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Calculating failure probabilities for TRISO-coated fuel particles using an integral formulation

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ABSTRACT

The fundamental design for a gas-cooled reactor relies on the safe behavior of the coated particle fuel. The coating layers surrounding the fuel kernels in these spherical particles, termed the TRISO coating, act as a pressure vessel that retains fission products. The quality of the fuel is reflected in the number of particle failures that occur during reactor operation, where failed particles become a source for fission products that can then diffuse through the fuel element. The failure probability for any batch of particles, which has traditionally been calculated using the Monte Carlo method, depends on statistical variations in design parameters and on variations in the strengths of coating layers among particles in the batch. An alternative approach to calculating failure probabilities is developed herein that uses direct numerical integration of a failure probability integral. Because this is a multiple integral where the statistically varying parameters become integration variables, a fast numerical integration approach is also developed. In sample cases analyzed involving multiple failure mechanisms, results from the integration methods agree closely with Monte Carlo results. Additionally, the fast integration approach, particularly, is shown to significantly improve efficiency of failure probability calculations. These integration methods have been implemented in the PARFUME fuel performance code along with the Monte Carlo method, where each serves to verify accuracy of the others.

1. Introduction

The success of gas-cooled reactors depends largely upon the safety and quality of the coated particle fuel. The coating layers of a particle, which surround the fuel and buffer, consist of an inner pyrolytic carbon (IPyC) layer, a silicon carbide (SiC) layer, and outer pyrocarbon (OPyC) layer. These layers act as a pressure vessel for fission product gases as well as a barrier to the migration of other fission products. The quality of the fuel can be characterized by the number of particle failures that occur during reactor operation. Fuel performance codes, such as Idaho National Laboratory's PARFUME [1], are needed to determine the failure probability of a population of fuel particles. Other performance codes are described in Ref. [2].

The failure probability for a batch of TRISO-coated fuel particles generally depends on statistical variations in a number of design parameters and on variations in the strengths of the coating layers among particles in the batch. The probability is traditionally calculated using the Monte Carlo method wherein a large number of particles are statistically sampled to account for the variations. In these calculations the design parameters are typically sampled from Gaussian statistical distributions, while the coating layer strengths are sampled from Weibull statistical distributions [3,4]. The parameters that can currently be varied statistically in the PARFUME code include the thicknesses of the three coating layers, densities of the pryocarbons, degree of anisotropy in the pyrocarbon layers (as measured by the Bacon anisotropy factor [BAF]), irradiation temperature, the creep coefficient for the pyrocarbons, kernel diameter, buffer thickness, Poisson's ratio in creep for the pyrocarbons, bond strength between the IPyC and SiC coating layers, and the degree of asphericity (as measured by aspect ratio) for aspherical particles. This list can be modified as desired. Only rarely would statistical variations in all of these parameters be considered in a single analysis.

A significant disadvantage of the Monte Carlo approach has been that a low failure probability requires a large particle sample to produce an accurate estimate of the probability. With the capabilities contained in an integrated fuel performance modeling code such as PARFUME, sampling a large number of particles to calculate small failure probabilities can be a time consuming effort. A further consideration is that failure probabilities may have to be calculated for a multitude of potential failure mechanisms (such as internal pressure loading, cracking of the IPyC, partial debonding of the IPyC from the SiC, asphericity effects, the amoeba effect, and

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degradation of the SiC). Multi-dimensional failure mechanisms are described in detail in Refs. [5–7]. These mechanisms complicate the calculations to the point that an independent method is needed to verify that the probabilities are determined accurately. Therefore, an alternative approach to the Monte Carlo method has been developed. In this approach, the failure probability for a particle batch is formulated in terms of an integral and methods for evaluating the integral have been developed as described below. Both the Monte Carlo and numerical integration methods have been implemented in the PARFUME code. The theory behind the PARFUME code is explained in Ref. [8], which more thoroughly describes implementation of the integration method.

2. Failure probability for Gaussian distribution of strengths

Failure of a particle is assumed to occur when the maximum stress σ in the SiC layer exceeds the SiC strength μ. Though the strengths for the SiC layer in a fuel particle batch are generally assumed to follow a Weibull statistical distribution, we will initially assume the strength levels μ to be distributed according to a Gaussian distribution with a mean strength μ_s and a standard deviation D_s. If the stress σ is a function of a parameter υ_k, which is also assumed to vary according to some statistical distribution, then the stress in a particle can be expressed as follows:

$$\sigma = g(\upsilon_k) \tag{1}$$

Assuming momentarily that the parameter υ_k is fixed for a batch of particles, then the probability that the stress in a particle exceeds its strength is [9]:

$$P_f(\upsilon_k) = \int_{-\infty}^{g(\upsilon_k)} \frac{1}{\sqrt{2\pi}D_s} e^{-(s-\mu_s)^2/2D_s^2}\, ds \tag{2}$$

This is the failure probability associated with a specific value for the parameter υ_k. Considering statistical variations in υ_k, if a_i is the fraction of particles within the batch having parameter υ_k equal to υ_{ki}, then the total failure probability for the batch is

$$P_f = a_1 P_f(\upsilon_{k1}) + a_2 P_f(\upsilon_{k2}) + a_3 P_f(\upsilon_{k3}) + \dots \tag{3}$$

This summation is converted to an integral by writing the a_i as a density function for the parameter υ_k:

$$P_f = \int_{-\infty}^{\infty} a(\upsilon_k) P_f(\upsilon_k)\, d\upsilon_k \tag{4}$$

If the parameter υ_k is assumed to be distributed normally with a mean value μ_k and a standard deviation D_k, then

$$P_f = \int_{-\infty}^{\infty} \int_{-\infty}^{g(\upsilon_k)} \frac{1}{\sqrt{2\pi}D_k} e^{-(\upsilon_k-\mu_k)^2/2D_k^2} \frac{1}{\sqrt{2\pi}D_s} e^{-(s-\mu_s)^2/2D_s^2}\, ds\, d\upsilon_k \tag{5}$$

The failure probability for this batch of particles is then determined by evaluating the integral above. Since Eq. (5) cannot be integrated in closed form, the accuracy of the calculated failure probability depends on the level of precision in the integration performed.

The formulation above can be extended to situations where the stress σ is a function of several parameters that vary according to some statistical distribution. Considering the case of a batch of particles where the stress is a function of two such parameters, υ_j and υ_k:

$$\sigma = g(\upsilon_j, \upsilon_k) \tag{6}$$

The probability of failure associated with specific values υ_j and υ_k for the two parameters is

$$P_f(\upsilon_j, \upsilon_k) = \int_{-\infty}^{g(\upsilon_j,\upsilon_k)} \frac{1}{\sqrt{2\pi}D_s} e^{-(s-\mu_s)^2/2D_s^2}\, ds \tag{7}$$

If a_m is the fraction of particles having parameter υ_j equal to υ_{jm}, and a_n is the fraction of particles having parameter υ_k equal to υ_{kn}, then the total batch failure probability is

$$P_f = \sum_m \sum_n a_m a_n P_f(\upsilon_{jm}, \upsilon_{kn}) \tag{8}$$

Again, this is converted to an integral by writing a_m and a_n as density functions for the parameters υ_j and υ_k. Then,

$$P_f = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} a(\upsilon_j) a(\upsilon_k) P_f(\upsilon_{j,} \upsilon_k)\, d\upsilon_k\, d\upsilon_j \tag{9}$$

Assuming that the parameters υ_j and υ_k are both normally distributed, then the failure probability becomes

$$\begin{aligned} P_f = {} & \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{g(\upsilon_j,\upsilon_k)} \frac{1}{\sqrt{2\pi}D_j} e^{-(\upsilon_j-\mu_j)^2/2D_j^2} \\ & \times \frac{1}{\sqrt{2\pi}D_k} e^{-(\upsilon_k-\mu_k)^2/2D_k^2} \frac{1}{\sqrt{2\pi}D_s} e^{-(s-\mu_s)^2/2D_s^2}\, ds\, d\upsilon_k\, d\upsilon_j \end{aligned} \tag{10}$$

A pattern is established in comparing Eqs. (5) and (10). Each parameter considered adds a density function to the integrand and increases the level of integration by one. Therefore, any number of parameters can be accommodated in this formulation.

The limits of integration in the mathematical expression above extend to infinity. In reality, of course, these parameters do not physically cover this range. It is found that an accurate value for the integral can be attained by integrating over a range of four standard deviations to each side of the mean value for each parameter. Outside this range, the density functions are so small that contributions to the integral become negligible. An integral for n parameters then appears as follows:

$$\begin{aligned} P_f = {} & A \int_{\mu_j-4D_j}^{\mu_j+4D_j} \int_{\mu_k-4D_k}^{\mu_k+4D_k} \dots \int_{\mu_s-4D_s}^{g(\upsilon_j,\upsilon_k\dots)} \\ & \times e^{-(\upsilon_j-\mu_j)^2/2D_j^2-(\upsilon_k-\mu_k)^2/2D_k^2\dots-(s-\mu_s)^2/2D_s^2}\, ds \dots d\upsilon_k\, d\upsilon_j \end{aligned} \tag{11}$$

where

$$A = \frac{1}{\sqrt{2\pi}^{\,n+1} D_j D_k \dots D_s} \tag{12}$$

3. Failure probability for Weibull variation of strengths

Because of the brittle nature of the graphitic materials in fuel particles, the material strengths generally follow a Weibull distribution rather than the Gaussian distribution assumed above [3,4]. In the Weibull theory, the probability of failure for the particles in a batch is [10]:

$$P_f = 1 - e^{-\left(\frac{\sigma_{\max}}{\sigma_{ms}}\right)^m} \tag{13}$$

where $\sigma_{\max}$ = maximum principal stress in the SiC layer, σ_{ms} = mean strength for the SiC, or the stress at which 63.2% of the particles fail and m = Weibull modulus for the SiC.

We now consider the case where the maximum stress is a function of a parameter (υ_k) that varies with some statistical distribution.

$$\sigma_{\max} = g(\upsilon_k) \tag{14}$$

The failure probability associated with a specific value ν_k for this parameter is

$$P_f(\upsilon_k) = 1 - e^{-\left(\frac{g(\upsilon_k)}{\sigma_{ms}}\right)^m} \tag{15}$$

The total failure probability for a batch of particles is

$$P_f = \int_{-\infty}^{\infty} a(\upsilon_k) P_f(\upsilon_k)\, d\upsilon_k \tag{16}$$

where $a(\nu_k)$ is a density function for the parameter ν_k.

In the situation where the stress is a function of multiple parameters having normal statistical distributions, the total failure probability becomes

$$P_f = B\int_{\mu_j-4D_j}^{\mu_j+4D_j}\int_{\mu_k-4D_k}^{\mu_k+4D_k}\dots e^{-(v_j-\mu_j)^2/2D_j^2-(v_k-\mu_k)^2/2D_k^2\cdots} \times\left[1-e^{-\left(\frac{g(v_j,v_k,\dots)}{\sigma_{ms}}\right)^m}\right]dv_1\dots dv_k\,dv_j \tag{17}$$

where

$$B = \frac{1}{\sqrt{2\pi}^n D_j D_k \dots D_1}$$

According to Ref. [11], an integral of this form gives the "expectation value" for the function in brackets, i.e. the failure probability.

In addition to the use of a Weibull distribution for the coating layer strengths, another exception to the use of a Gaussian distribution to characterize the statistical variation in a parameter is in the temperature distribution among particles. The temperature of a particle in a fuel pebble, for example, is dependent on its radial position in the pebble. The distribution used to represent the radial density of particles in a pebble is $3r^2/R^3$, where r is any radial location in the pebble and R is the outside radius of the fueled region of the pebble. The corresponding radial density of particles in a cylinder is $2r/R^2$. When integrated over the range of 0–R, these densities sum to 1.

Determining the failure probability with Monte Carlo statistical sampling of the integration variables is a means of evaluating the integral in Eq. (17). The other approach exercised in PARFUME is a direct numerical integration where the integration is typically performed at eleven Gaussian quadrature points over the range of $\mu_i - 4D_i$ to $\mu_i + 4D_i$ for each parameter v_i. An odd number of points is used so that an integration is performed at the mean value μ_i for each parameter, which is essential to achieving maximum accuracy in the calculation. An exception to the use of Gaussian quadrature points in PARFUME is in the integration of particle radial position over the radius of a sphere (pebble) or cylinder (prismatic block). These integrations are performed at equal intervals over the radius (dependent on user specified nodalization).

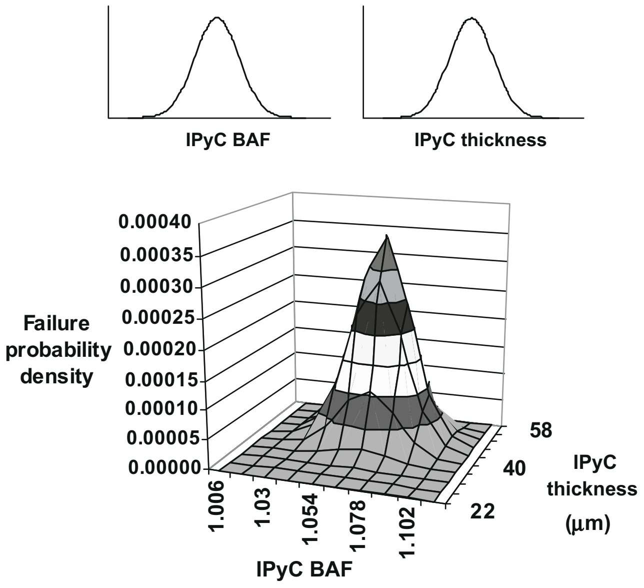

Fig. 1. Failure probability density obtained from numerical integration.

Fig. 1 plots a representative failure probability density obtained from numerical integration when the IPyC thickness and BAF were assumed to vary according to a Gaussian statistical distribution. The largest concentration of particles occurs around the mean values of 1.054 and 40 for the IPyC BAF and IPyC thickness, respectively. The peak of the failure probability density is shifted somewhat from the point where these mean values intersect in the BAF/thickness plane.

4. Implementation of the integration method in PARFUME

In principle, determining the failure probability by numerically integrating Eq. (17) should produce the same failure probability as that calculated by the Monte Carlo method (discounting numerical error). This method is implemented in PARFUME by integrating over a parameter space consisting of those parameters v that exhibit a statistical variation about a mean value. For each differential volume element (in parameter space), PARFUME solves incrementally (through time) for stresses in a particle from the beginning to the end of irradiation. The particle analyzed has parameters that correspond to that differential volume element. It then determines a failure probability for each of several failure modes (such as IPyC cracking, partial debonding, internal pressure, and the amoeba effect) at the end of each time increment of the stress solution. Thinning of the SiC due to corrosion is an additional failure mechanism that is currently under development. If the failure probability at the end of a time increment exceeds the accumulated probability at the beginning of the increment, the cumulative probability for the volume element is incremented accordingly.

To determine the probability that particles will fail due to IPyC cracking, the code first determines the probability that cracking of the IPyC will occur. It then determines the probability that the SiC layer of the particle will fail due to the presence of the IPyC crack. The product of these probabilities then gives a probability for particle failure due to IPyC cracking. The probability that particles will fail due to partial debonding of the IPyC layer is likewise determined by first calculating the probability that debonding occurs, then determining the probability that a debonded particle will fail. A complication in these calculations is that there are times when IPyC cracking or IPyC debonding would occur in the same particle, introducing overlap in the probabilities of these two mechanisms. To develop an appropriate split between the probabilities of IPyC cracking and IPyC debonding, the code uses the process described as follows. It determines maximum values for the IPyC hoop stress and the radial stress at the interface between IPyC and SiC layers occurring throughout irradiation. It uses the maximum IPyC hoop stress in Eq. (13) to determine the probability (within a differential volume element) that the IPyC layer would crack, where $\sigma_{\max}$, σ_{ms}, and m are now maximum stress, mean strength, and Weibull modulus for the IPyC layer. Because the bond strength is currently treated in PARFUME as having a normal statistical distribution, the code uses Eq. (11) to determine the probability that the IPyC layer would debond from the SiC, where g is now the maximum radial stress at the interface and μ_s is the mean bond strength.

Having determined probabilities that a particle within the differential volume element would crack (P_a) or debond (P_b), the code now determines what fraction of particles within the volume will crack (a), debond (b), or do neither (c). The sum of the fractions a, b, and c must be 1:

$$a + b + c = 1 \tag{18}$$

There may be some particles that mathematically could both crack and debond. PARFUME currently allows a particle to do one or the other, but not both. Thus, the fraction of particles that crack is something less than the probability of cracking if the probability of debonding is non-zero (and vice versa). If the probability of cracking is n times the probability of debonding, then cracking will occur n times as often. A second condition, then, is that the ratio between the fraction of particles that crack and the fraction of particles that debond is equal to the ratio between the probability of cracking and the probability of debonding:

$$a = \frac{P_a}{P_b} b \tag{19}$$

A third condition comes from recognizing that the probability that a particle neither cracks nor debonds (P_c) is

$$P_c = (1 - P_a)(1 - P_b) \tag{20}$$

A particle that would crack may also be a particle that would debond. However, a particle that would do neither has no such overlap. Hence

$$c = P_c \tag{21}$$

Substituting Eqs. (19)–(21) into Eq. (18) gives

$$b = P_b \left(1 - \frac{P_a P_b}{P_a + P_b}\right) \tag{22}$$

The fractions a and b are calculated above as if the values for the quantities are developed in a single time step. Since PARFUME solves through irradiation in time increments, the process described above has to be modified accordingly. Within a time increment, the probabilities for cracking and debonding increase incrementally by ΔP_a and ΔP_b, respectively, resulting in corresponding increases to fractions a and b of Δa and Δb. Then Eqs. (18) and (19) are modified as follows:

$$a + \Delta a + b + \Delta b + c = 1 \tag{23}$$

$$\Delta a = \frac{\Delta P_a}{\Delta P_b} \Delta b \tag{24}$$

where a and b are the crack and debond fractions at the beginning of the increment. The quantity c is the fraction of particles that have neither cracked nor debonded at the end of the time increment, meaning that its value has decreased by $\Delta a + \Delta b$ during the increment. Eqs. (20) and (21) remain unchanged, and the probabilities in these equations are those occurring at the end of the time increment. Substituting Eqs. (20), (21), and (24) into Eq. (23) results in:

$$\Delta b = \frac{\Delta P_b (P_a + P_b - P_a P_b - a - b)}{\Delta P_a + \Delta P_b} \tag{25}$$

The incremental fractions Δa and Δb are then added to a and b, respectively, to produce new failure fractions at the end of the increment.

Once the fractions a, b, and c are determined for the volume element, the program computes a differential failure probability (of the SiC) for each of three failure mechanisms, i.e., IPyC cracking, IPyC debonding, and internal gas pressure loading. To do this it first calculates the maximum stress in the SiC layer for each of these mechanisms in a particle corresponding to the volume element. For IPyC cracking or debonding, this is done using the statistical methodology described in Ref. [12]. For internal pressure loading, the maximum stress in the SiC layer for a spherical particle is calculated using the solution of Ref. [13]. If asphericity in the particles is considered, then the maximum SiC stress due to internal pressure is calculated using methodology described in Ref. [6]. Asphericity can be treated as a statistical parameter, where the aspect ratio becomes one of the parameters of Eq. (17).

For each of the three failure mechanisms, the program then applies the maximum SiC stress in the integrand of Eq. (17) to calculate a differential failure probability. It applies the factors a and b (corresponding to the end of the time increment) to the probabilities of SiC failure due to IPyC cracking and debonding, respectively. It then applies the following factor to the probability of SiC failure due to internal pressure loading:

$$c + a e^{-\left(\frac{\sigma_{\max a}}{\sigma_{msa}}\right)^m} + b e^{-\left(\frac{\sigma_{\max b}}{\sigma_{msb}}\right)^m} \tag{26}$$

where $\sigma_{\max\,a}$ = maximum principal stress in the SiC layer of a particle having a cracked IPyC, σ_{msa} = mean strength for the SiC layer of a particle having a cracked IPyC, $\sigma_{\max\,b}$ = maximum principal stress in the SiC layer of a particle having a cracked IPyC, σ_{msb} = mean strength for the SiC layer of a particle having a cracked IPyC and m = Weibull modulus for the SiC.

The exponential in the second term of Eq. (26) is the probability that the SiC layers among cracked particles have survived potential failure due to the crack (assuming a Weibull strength distribution for the SiC layer). The second term itself then represents that fraction of particles that incurred an IPyC crack but did not experience failure of the SiC due to the presence of the crack. These particles that have survived are thus allowed the possibility to fail later due to internal pressure loading. The third term treats particles that have debonded in like manner.

In executing the integration method, PARFUME accumulates a failure probability for each failure mechanism considered (IPyC cracking, failure of the SiC due to IPyC cracking, etc.). To do this, the incremental failure probability for each time increment in the analysis of each particle is weighted by the appropriate probability density functions for the particle, and is then added to a cumulative probability for that time increment. At the end of the integration, then, each time increment has a cumulative failure probability for that failure mechanism. The cumulative failure probabilities for all increments up to a time t_i are then summed to produce a total failure probability at time t_i.

If failure due to the amoeba effect is found to occur in a differential volume element during any time increment, the probability of SiC failure jumps to 1.0 for that element. Therefore, no further consideration of SiC failure is required for that element beyond that time increment.

5. Fast integration method

The time required to execute the probability calculation of Eq. (17) depends on how many parameters are given a statistical variation. For example, the execution time is just a fraction of a second when only one parameter is statistically varied, regardless of the magnitude of the failure probability. The computation time can, though, become inordinately large when a large number of parameters are considered. Therefore, an approximation is developed below that can substantially reduce the time required to perform the integration with only a minimal loss of accuracy.

Considering for the moment statistical variations in four parameters, Eq. (17) can be expressed as the following integral:

$$\begin{aligned} I_{1,2,3,4} = {} & \frac{1}{\sqrt{2\pi}^4 D_1 D_2 D_3 D_4} \int_{-4D_4}^{4D_4} \int_{-4D_3}^{4D_3} \int_{-4D_2}^{4D_2} \\ & \times \int_{-4D_1}^{4D_1} e^{-\Delta v_1^2/2D^2 - \Delta v_2^2/2D^2 - \Delta v_3^2/2D^3 - \Delta v_4^2/2D^2} \\ & \times \left[1 - e^{-\left(\frac{g(\Delta v_1, \Delta v_2, \Delta v_3, \Delta v_4)}{\sigma_{ms}}\right)^m}\right] d\Delta v_1\, d\Delta v_2\, d\Delta v_3\, d\Delta v_4 \end{aligned} \tag{27}$$

or in the basic form

$$\begin{aligned} I_{1,2,3,4} = {} & \int_{-4D_4}^{4D_4} \int_{-4D_3}^{4D_3} \int_{-4D_2}^{4D_2} \\ & \times \int_{-4D_1}^{4D_1} f(\Delta v_1, \Delta v_2, \Delta v_3, \Delta v_4)\, d\Delta v_1\, d\Delta v_2\, d\Delta v_3\, d\Delta v_4 \end{aligned} \tag{28}$$

where Δv_i is the variation in parameter i from its mean value μ_i. Additionally, the subscript 1–4 on the integral I indicates that the integral entails variations in the parameters 1–4.

The integrand $f(\Delta v_1, \Delta v_2, \Delta v_3, \Delta v_4)$ can be expanded into a Taylor series having the following form:

$$\begin{aligned} &f(\Delta v_1,\Delta v_2,\Delta v_3,\Delta v_4)\\ &\quad= f(0,0,0,0)\left(1+\sum_{i=1}^{\infty}\sum_{p=1}^{4}a_{ip}\Delta v_p^i+\sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{p=1}^{3}\sum_{q=2}^{4}b_{ijpq}\Delta v_p^i\Delta v_q^j\right.\\ &\qquad+\sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\sum_{p=1}^{2}\sum_{q=2}^{3}\sum_{r=3}^{4}c_{ijkpqr}\Delta v_p^i\Delta v_q^j\Delta v_r^k\\ &\qquad\left.+\sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}d_{ijkl}\Delta v_1^i\Delta v_2^j\Delta v_3^k\Delta v_4^l\right)\quad(p<q<r) \end{aligned}\tag{29}$$

The coefficients in this series (a_{ip}, b_{ijpq}, c_{ijkpqr} and d_{ijkl}) are composed of derivatives of the function f with respect to the parameters v_i. The error that would be incurred in dropping some of the summations in this series may be small, depending on the degree of coupling between the parameters v_i. The maximum stress $g(\Delta v_1, \Delta v_2, \Delta v_3, \Delta v_4)$ can similarly be expanded into a Taylor series. A study of the stresses in the coating layers has revealed that g can be well approximated by carrying only terms involving variations in two or fewer parameters. In this case, summations in the series involving variations in three or more parameters can reasonably be neglected. Because the integrand f is strongly a function of the stress g, it can be expected that summations in its series involving variations in three or more parameters can be neglected as well.

Prior to eliminating these summations, the following relations can be established from Eqs. (28) and (29):

$$I = f(0,0,0,0) = 1 - e^{-\left(\frac{g(0,0,0,0)}{\sigma_{ms}}\right)^m}\tag{30a}$$

$$\begin{aligned} I_1 &= \int_{-4D_1}^{4D_1} f(\Delta v_1,0,0,0)\,d\Delta v_1\\ &= \int_{-4D_1}^{4D_1} e^{-(\Delta v_1)^2/2D_1^2}\left[1-e^{-\left(\frac{g(\Delta v_1)}{\sigma_{ms}}\right)^m}\right]d(\Delta v_1)\\ &= I\left(1+\int_{-4D_1}^{4D_1}\sum_{i=1}^{\infty}a_{i1}\Delta v_1^i\,d\Delta v_1\right) \end{aligned}\tag{30b}$$

$$\begin{aligned} I_{1,2} &= \int_{-4D_2}^{4D_2}\int_{-4D_1}^{4D_1} f(\Delta v_1,\Delta v_2,0,0)\,d\Delta v_1 d\Delta v_2\\ &= I\left(1+\sum_{p=1}^{2}\int_{-4D_p}^{4D_p}\sum_{i=1}^{\infty}a_{ip}\Delta v_p^i\,d\Delta v_p\right.\\ &\qquad\left.+\int_{-4D}^{4D_2}\int_{-4D_1}^{4D_1}\sum_{i=1}^{\infty}\sum_{j=1}^{\infty}b_{ij12}\Delta v_1^i\Delta v_2^j\,d\Delta v_1 d\Delta v_2\right)\\ &= I_1+I_2-I+I\int_{-4D}^{4D_2}\int_{-4D_1}^{4D_1}\sum_{i=1}^{\infty}\sum_{j=1}^{\infty}b_{ij12}\Delta v_1^i\Delta v_2^j\,d\Delta v_1 d\Delta v_2 \end{aligned}\tag{30c}$$

Substituting Eq. (29) into Eq. (28), neglecting all summations involving more than two parametric variations, and utilizing the relations of Eqs. (30a), (30b) and (30c), the failure probability integral becomes

$$I_{1,2,3,4} \cong I + \sum_{p=1}^{4} I_p - 4I + \sum_{p=1}^{3}\sum_{q=2}^{4}(I_{p,q} - I_p - I_q + I)\quad (p<q)\tag{31}$$

where only those parameters having a Δv that deviates from zero are shown in subscripts. On simplification,

$$I_{1,2,3,4} \cong 3I - 2\sum_{p=1}^{4} I_p + \sum_{p=1}^{3}\sum_{q=2}^{4} I_{p,q}\quad (p<q)\tag{32}$$

For the more general case of N variables of integration, Eq. (31) becomes

$$I_{1,2,\ldots N} \cong I + \sum_{p=1}^{N} I_p - NI + \sum_{p=1}^{N-1}\sum_{q=2}^{N}(I_{p,q} - I_p - I_q + I)\quad (p<q)\tag{33}$$

which is simplified to

$$I_{1,2,\ldots N} \cong \frac{(N-2)(N-1)}{2}I - (N-2)\sum_{p=1}^{N} I_p + \sum_{p=1}^{N-1}\sum_{q=2}^{N} I_{p,q}\quad (p<q)\tag{34}$$

This resolves the multiple integral (over N variables) into a number of subintegrals that each requires integration over two or fewer variables.

It is noted that this approximation equation could apply to any multiple integration, not just the failure probability integral for TRISO-coated fuel particles. The general equation for estimating an N-dimension integral with integrals up to level k (where $k < N$) can be similarly developed to give

$$\begin{aligned} I_{1,2,\ldots N} &\cong \frac{(-1)^k(N-1)!}{(N-k-1)!k!}I + \frac{(-1)^{k-1}(N-2)!}{(N-k-1)!(k-1)!}\sum_{p=1}^{N} I_p\\ &\quad+\frac{(-1)^{k-2}(N-3)!}{(N-k-1)!(k-2)!}\sum_{p=1}^{N-1}\sum_{q=2}^{N} I_{p,q} + \cdots\\ &\quad+\sum_{p=1}^{N-k+1}\sum_{q=2}^{N-k+2}\cdots\sum_{z=k}^{N} I_{p,q,\ldots z}\quad (p<q<\cdots<z) \end{aligned}\tag{35}$$

The level k that may be needed in a particular case is dependent upon the degree of coupling among the integration variables. When the integration is carried out to an appropriate level k, the estimate should be very accurate. For the failure probability integral of Eq. (17), a value of $k = 2$ has been sufficient.

The time required to perform the integration using Eq. (34) relative to the full integration can be measured in terms of the number of integration points required for each. It has been found that the integrations for a fuel particle can generally be carried out to a high degree of accuracy in PARFUME using eleven integration points over the range of each statistically varying parameter. The number of integration points n needed to perform the full integration of Eq. (17), then, is

$$n = 11^N\tag{36}$$

Resolving the integral into subintegrals up to level two, as in Eq. (34), reduces the number of integration points to

$$n = 1 + N(11) + \frac{N(N-1)}{1(2)}(11)^2\tag{37}$$

Based on these equations, PARFUME would execute a 2-level integration in approximately 1/(4.67 × 10^6) the time required to execute the full integration if 10 variables are considered.

The full integration method is executed in the code with a set of nested DO loops, one for each statistically varying parameter. Each parameter is cycled through its full range of values within its respective loop. The two-level method is executed with two nested loops. These loops execute subintegrals involving all possible combinations of parameters taken two at a time [the third term on the right-hand side of Eq. (34)]. They are also used to execute subintegrals involving variations in one or no parameters [the second and first terms of Eq. (34), respectively]. The two-level approach is referred to as the "fast integration" approach.

6. An improved means of implementing the Monte Carlo method

The Monte Carlo method has traditionally been executed by statistically sampling the coating layer strengths along with the integration variables of Eq. (17). With this approach, the integral of Eq. (17) is actually evaluated in the following modified form:

$$P_f = B\int_{\mu_j-4D_j}^{\mu_j+4D_j}\int_{\mu_k-4D_k}^{\mu_k+4D_k}\cdots\int_0^{g(\nu_j,\nu_k,\ldots)} e^{-(\nu_j-\mu_j)^2/2D_j^2-(\nu_k-\mu_k)^2/2D_k^2\cdots} \times\left[\frac{m}{(\sigma_{ms})^m}s^{m-1}e^{-\left(\frac{s}{\sigma_{ms}}\right)^m}\right]ds\ldots d\nu_k\,d\nu_j \qquad (38)$$

where the expression for failure probability [within brackets on the right-hand side of Eq. (17)] has been differentiated with respect to the stress s and integrated from 0 to the stress level $g(\nu_j, \nu_k, \ldots)$. As with Eq. (11), the stress s within the integral of Eq. (38) is the strength variable for the coating layer, except that the strength has a Weibull distribution rather than a Gaussian distribution. In exercising the Monte Carlo method according to Eq. (38), the calculated stress in the coating layer is compared to the sampled strength value to determine whether a coating layer fails. As noted above, though, a disadvantage to this approach is that a large statistical sample is required to capture a small failure probability. If the Monte Carlo method is executed instead according to Eq. (17), then statistical sampling on strength is not needed since it is not an integration variable. Consequently, the size of the sample can be greatly reduced in cases where the failure probability is low. Eq. (17) is also more desirable for the numerical integration approaches since it does not require integration over strength variables. A further advantage of the use of Eq. (17) is that a closed-form integration on the strength variables is more exacting than the use of discrete strength values. Therefore, the desired approach to calculating failure probabilities, whether using the Monte Carlo or numerical integration approaches, is to use Eq. (17) implemented according to the method of Section 4. It is noted that the stress function $g(\nu_j, \nu_k, \ldots)$ must be continuous (integrable) across the full range (generally $-4D$ to $4D$) of all parameters ν_i through the time over which the analysis is conducted. When using the Monte Carlo approach in the method of Section 4, the parameters for each particle analyzed are selected by statistical sampling. There is, though, no statistical sampling of the coating layer strengths. Using Eq. (17) to determine failure probabilities with the fast, full, and Monte Carlo integration approaches is demonstrated in two sample cases below.

7. Application to sample cases

The integration methods developed herein for calculating fuel particle failure probabilities were applied to two cases of particles in a fuel pebble to demonstrate that they produce results that agree with results from the Monte Carlo approach. The input parameters considered in these cases are summarized in Table 1. These constitute only hypothetical cases intended to test the methodology, not to represent actual fuel particle batches. In these cases, a period of irradiation is followed by a post-irradiation heatup with boundary temperatures as shown in Table 2. The post-irradiation temperatures varied significantly over a very short time. The basic differences between the cases are that Case 2 has a higher fluence, irradiation temperature, and burnup than Case 1.

The strengths of the IPyC and SiC layers were treated with Weibull statistical distributions having the characteristic strengths and moduli shown in the table. (Ref. [10] gives a description of these parameters.) The characteristic strengths shown were used to determine mean strengths for the IPyC and SiC layers that corresponded to stress distributions resulting from internal pressure loading. (Ref. [12] gives a description of the method used to determine the mean strength for a stress distribution.) In Case 1, the mean strengths for stress distributions in the SiC that resulted from a cracked IPyC and from a debonded SiC were arbitrarily set to values of 1544 MPa and 1000 MPa, respectively. In Case 2, these mean strength values were arbitrarily set to 544 and 500 MPa, respectively.

As shown in Table 1, five input parameters were given statistical variations in these analyses, i.e. IPyC thickness, SiC thickness, IPyC BAF, IPyC/SiC bond strength, and particle temperature. The first four of these parameters were treated with a Gaussian distribution having the mean values and standard deviations shown in the table. A time-dependent global temperature distribution was calculated across the radius of the pebble. The temperatures of the particles, then, varied with radial position in the pebble. The distribution used to represent the radial density of particles in the pebble was $3r^2/R^3$, where r is the radial position of a particle and R is the outside radius of the fueled region of the pebble.

Three particle failure mechanisms were considered in these calculations, i.e. failure of the SiC due to (1) internal pressure loading,

Table 1
Input parameters for failure probability calculations.

Parameter	Units	Mean value Case 1	 Case 2[a]	Standard deviation
Kernel diameter	μm	497	Same	
Buffer thickness	μm	94	Same	
IPyC thickness	μm	41	Same	4
SiC thickness	μm	36	Same	1.7
OPyC thickness	μm	40	Same	
IPyC density	Mg/m^3	1.90	Same	
OPyC density	Mg/m^3	1.88	Same	
IPyC BAF		1.053	Same	0.01
OPyC BAF		1.019	Same	
Weibull characteristic strength, IPyC	MPa $\mu m^{3/9.5}$	1316.7	Same	
Weibull modulus, IPyC		9.5	Same	
Weibull characteristic strength, SiC	MPa $\mu m^{3/8.02}$	9640	Same	
Weibull modulus, SiC		8.02	Same	
Pyrocarbon Poisson's ratio in creep		0.5	Same	
Oxygen to uranium ratio	Atom ratio	2	Same	
Carbon to uranium ratio	Atom ratio	0	Same	
End-of-life fluence	10^{25} n/m^2 $E > 0.18$ MeV	5.00	6.82	
Ambient pressure	MPa	0.1	Same	
Boundary temperature during irradiation	K	1113.2	1348.0	Distributed according to the geometry of a pebble
IPyC/SiC bond strength	MPa	30	32	4
Burnup	% FIMA	11.1	13.9	

[a] The irradiation conditions of Case 2 were set to be more severe than those of Case 1.

Table 2
Post-irradiation boundary temperatures.

Case 1		Case 2	
Fluence (10^{25} n/m^2, $E > 0.18$ MeV)	Temperature (K)	Fluence (10^{25} n/m^2, $E > 0.18$ MeV)	Temperature (K)
5.0	1113.2	6.82	1348
5.0+	999.667	6.82+	1089.67
5.0+	786.333	6.82+	831.34
5.0+	573	6.82+	573
5.0+	573	6.82+	573
5.0+	823	6.82+	823
5.0+	1073	6.82+	1073
5.0+	1323	6.82+	1323
5.0+	1323	6.82+	1323
5.0+	1523	6.82+	1523
5.0+	1523	6.82+	1523
5.0+	1698	6.82+	1698
5.0+	1873	6.82+	1873
5.0+	1873	6.82+	1873

(2) cracking of the IPyC layer, and (3) partial debonding of the IPyC from the SiC. Though no asphericity effects were considered, pressure vessel failures occur because of the significant internal pressures that occur during heatup following irradiation. The failure probabilities in all cases were calculated using the approaches described in Sections 3 through 6, which entail implementing Eq. (17) as described in Section 4.

Results for Case 1, where only two of the five input parameters (i.e., temperature and bond strength) were varied statistically, are presented in Table 3. In these calculations, the other three parameters were set to their mean values. The magnitudes of the calculated probabilities are not as important as how well the results compare for the three integration methods. Because there are only two integration variables, there is no distinction between the fast and full integration approaches and their results are identical. The results for the fast and full methods compare very closely with those from the Monte Carlo approach where 100,000 particles were sampled. The Monte Carlo method was able to capture very small failure probabilities in this case with only a 100,000-particle sample because the IPyC and SiC strengths were not treated as integration variables. Had these been treated as integration variables, the sample size required to capture these small probabilities would have been several orders of magnitude larger. The execution time for the fast and full integration solutions (which are identical in this case) was about 4 s, while that of the Monte Carlo solution was about 13 min.

Results for Case 1, where all five input parameters were varied statistically, are presented in Table 4. The results for the fast and full integration approaches are identical to the four digits shown,

Table 3
Results for Case 1, two-variable case.

Variables: temperature, bond strength			
Probability of	Integration method		
	Fast	Full	Monte Carlo (100,000 particles)
IPyC cracking	0.2125	0.2125	0.2125
IPyC debonding	0.7820	0.7820	0.7820
SiC failure due to IPyC cracking	5.050×10^{-8}	5.050×10^{-8}	5.037×10^{-8}
SiC failure due to IPyC debonding	8.003×10^{-9}	8.003×10^{-9}	7.986×10^{-9}
SiC failure due to internal pressure	7.602×10^{-6}	7.602×10^{-6}	7.592×10^{-6}
SiC failure, total	7.661×10^{-6}	7.661×10^{-6}	7.650×10^{-6}
Execution time	4 s	4 s	13 min

Table 4
Results for Case 1, five-variable case.

Variables: temperature, bond strength, IPyC BAF, IPyC thickness, SiC thickness			
Probability of	Integration method		
	Fast	Full	Monte Carlo (100,000 particles)
IPyC cracking	0.2058	0.2058	0.2059
IPyC debonding	0.7621	0.7621	0.7621
SiC failure due to IPyC cracking	7.110×10^{-8}	7.110×10^{-8}	7.062×10^{-8}
SiC failure due to IPyC debonding	1.007×10^{-8}	1.007×10^{-8}	1.001×10^{-8}
SiC failure due to internal pressure	1.883×10^{-5}	1.883×10^{-5}	1.890×10^{-5}
SiC failure, total	1.891×10^{-5}	1.891×10^{-5}	1.898×10^{-5}
Execution time	15 s	28.5 min	13 min

Table 5
Results for Case 2, two-variable case.

Variables: temperature, bond strength				
Probability of	Integration method			
	Fast	Full	Monte Carlo (100,000 particles)	Monte Carlo (1,000,000 particles)
IPyC cracking	0.01693	0.01693	0.01689	0.01690
IPyC debonding	0.07574	0.07574	0.07548	0.07553
SiC failure due to IPyC cracking	1.799×10^{-5}	1.799×10^{-5}	1.787×10^{-5}	1.788×10^{-5}
SiC failure due to IPyC debonding	5.502×10^{-5}	5.502×10^{-5}	5.456×10^{-5}	5.462×10^{-5}
SiC failure due to internal pressure	0.06202	0.06202	0.06209	0.06204
SiC failure, total	0.06209	0.06209	0.06216	0.06212

Table 6
Results for Case 2, five-variable case.

Variables: temperature, bond strength, IPyC BAF, IPyC thickness, SiC thickness				
Probability of	Integration method			
	Fast	Full	Monte Carlo (100,000 particles)	Monte Carlo (1,000,000 particles)
IPyC cracking	0.01748	0.01748	0.01741	0.01745
IPyC debonding	0.11870	0.11877	0.11802	0.11872
SiC failure due to IPyC cracking	4.538×10^{-5}	4.577×10^{-5}	4.503×10^{-5}	4.571×10^{-5}
SiC failure due to IPyC debonding	1.654×10^{-4}	1.667×10^{-4}	1.640×10^{-4}	1.664×10^{-4}
SiC failure due to internal pressure	0.06593	0.06593	0.06599	0.06589
SiC failure, total	0.06614	0.06614	0.06620	0.06610

indicating that the fast integration approximation gave a very good estimate of the failure probability. Again, the results also agree well with those from the Monte Carlo approach. Because of the increase in integration variables, the execution time for the fast integration method increased to 15 s, while that of the full integration method increased to 28.5 min. The execution time for the Monte Carlo solution remained at 13 min. These execution times demonstrate the advantage of the fast integration method.

Tables 5 and 6 show corresponding results for Case 2. In this case, failure probabilities were higher due to more severe input conditions. Again, the calculated failure probabilities among the three integration methods agree closely. Results also show that increasing the Monte Carlo sample size from 100,000 to 1,000,000 particles further improves this agreement. The execution times for Case 2 were similar to those of Case 1. The execution time for a 1,000,000-particle Monte Carlo sample is about 10 times that of a 100,000-particle sample.

8. Conclusions

An alternative approach to the traditional Monte Carlo method has been developed for calculating failure probabilities for TRISO-coated fuel particles in the PARFUME fuel performance modeling code. In this approach, the failure probability is formulated in terms of an integral. The integral can be evaluated with either the Monte Carlo method or a direct numerical integration over the range of variation of all statistically varying parameters that characterize a batch of particles. This numerical integration can be much faster than the Monte Carlo approach, and provides an independent means of verifying that failure probabilities are calculated correctly in a comprehensive performance code.

Numerical integration can require long execution times when a large number of statistically varying parameters are considered in the failure probability calculation. Therefore, an approximation to full integration has been developed that involves subintegrals having no more than two integration variables. This approach, referred to as the fast integration approach, can greatly reduce the execution times required to calculate failure probabilities with only a minimal loss of accuracy.

In sample cases analyzed, both the fast and full integration approaches produced results that are in close agreement with the Monte Carlo approach. It was also shown that the fast integration method can save substantial computational time relative to the full integration and Monte Carlo approaches, which is a strong advantage of this method.

A modification to the traditional Monte Carlo method can greatly reduce the required particle sample size when calculating a small failure probability. This modification entails treating a coating layer strength as a Weibull statistical parameter but not as an integration variable. Using this approach in the sample calculations, the Monte Carlo results compared very well with results from the numerical integration methods.

All three integration methods have been incorporated into the PARFUME code.

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