Random Particle Generation for a Failure Analysis on the Coated Fuel Particles of an HTR

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1. Introduction

A large number of coated fuel particles (CFPs) are contained in a fuel element of a high temperature reactor (HTR). The integrity of CFPs greatly affects the characteristics of the fission product migration in a fuel element. It should be evaluated how various mechanical and chemical hazards deteriorate the integrity of the CFPs during the operation of an HTR.

The CFP usually consists of a fuel kernel in its innermost center and four surrounding coating layers such as a low-density pyrocarbon called buffer, an inner high-density pyrocarbon (IPyC), a silicon carbide (SiC), and an outer high-density pyrocarbon (OPyC) from its inside part. The sizes and material properties of the CFP components are statistically variable. Those statistical variations must be considered when doing a performance analysis on a batch of CFPs.

This study describes how to generate random CFPs for a fuel performance analysis, and shows an example of the random particle calculations.

2. Random Particle Generation

The CFP quantities with normal distribution are the diameter of a kernel, the thickness and density of a buffer, the thicknesses, densities, and bacon anisotropy factors (BAFs) of coating layers. The CFP quantities with Weibull distribution are the strengths of coating layers. They are stochastically independent of each other. They can be generated using uniform deviates whose range is from 0 to 1, where uniform deviates are just random numbers that come from a uniform distribution.

2.1. Generating normal deviates from uniform deviates

Two independent standard normal distribution deviates are produced from two independent uniform distribution deviates using the Box-Muller method [1]:

$$y_1 = \sqrt{-2\ln R^2 / R^2} \left(2x_1 - 1 \right), \tag{1}$$

$$y_2 = \sqrt{-2\ln R^2 / R^2} \left(2x_2 - 1 \right), \tag{2}$$

where $R^2 = (2x_1 - 1)^2 + (2x_2 - 1)^2$, y = the standard normal distribution deviate \in (- ∞ , ∞), and x = the uniform distribution deviate \in (0, 1). A usual random number generator (RNG) produces x_1 and x_2 .

The CFP quantities with normal distribution can be calculated using a standard normal distribution deviate *y*:

$$t = \bar{t} + y \cdot STD_t , \qquad (3)$$

where \bar{t} and STD_t = the mean value and standard deviation of t, respectively, that are experimentally given.

2.2. Generating Weibull deviates from uniform deviates

The random variable y with a probability distribution f(y) is related to the uniform random variable x on (0, 1) by the fundamental transformation law of probabilities [2]:

$$f(y) = \frac{dx}{dy},\tag{4}$$

where f = the probability density function of y. Solving Eq. (4) gives the random variables x and y:

$$x = F(y) = \int_{-\infty}^{y} f(z) dz , \qquad (5)$$

$$y = F^{-1}(x)$$
, (6)

where F = the cumulative distribution function of y, and F^{-1} = the inverse function of F. The random variable y is expressed by Eq. (7) if it is in a Weibull distribution of Table I [3]:

$$y = \lambda [-ln(1-F)]^{1/m}.$$
 (7)

A usual RNG produces F on (0, 1).

The probability distribution for the strength of a CFP coating layer is defined by a Weibull distribution. Table II shows the strength distributions according to the scale parameter of a Weibull distribution. Fig. 1 shows the variation of random Weibull strength deviate over uniform deviate.

$$f(y) = \begin{cases} \frac{m}{\lambda^m} y^{m-1} e^{-(y/\lambda)^m} &, y \ge 0\\ 0 &, y < 0 \end{cases},$$

$$F(y) = \begin{cases} 1 - e^{-(y/\lambda)^m} &, y \ge 0\\ 0 &, y < 0 \end{cases},$$

$$y_{mean} = \lambda \Gamma(1 + 1/m)$$

$$y_{med} = \lambda (ln2)^{1/m}$$

$$V_y = \lambda^2 \{ \Gamma(1 + 2/m) - [\Gamma(1 + 1/m)]^2 \}$$





Fig. 1. Random Weibull strength deviate (case 1: $\lambda = s_{med}/(\ln 2)^{1/m}$, case 2: $\lambda = s_{mean}/\Gamma(1+1/m)$)

2.3. Generating uniform deviates

The uniform deviates are generated using a RNG. Some useful RNGs were developed in Ref. [2]. The authors of the reference recommend that you use *ran2* if you are going to generate more than 100,000,000 random numbers in a single calculation. The *ran2* has much longer period. It is initialized using a negative integer seed number, and it produces a different random number every time it receives a different seed number.

In a failure analysis on a batch of CFPs of an HTR, the number of *ran2* calls is the number of CFPs multiplied by the total number of the stochastic quantities of a CFP. Because of the large number of RNG calls, it is highly recommend to use a parallel computing to perform the failure analysis. In an MPI parallel computing using a block distribution [4], the generation of random particles is appropriately distributed to the processors involved. The seed number in the calculation part of each processor can be - $1000 \times (myrank+1)$, where *myrank* is a rank that is a processor identification number between zero and the number of processors involved minus one. The random numbers thus generated are all statistically independent of each other.

3. Random Particle Calculation

It is assumed in this example calculation of random particles that the total number of particles is ten, and only the thickness and strength of a coating layer are statistically variable. Table III lists the statistical thicknesses and strengths of the coating layers of a CFP. Table IV lists ten random particles calculated. The thicknesses of a CFP coating layer are statistically independent of each other and the strengths are the same.

Table III: An example of CFP stochastic variables

Conting laware	Thickness (um)	Strength		
Coating layers	$\Gamma \Pi CKIESS (\mu \Pi)$	т	s _{med} (MPa)	
IPyC	40±0.04	9.5	350	
SiC	35±0.035	6	770	
OPyC	40±0.04	9.5	350	

Table	IV	Calcui	lated	ten	random	CFPs
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No	Thickness (µm)		Strength (MPa)			
	IPyC	SiC	OPyC	IPyC	SiC	OPyC
1	40.094	35.012	39.890	331.858	925.776	386.294
2	39.528	34.387	40.053	277.155	921.432	319.319
3	39.893	35.376	39.911	347.581	724.465	398.108
4	39.885	35.088	39.317	244.809	738.773	368.401
5	39.278	34.875	39.861	384.857	603.836	198.999
6	40.234	34.774	40.622	375.566	902.519	335.816
7	39.618	35.275	40.508	331.89	597.887	272.041
8	39.559	35.259	39.745	351.084	808.441	198.516
9	40.641	34.900	40.062	353.203	955.375	342.118
10	40.282	35.494	40.661	283.092	651.206	363.768

4. Summary

A method generating random CFPs has been developed that use only a random number generator during a fuel performance analysis. The method produces statistical properties of a batch of CFPs using a uniform random number produced by a usual random number generator. The method is utilized in a statistical fuel performance analysis on a batch of CFPs.

ACKNOWLEDGEMENTS

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIP) (No. 2018M2A8A1084251).

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Scale parameter λ	$\frac{S_{med}}{(ln2)^{1/m}}$	$\frac{S_{mean}}{\Gamma(1+1/m)}$		
f(s)	$ \begin{cases} \frac{m \ln 2}{s_{med}} \left(\frac{s}{s_{med}}\right)^{m-1} e^{-\ln 2 \left(s/s_{med}\right)^m} & , s \ge 0 \\ 0 & s < 0 \end{cases} $	$\begin{cases} \frac{m[\Gamma(1+1/m)]^m}{s_{mean}} \left(\frac{s}{s_{mean}}\right)^{m-1} e^{-[\Gamma(1+1/m)]^m (s/s_{mean})^m} , s \ge 0 \\ 0 \qquad s < 0 \end{cases}$		
F(s)	$\begin{cases} 1 - e^{-\ln 2 (s/s_{med})^m} & , s \ge 0\\ 0 & , s < 0 \end{cases}$	$\begin{cases} 1 - e^{-[\Gamma(1+1/m)]^m (s/s_{mean})^m} &, s \ge 0\\ 0 &, s < 0 \end{cases}$		
Smean Or Smed	$s_{mean} = \frac{s_{med}}{(ln2)^{1/m}} \Gamma(1+1/m)$	$s_{med} = s_{mean} (ln2)^{1/m} / \Gamma(1+1/m)$		
Vs	$\frac{s_{med}^2}{(ln2)^{2/m}} \{ \Gamma(1+2/m) - [\Gamma(1+1/m)]^2 \}$	$\frac{s_{mean}^2}{[\Gamma(1+1/m)]^2} \{ \Gamma(1+2/m) - [\Gamma(1+1/m)]^2 \}$		
S	$S_{med} \left[-\frac{ln(1-F)}{ln2} \right]^{1/m}$	$S_{mean} \left[-\frac{ln(1-F)}{[\Gamma(1+1/m)]^m} \right]^{1/m}$		
$s =$ the strength (MPa), $s_{med} =$ the median strength (MPa) > 0, $s_{mean} =$ the mean strength (MPa) > 0, $m =$ the shape parameter > 0,				
f = the Weibull probability density function of s , F = the Weibull cumulative distribution function of s , V_s = the variance of s				

Table II: Weibull distribution for the strength of a CFP coating layer

f = the Weibull probability density fu (MPa)² > 0, Γ = the gamma function.