and Physics (92nd ed.)*. Boca Raton, FL: CRC Press.
- Hunn, JD; Gerczak, TJ; Montgomery, FC; Skitt, DJ; Baldwin, CA; Helmreich, GWI Eckhart, BD; Dyer, JA. (2018). *AGR-2 As-Irradiated UCO Compact 5-4-2 PIE Report, ORNL/TM-2108/863*. Oak Ridge, TN.: Oak Ridge National Laboratory.
- IAEA. (2012). *Advances in High Temperature Gas Cooled Reactor Fuel Technology, IAEA-TECDOC-CD-1674*. Vienna, Austria: International Atomic Energy Agency.
- Japan Atomic Energy Agency. (2021, May 11). *Graph of Fission Product Yields*. Retrieved from Nuclear Data Center Japan Atomic Energy Agency: <https://www.ndc.jaea.go.jp/cgi-bin/FPYfig?lib=11&mode=s&iso=nU235&typ=g2&ynuc=Kr-85&ysub=Show+Yield&yld=c&zlog=set&yflow=12&part=n&xrot=40&zrot=30&eng=e1>
- Jayanta, S. (2021). *Conduction with Heat Generation | Thermal Engineering*. Retrieved from engineeringnotes.com: <https://www.engineeringnotes.com/thermal-engineering/heat-conduction/conduction-with-heat-generation-thermal-engineering-2/30250>
- Miller, G., Petti, D., Maki, D., & Skerjanc, W. (2018). *PARFUME Theory and Model Basis Report, INL/EXT-08-14497*. Idaho Fall, ID: Idaho National Laboratory.
- Proksch, E., & Strigl, A. (1982). Production of Carbon Monoxide during Burn-up of UO<sub>2</sub> Kerneled HTR Fuel PArticles. *Journal of Nuclear Materials*, 280-285.

- Skerjanc, W. (2019). *CO Production Model Analysis for Correlations into PARFUME*, INL/MIS-19-55748-Rev000. Idaho Falls, ID: Idaho National Laboratory.
- Snead, L., Nozawa, T., Kato, Y., Buyn, T., Kondo, S., & Petti, D. (2007). Handbook of SiC Properties for Fuel Performance Modeling. *Journal of Nuclear Materials*, 329-337.
- Turnbull, J., & Beyer, C. (2010). *Background and Derivation of ANS-5.4 Standard Fission Product Release Model*, NUREG/CR-7003, PNNL-18490. Richland, WA: Pacific Northwest National Laboratory.
- Wells, B., Phillips, N., & KJ, G. (2021). *TRISO Fuel: Properties and Failure Modes*. PNNL-31427. Richland, WA: Pacific Northwest National Laboratory.

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