A Constrained Sampling Methodology for TRISO Microspheres with Continuous Distributions of Diameters

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INTRODUCTION

The Fort St. Vrain (FSV) High Temperature Gas Reactor (HTGR) consisted of a mixture of two TRISO fuel particles: fissile particles containing fuel kernels with highly enriched uranium and thorium, and fertile fuel particles consisting of fuel kernels with thorium. There were small and large kernels for both fissile and fertile particles [1-2]. Table I lists the properties of the FSV fuel particles. The average Th:U weight ratio was known for the mixture of fissile and fertile particles, but there was considerable uncertainty in the diameters of the fissile and fertile particles which were only known within the relatively large diameter ranges shown in Table I. In particular, the distributions of kernel diameters over these diameter ranges were not known and even the average diameters were not known, since detailed fabrication records do not exist for the FSV fuel. In order to assess the effect of these uncertainties, a study was undertaken to assess the sensitivity of the neutronic analysis of the FSV fuel to the uncertainty in the kernel diameter distributions of the TRISO fissile and fertile fuel particles.

A constrained sampling methodology was developed that allowed arbitrary probability density functions (PDFs) over the given diameter ranges, but which preserved specified uranium and thorium fuel loadings and overall packing fraction, thus allowing an assessment of the sensitivity of the neutronic analysis to the choice of kernel diameter PDF.

The results indicate that the kernel diameter PDF is not a sensitive quantity for the neutronic analysis of a FSV fuel compact but the methodology used to arrive at this conclusion may have application beyond this study.

Table I. FSV TRISO Particle Geometry Data (μm)

	Fissile		Fertile	
Dimensions	**Small**	**Large**	**Small**	**Large**
Kernel Diameter	100-175	175-275	300-450	450-600
Buffer Coating	50	50	50	50
PyC Coating	20	20	20	20
SiC Coating	20	20	20	20
PyC Coating	30	40	40	50
Total Coating	120	130	130	140

FUEL PARTICLE CONSTRAINTS

Since the average uranium and thorium fuel loadings, the average Th:U weight ratio in the fissile kernel, and the overall packing fraction (58%) were known, these quantities were treated as constraints for the sensitivity studies for the kernel diameter PDFs.

The methodology for imposing the constraints on the thorium and uranium loadings and the overall Th:U ratio was based on prior knowledge of an acceptable fuel configuration consisting of single diameter kernels for each of the four fuel types given in Table I. The single diameter selected for each of the particle types was the midpoint diameter given for the diameter range given in Table I. By construction, this reference system satisfied the constraints but was not necessarily an accurate model since all kernels had the same diameter for a given particle type.

CONSTRAINED SAMPLING METHODOLOGY

The goal is to sample kernel diameters from arbitrary probability density functions (PDFs) for each of the four particle types, but satisfying the known packing factor and fuel loading constraints. Since the true kernel diameter PDFs are not known, several different PDFs were chosen to assess the sensitivity of the results to the kernel diameter PDF. The sampling methodology was developed for uniform, piecewise polynomial, and Gaussian PDFs, and is described below.

Piecewise polynomial PDFs

The PDFs $f_1(D)$ and $f_2(D)$ were constrained to peak at D=x and monotonically go to zero at D=a and D=b, respectively, where [a,b] is the diameter range from Table I for the particle type and x=(a+b)/2 is the midpoint of the corresponding diameter range. Figure 1 gives a notional description of the kernel diameter PDFs $f_1(D)$ and $f_2(D)$. The variables y_1 and y_2 are local variables for the two PDFs.

Now define the following PDF for kernel diameters over the full range [a,b]:

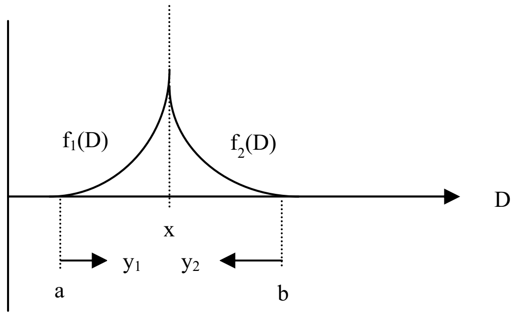

Figure 1. Piecewise Polynomial Kernel Diameter PDFs

$$f(D) = Pf_1(D) + (1-P)f_2(D) \tag{1}$$

where P is the probability that the diameter is in the lower range. If one only wants to preserve the kernel volume, it is sufficient to require $\overline{D} = x$, which yields the following expression for P in terms of the average diameters for the two ranges:

$$P = \frac{\overline{D_2^3} - x^3}{\overline{D_2^3} - \overline{D_1^3}} \tag{2}$$

Since the average kernel volume is preserved, this guarantees that the fuel loadings are preserved. Kernels are sampled until the fuel loading constraint is satisfied, yielding (statistically) the same number of kernels for each particle type as the reference system.

However, this method does not preserve the packing fraction because larger kernels will have proportionally less coating volume per kernel volume than smaller kernels, and this will result in a smaller packing fraction for the same kernel volume. This can be addressed by requiring both the total sampled kernel volume and the resultant total coating volume be the same as in the reference system [3]:

$$N\frac{1}{6}\pi x^3 = N'\frac{1}{6}\pi\left[\overline{D^3}\right] \tag{3}$$

$$N\frac{1}{6}\pi\left[(x+2t)^3 - x^3\right] = N'\frac{1}{6}\pi\left[\overline{(D+2t)^3 - D^3}\right] \tag{4}$$

where t is the total coating thickness, N is the number of single diameter kernels of diameter x in the reference system, N' is the number of sampled kernels, and the overbars represent averages with respect to the PDF f(D).

Gaussian PDFs

A slightly different approach was taken for the Gaussian kernel diameter PDF. A single Gaussian was chosen for the entire diameter range [a,b], eliminating the unlikely spike in the PDF near D=x for the piecewise polynomial PDFs. Since a Gaussian PDF has two parameters, the mean μ and standard deviation σ, the standard deviation was chosen using the reasonable assumption that the diameter range be four standard deviations wide independent of the location of the mean, or $\sigma = (b-a)/4$. Preserving both the kernel and coating volumes, as shown in Eqs. (3) and (4), resulted in a nonlinear equation that could be solved numerically for the mean μ [4].

GENERATION OF STOCHASTIC MIXTURES

The stochastic fuel compact model is based on methodology developed by Li and Ji at Rensselaer Polytechnic Institute [5]. This methodology, which was originally developed to pack spheres in a pebble bed reactor while accounting for interparticle forces such as friction and wall forces, was adapted to pack TRISO fuel particles in a cylindrical fuel compact. The methodology packs kernels up to a 60% packing fraction with its unique "settling" approach, where interparticle forces and wall forces allow an initial overlapping particle distribution to approach a realistic distribution that has no overlap and is entirely within the container, which in this case is a finite cylinder. It also has the capability to pack a fuel compact with different sized particles including those with a continuous distribution of kernel diameters sampled from PDFs, which was needed for this study.

The particle packing code writes out MCNP5 [6] input files describing the coordinates of all the TRISO particles in the fuel compact, which is a cylinder of radius 0.625 cm and height 5.0 cm. MCNP5 was used to model a fuel compact cell, consisting of the fuel compact surrounded by a hexagonal graphite region representing its share of the graphite in a fuel block. The fuel compact cell has reflecting boundary conditions on all surfaces.

NUMERICAL RESULTS

Verification of sampling methodology

Table II gives the results of sampling using uniform, piecewise linear through quartic polynomial, and Gaussian PDFs for each of the four particle types in Table II. The only results shown in Table II are the numbers of sampled particles of each type because the packing fractions and fuel volumes were essentially the same as the reference system, with deviations less than .2% for all cases, indicating that the sampling methodology was correct. It should be noted that only one geometry realization was sampled, and each particle type is sampled independently using the methodology described above. The resultant fuel compact consists of four different particle types, with the number of each given in Table II.

Table II. Constrained Sampling Results

	Number of Kernels			
	Fissile		Fertile	
PDF	**Small**	**Large**	**Small**	**Large**
Constant	56,025	4,738	10,814	1,020
Linear	55,231	4,691	10,659	1,030
Quadratic	55,142	4,660	10,579	1,016
Cubic	54,991	4,665	10,608	1,014
Quartic	54,904	4,662	10,561	1,018
Gaussian	55,357	4,717	10,710	1,025
# kernels in reference 4-particle system	54,659	4,637	10,542	1,013

Results of Sensitivity Studies

The fuel compacts were modeled in MCNP5 with 10,000 source particles per cycle with 400 active cycles. Table III contains the results, where the quadratic PDF was chosen as the reference case. As can be seen, the observed eigenvalue differences are within a two standard deviation (~ 60 pcm) uncertainty.

Table III. MCNP5 Results for Fuel Compact Cell

PDF	keff	σ (pcm)	Difference (pcm)
Uniform	1.18311	32	43
Linear	1.18275	32	7
Quadratic	1.18268	33	0
Cubic	1.18275	33	7
Quartic	1.18314	30	46
Gaussian	1.18218	32	-50

CONCLUSIONS

Given the substantial differences in the PDFs, ranging from a uniform distribution over the diameter range to a Gaussian, this deviation is considered to be relatively small. Therefore, the eigenvalues for the FSV fuel compact cells are relatively insensitive to the choice of kernel diameter PDFs for the fuel compact cell cases.

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