

On Using Code Emulators and Monte Carlo Estimation to Predict Assembly Attributes of Spent Fuel Assemblies for Safeguards Applications

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Abstract—*The quantification of the plutonium mass in spent nuclear fuel assemblies is an important measurement for nuclear safeguards practitioners. A program is well underway to develop nondestructive assay instruments that, when combined, will be able to quantify the plutonium content of a spent nuclear fuel assembly. Each instrument will quantify a specific attribute of the spent fuel assembly, e.g., the fissile content. In this paper, we present a Monte Carlo–based method of estimating the mean and distribution of some assembly attributes. An MCNPX model of each instrument has been created, and the response of the instrument was simulated for a range of spent fuel assemblies with discrete parameters (e.g., burnup, initial enrichment, and cooling time). The Monte Carlo–based method interpolates between the modeled results for an instrument to emulate a response for parameters not explicitly modeled. We demonstrate the usefulness of this technique in applying the technique to six different instruments under investigation. The results show that this Monte Carlo–based method can be used to estimate the assembly attributes of a spent fuel assembly based upon the measured response from the instrument.*

I. INTRODUCTION

Quantifying the plutonium mass in spent nuclear fuel assemblies is a problem of concern to the International Atomic Energy Agency (IAEA). Ensuring that no nuclear material is maliciously diverted from an assembly requires close monitoring of the spent fuel assemblies after their removal from nuclear reactors around the world.

The IAEA already monitors spent nuclear fuel reprocessing plants and storage facilities, typically by using cameras and visual inspections. In addition, gamma and neutron measurements are taken, but the operator's declaration of the parameters (i.e., burnup, initial enrichment, and time since removed from a reactor) are used as a reference to the measurements. These radiation measurements and visual inspection cannot measure the plutonium content of the spent nuclear fuel assembly; they can only detect some types of changes to the assembly.

Under the sponsorship of the Next Generation Safeguards Initiative (NGSI), an effort is underway¹ to mea-

sure the plutonium content of spent nuclear fuel assemblies without relying on the operator's declaration of the operating parameters of the nuclear reactor and without previous measurements of the spent nuclear fuel assembly. This effort is focusing on a variety of nondestructive assay (NDA) techniques that can be used in a variety of surroundings (e.g., air, water, and bated water) and are fast enough to not be a burden on the operational procedures in a nuclear reactor, spent fuel storage, or reprocessing facility. A few of these techniques will be integrated into one instrument to allow a safeguards inspector to measure the mass of plutonium in a spent nuclear fuel assembly and determine whether spent fuel pins have been removed from the assembly.

The program to develop a combination of instruments—integrated in such a way as to quantify the mass of plutonium—is, recognizably, a grand challenge.² We are currently investigating 14 different NDA instruments as part of this program. No single instrument can measure the plutonium mass directly, but each instrument provides a measurement that contributes a piece of the puzzle necessary to quantify the plutonium mass.

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Some of the quantities that can be measured from an individual measurement are the average burnup of an assembly; the ratio of the mass of the fissile isotopes to the mass of the fertile isotopes (fissile/fertile ratio); the ratio of the mass of elemental uranium to the mass of elemental plutonium (elemental U/Pu ratio); the mass of ^{235}U to the mass of ^{239}Pu ($^{235}\text{U}/^{239}\text{Pu}$ ratio); and a combination of the masses of the three fissile isotopes ^{235}U , ^{239}Pu , and ^{241}Pu (fissile content).

In order to determine the response of each of the 14 NDA techniques to spent nuclear fuel assemblies, we have created an MCNPX model³ of each instrument. A library of spent fuel assemblies has been created⁴ that contains a wide variety of spent fuel assemblies. The models are 17×17 , pressurized water reactor assemblies with assembly parameters of 15, 30, 45, or 60 GWd/t U burnup; 2, 3, 4, or 5 wt% ^{235}U initial enrichment; and 1-, 5-, 20-, or 80-yr cooling time. The parameters of burnup, initial enrichment, and cooling time define the mass and spatial distribution of the many isotopes in the spent fuel assembly.

The combination of assembly parameters of burnup, initial enrichment, and cooling time give 64 different models of spent nuclear fuel assemblies that are representative of spent nuclear fuel assemblies in existence in nuclear reprocessing, storage facilities, or reactor sites. The models are combined with the geometry of the detectors, and a fixed-source MCNPX calculation is performed with a variety of tallies to estimate the response of the detectors used in the technique. The detector re-

sponses can then be used to estimate the measured quantity of the technique. The MCNPX simulations can be performed with the assembly surrounded by either water, borated water (2200 ppm), or air.

Each of the 14 NDA instruments has some detector response that changes with some attribute of the assembly (e.g., fissile content, elemental U/Pu ratio, etc.). The goal for each instrument is to accurately predict an assembly attribute for a given detector response. One detector may measure neutrons while the instrument response scales with the fissile content. Another detector may preferentially measure delayed neutrons that scales with the $^{235}\text{U}/^{239}\text{Pu}$ ratio. Both the fissile content and $^{235}\text{U}/^{239}\text{Pu}$ ratio are assembly attributes. Though an individual MCNPX simulation can estimate the detector response and can estimate or calculate a particular assembly attribute, it can be computationally expensive. However, a single simulation cannot estimate a *distribution* of assembly attributes for a measured detector response. Furthermore, one MCNPX simulation estimates the detector response from a single set of parameters defining a spent fuel assembly, and there can be many sets of parameters that produce the same detector response.

To illustrate, we plot in Fig. 1 a typical detector response against an assembly attribute. These are the results of simulating one of our instruments using the 64 spent fuel assembly models surrounded by water. The colors in Fig. 1 represent the burnup parameter, and the marker shape represents the initial enrichment. (Note

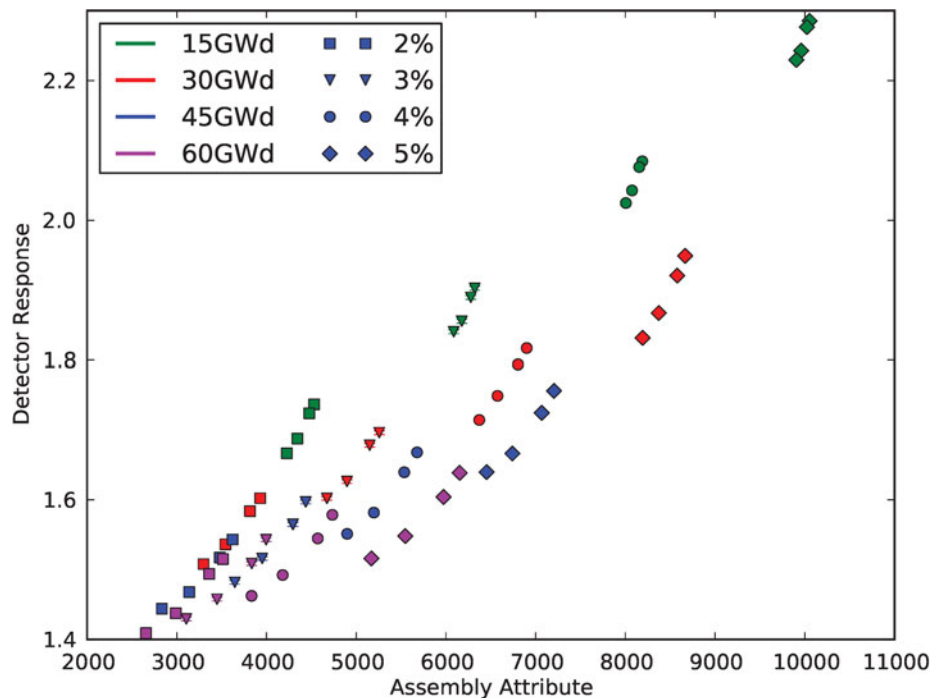


Fig. 1. Sample data showing detector response scaling with assembly attribute.

that the remaining figures are not shown in color, but in grayscale. The burnup value for each result should be clear from the context.) The difference in cooling time is not explicitly shown, but it is known that the assembly attribute decreases as the cooling time increases. Error bars arising from using a finite number of MCNPX histories are shown in Fig. 1 (and in all the figures of this paper) but are smaller than the plot markers. The statistical uncertainty (the standard deviation of the reproducibility of the MCNPX results) in these calculations is $\sim 0.2\%$ relative to the true value. If a measurement was made and the detector gave a response of 1.600 ± 0.008 , there are no fewer than five assemblies that would give the same detector response, and each has a different value for the assembly attribute such as ^{235}U or elemental Pu mass. As well, there are many additional assemblies not specifically modeled that would have the same detector response, e.g., a spent fuel assembly with 30 GWd/t U, 2.5 wt% ^{235}U initial enrichment, and 5-yr cooling time parameters. We see, therefore, the difficulty in using the measured detector response to predict the assembly attribute for an unknown spent fuel assembly.

This paper reports on a Monte Carlo–based method developed to predict certain assembly attributes from a measured detector response. The method relies on explicit modeling of the detector response for a variety of spent fuel assemblies for which the assembly attribute is known or can be estimated in the MCNPX simulation. This Monte Carlo method of estimating assembly attributes from modeled data requires interpolation between the modeled data points and is akin to emulating MCNPX simulations. In Sec. II we discuss the emulation of MCNPX simulations and the interpolation between explicitly simulated results. We also introduce the Monte Carlo–based method of estimating the assembly attributes.

We present some numerical results in Sec. III for several of the NDA techniques that we have simulated to demonstrate the effectiveness of the Monte Carlo method. Finally, in Sec. V we draw some conclusions and discuss future work.

II. CODE EMULATION AND MONTE CARLO ESTIMATES

In each of the instruments being explored as part of the effort to quantify the plutonium content of spent nuclear fuel assemblies, some assembly attribute is desired from some measured detector response. We only have the detector response (e.g., total neutron count), and we must infer some assembly attribute (e.g., fissile content). A one-to-one relationship between the detector response and assembly attribute is ideal as the assembly attribute mean and distribution would be known exactly from the measured detector response and its associated uncertainty.

In dealing with the complexity of spent nuclear fuel, we are not so fortunate as to work with such ideal assemblies. A spent nuclear fuel assembly has myriad dif-

ferent isotopes; some are fissile, and others have large absorption cross sections. Each isotope behaves differently as the assembly parameters change. Nevertheless, it is possible to estimate a mean value and distribution for a particular assembly attribute given a measured detector response. An example of the complexity in the relationship between the detector response and the assembly attribute is shown in Fig. 1. We can see that there are some general trends in the data with regard to burnup, initial enrichment, and cooling time. However, we do not have a one-to-one relationship between the detector response and the assembly attribute.

II.A. Interpolation and Code Emulation

The 64 models in our library of spent fuel assembly models span a wide range of burnup, cooling time, and initial enrichment and encompass most of the spent fuel assemblies expected in spent fuel storage facilities. Despite the broad range of assemblies modeled, it is in no way a complete set of spent nuclear fuel assemblies. Reactor operators are free to operate their reactor and burn their fuel to whatever specifications for which the reactor was designed; they are not limited to 15, 30, 45, or 60 GWd/t U. Similarly, it is unlikely that measurements of a spent fuel assembly will be made at exactly 1, 5, 20, or 80 yr since the assembly was removed from the reactor or that the assembly will initially have had an enrichment of 2, 3, 4, or 5 wt% ^{235}U .

Many of the simulations performed in our investigation of the 14 NDA techniques require >200 CPU hours to reduce the level of statistical uncertainty in our calculations to acceptable values. This is in addition to computer time required to create the assembly model. The computational expense of performing such a simulation is too great to be used for every measurement of a spent fuel assembly.

Instead of running MCNPX for every measured spent fuel assembly, the results of the simulations of the 64 spent fuel assembly models can be interpolated to create functions that map assembly parameters (e.g., burnup, initial enrichment, and cooling time) to the detector response and desired assembly attribute. Once mapping functions have been created, through interpolation of existing data, new data can be inferred from the mapping functions.

The idea of using knowledge of a system from previous measurements or simulations with specific parameters to predict a system response at other parameters is not new. In geostatistics this is known as “kriging”^{5,6} and has been used for decades. In their paper, Heitmann et al.⁷ call this code “emulation” as compared to the explicit “simulation” of the system response. To the best of our knowledge, this is the first time this has been applied to safeguards applications.

We have chosen to use radial basis functions to perform the interpolation between the 64 spent fuel assembly models and the detector response or assembly

attribute. The interpolating function is a linear function between the data points. Radial basis functions are well suited for applications⁸

1. that depend on many variables or parameters
2. that are defined by possibly very many data
3. for which the data are “scattered” in their domain.

We see from Fig. 1 that our data are many, scattered, and depend on many parameters; thus, radial basis functions meet the needs for our interpolation. In addition, radial basis functions are capable of performing interpolations in many dimensions.

For our work, two different three-dimensional mapping functions are needed:

$$D = M_D(B, E, C) \quad (1a)$$

and

$$P = M_P(B, E, C) \quad (1b)$$

where

B, E, C = burnup, initial enrichment, and cooling time, respectively. Together, these three parameters define an assembly model A .

M_D = mapping function from the assembly model to the detector response D

M_P = mapping function from the assembly model to the assembly attribute P .

II.B. Monte Carlo Estimate of Assembly Attributes

With the mapping functions defined, we can estimate the mean and distribution of an assembly attribute via a Monte Carlo-based method given a detector response. Typically, the detector response will be measured by an instrument in the field, and the assembly attribute must be inferred from the detector response. Since none of our NDA techniques have yet been built, all detector responses in this paper are the results of MCNPX simulations. Regardless of whether the detector response is measured or simulated, we refer to it as the measured detector response.

The mean assembly attribute can be calculated as

$$\bar{P} = \int_{\Delta B} \int_{\Delta E} \int_{\Delta C} R(D, \mu, \sigma) M_P(B, E, C) \times f(B, E, C) dC dE dB \quad (2)$$

where

$\Delta B, \Delta E, \Delta C$ = ranges of possible burnup, initial enrichment, and cooling time for the assembly, respectively

M_P = mapping function from assembly parameters to the assembly attribute [Eq. (1b)]

$f(B, E, C)$ = three-dimensional probability density function (pdf) defining the probability of each B, E , and C .

The function $R(D, \mu, \sigma)$ in Eq. (2) is the response function and is defined to be

$$R(D, \mu, \sigma) = e^{-(D-\mu)^2/2\sigma^2} \quad (3)$$

where μ and σ are the measured detector response and its standard deviation and D comes from Eq. (1a). The response is dependent on the assembly parameters B, E , and C . We can see that the response function ranges from 0, when D is infinitely far away from the measured detector response μ , to 1, when $D = \mu$. The response function serves to reduce the importance of assemblies with a simulated detector response far from the measured detector response.

To illustrate why we have included the response function, we refer again to Fig. 1 and suppose that our measured response is approximately 1.65. This measured response could be produced by an assembly with 45 GWd/t U burnup, 5 wt% ²³⁵U, and 80-yr cooling time, with an approximate assembly attribute value of 6500. However, any of the four assemblies with 15 GWd/t U burnup and 3 wt% ²³⁵U have a value for the assembly attribute close to 6500. The response function $R(D, \mu, \sigma)$ will have to be smaller for the assemblies with 15 GWd/t U burnup than the assemblies with 45 GWd/t U, and its contribution to \bar{P} is reduced.

The multidimensional integral in Eq. (2) can be estimated using a simple Monte Carlo integration⁹:

$$\hat{P} \approx \frac{1}{N} \sum_{k=1}^N R(D_k, \mu, \sigma) M_P(B_k, E_k, C_k) \quad (4)$$

where

B_k, E_k, C_k = random samples of burnup, initial enrichment, and cooling time that define a randomly sampled spent fuel assembly A_k

$D_k = M_D(B_k, E_k, C_k)$ = simulated detector response for A_k .

To calculate the distribution, or pdf, associated with \hat{P} , one can simply bin the individually sampled results and their weights and construct a frequency plot of the assembly attribute.

The values for the assembly parameters B_k, E_k , and C_k are randomly sampled from the pdf, $f(B, E, C)$. Without additional knowledge, we assume that these values are equally probable throughout the whole range of possible values, i.e., 15 to 60 GWd/t U, 2 to 5 wt% ²³⁵U, and 1 to 80 yr. The pdf, $f(B, E, C)$, would be defined as

$$f_{II} = \Pi_B \Pi_E \Pi_C \quad (5)$$

with Π_X being the uniform pdf of picking parameter X over its appropriate range:

$$\Pi_B = \frac{1}{60 - 15} , \quad (6a)$$

$$\Pi_E = \frac{1}{5 - 2} , \quad (6b)$$

and

$$\Pi_C = \frac{1}{80 - 1} . \quad (6c)$$

Suppose an independent measurement provided information about burnup, i.e., 45.00 ± 2.25 GWd/t U (5% uncertainty). Rather than sampling an assembly parameter from the uniform pdfs in Eqs. (6), we can sample from a pdf that uses information about the measured assembly parameter. Independent measurements of the other assembly parameters can also be included. With information about all three assembly parameters from independent measurements, our pdf, $f(B, E, C)$, can be defined as

$$f_A = \Lambda_B \Lambda_E \Lambda_C , \quad (7)$$

with Λ_X being the uniform pdf of picking parameter X over its appropriate range:

$$\Lambda_B = \frac{1}{\sqrt{2\pi}(\sigma_B)^2} e^{-(B-B_m)^2/2(\sigma_B)^2} , \quad (8a)$$

$$\Lambda_E = \frac{1}{\sqrt{2\pi}(\sigma_E)^2} e^{-(E-E_m)^2/2(\sigma_E)^2} , \quad (8b)$$

and

$$\Lambda_C = \frac{1}{\sqrt{2\pi}(\sigma_C)^2} e^{-(C-C_m)^2/2(\sigma_C)^2} , \quad (8c)$$

where

B_m, E_m, C_m = independent measurements of the burnup, initial enrichment, and cooling time, respectively

$\sigma_B, \sigma_E, \sigma_C$ = associated uncertainties.

The pdfs in Eqs. (8) are Gaussian, centered at the measured value, and the standard deviation is equal to the uncertainty in the measured value. When an independent measurement gives a value for one of the assembly parameters, this information can be used to reduce the range of values from which to sample the assembly parameter. The pdf from which the assembly parameter is sampled becomes a Gaussian instead of a uniform distribution that arises when no additional knowledge about the assembly parameter is known. We will see later that

the reduction in the range of possible values from which we can sample narrows the distribution of assembly attributes thus providing a more precise estimate of the assembly attribute.

The assembly parameters B , E , and C are sampled from the pdf, $f(B, E, C)$, N times. After each sample, values for D , P , and R are estimated using Eqs. (1) and (3). The results are separated into bins to estimate the distribution of the assembly attribute. Finally, the mean value of all the results is calculated using Eq. (4).

III. NUMERICAL SIMULATIONS

Results will be given for using the Monte Carlo-based method described in Sec. II, on several of the NDA instruments we are investigating, as listed below (descriptions of each instrument are beyond the scope of this paper; however, explanations can be found through the references of each instrument):

1. passive neutron albedo reactivity with fission chambers¹⁰ (PNAR-FC)
2. ²⁵²Cf interrogation with prompt neutrons¹¹ (CIPN)
3. differential die-away¹² (DDA)
4. delayed neutron¹³ (DN)
5. differential die-away self-interrogation¹⁴ (DDSI)
6. self-interrogation neutron resonance densitometry¹⁵ (SINRD).

In the discussion of the Monte Carlo-based method to estimate attributes of a spent fuel assembly, we have intentionally been vague regarding what an assembly attribute is. This was done to illustrate that the Monte Carlo-based method is useful for any assembly attribute and any detector response. Some assembly attributes quantified through simulation of various instruments were given in Sec. I; they are fissile/fertile ratio, elemental U/Pu ratio, ²³⁵Pu/²³⁹Pu ratio, and the fissile content. All of the instruments in the above list quantify the fissile content of an assembly except for the SINRD instrument, which quantifies the ²³⁹Pu mass or ²³⁵U mass, primarily from the outer few rows of an assembly.

We now show our results for this Monte Carlo-based method of estimating a mean and distribution for an assembly attribute (e.g., the fissile content) for instruments delineated above. For each instrument, the “measured” detector response will be the simulated detector response for a reference assembly with 45 GWd/t U burnup, 4 wt% ²³⁵U initial enrichment, and 5-year cooling time. For the results given in this paper, the uncertainty (the relative random error standard deviation) in the measured response was chosen to be 1.0% for all instruments. (In practice, each instrument will have a different uncertainty; a single value for the uncertainty

TABLE I

Results of Using a Monte Carlo–Based Estimator of an Assembly Attribute for the Independent NDA Instruments PNAR-FC, CIPN, DDA, DN, DDSI, and SINRD*

Figure	PNAR-FC	CIPN	DDA	DN	DDSI	SINRD
	2	3	4	5	6	7
Simulation	5535	5.76	5902	149	4956	2817
Full	5562 ± 386	5.35 ± 0.34	5480 ± 419	144.0 ± 7.7	4615 ± 297	2687 ± 174
Limited	5596 ± 177	5.75 ± 0.08	5901 ± 105	146.0 ± 2.3	4905 ± 77	2812 ± 35

*The “Simulation” results are the explicit MCNPX simulation results; the “Full” and “Limited” results are from the Monte Carlo calculations sampling from a full or limited range of parameter values, respectively. The figure numbers where the results are plotted are also given.

was chosen for simplicity and to allow for easy comparison.) The choice to pick the result from this assembly was made in order to have a known value to which we can compare the Monte Carlo estimates. In addition, picking the same assembly for each instrument makes for consistent and simple results across all the instruments. The reference assembly is still used to define the mapping functions from Eqs. (1). The number of Monte Carlo samples, or random assemblies emulated, is 1×10^5 . The individual results are separated into bins, and the frequency plot of the assembly attribute is calculated.

For each instrument, two calculations are performed. The first calculation samples assembly parameters from the full range of values, i.e., 15 to 60 GWd/t U, 2 to 5 wt% ^{235}U , and 1 to 80 yr. The second calculation samples assembly parameters from a limited range of values: 45.00 ± 2.25 GWd/t U, 4.0 ± 0.2 wt% ^{235}U , and $5 \pm$

1 yr. The results of the calculations are shown in Table I. The “Simulation” results are the explicit MCNPX simulations; the “Full” and “Limited” results are, respectively, those Monte Carlo calculations using either a full or limited range of parameter values as discussed.

We can see that for all the instruments, the estimated mean is well within 2σ —and sometimes within 1σ —of the explicit MCNPX simulation for the reference assembly. In addition, when sampling from a limited range of assembly parameters, the distribution of possible values of the assembly attribute is much narrower than for the simulation with the full sampling range of assembly parameters.

The results for all calculations are plotted in Figs. 2 through 7. For each instrument, two figures are plotted. The Figs. (a) show the calculation results from sampling from the full range of assembly parameter values, and

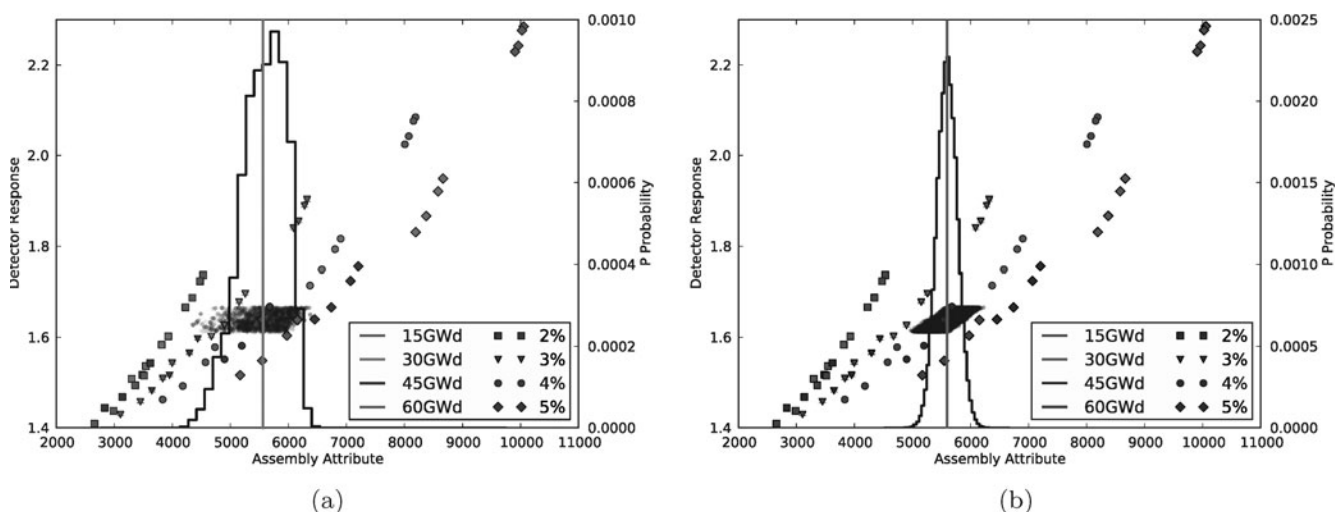


Fig. 2. Results of estimating the assembly attribute measured by the PNAR-FC instrument using the Monte Carlo–based method. The markers indicate the simulation results from the 64 spent fuel library models. The black smudge is the emulated results from the randomly sampled assemblies. (a) Full parameter range sampling. (b) Limited parameter range sampling.

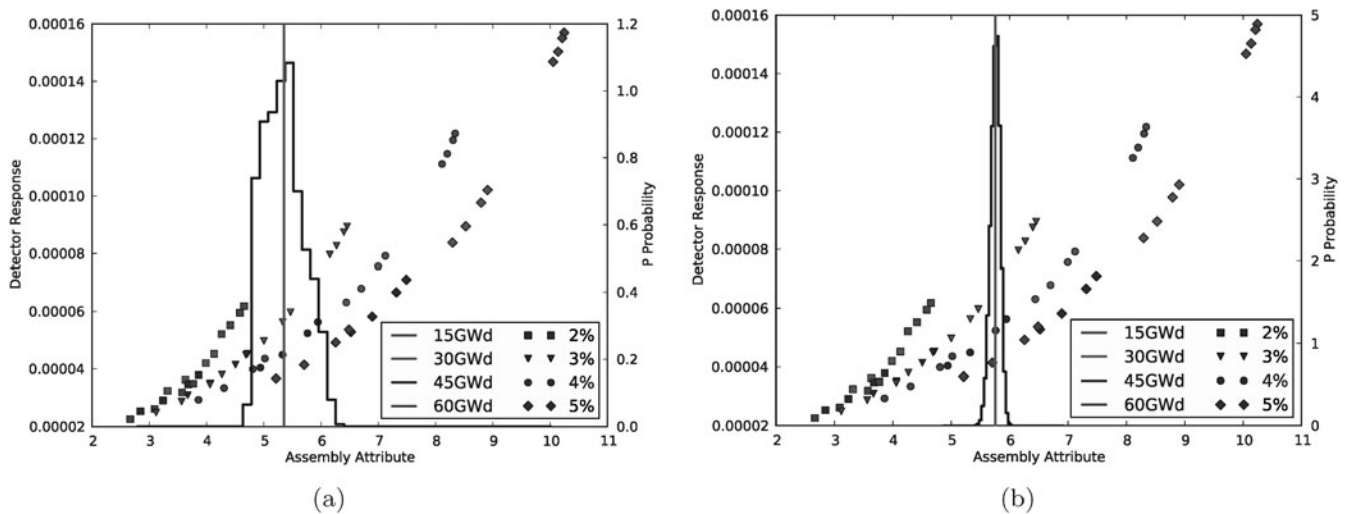


Fig. 3. Results of estimating the assembly attribute measured by the CIPN instrument. (a) Full parameter range sampling. (b) Limited parameter range sampling.

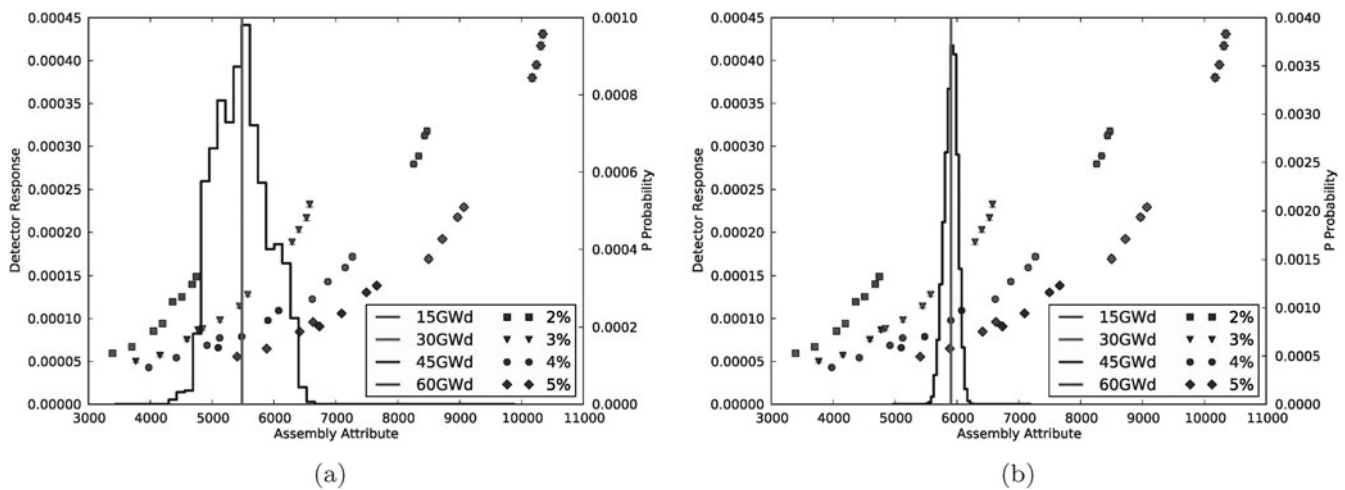


Fig. 4. Results of estimating the assembly attribute measured by the DDA instrument. (a) Full parameter range sampling. (b) Limited parameter range sampling.

the Figs. (b) show the calculation from sampling from the limited range of assembly parameter values. In both Figs. (a) and (b), the markers represent the MCNPX simulation results for the 64 models in the spent fuel library, and the mean (vertical line) and distribution of the assembly attribute are shown.

The distribution of possible assembly attributes is estimated by binning the results into 50 equally spaced bins of the assembly attribute. In each figure, the black line is a frequency plot of the assembly attribute as compared with all the calculated assembly attributes. We see that in the full simulations, the distribution is often asymmetric. The asymmetry of the distribution is due to the asymmetry of the explicitly simulated assemblies that

provide the data for the interpolation. We can see in Fig. 2a, for example, that the density of the markers is greater for smaller values of the assembly attribute; thus, we expect a tail of the distribution on the left side of the distribution. In Fig. 2b, the distribution is more symmetric because the assembly parameters are sampled from a limited range (as explained above).

Figure 2 shows the results from the PNAR-FC instrument. (These data are the same as in Fig. 1.) While not individually distinguishable, the emulated results from the randomly sampled assemblies are plotted with small black markers making a smudge across Fig. 2; the blackness of each point is equal to the weight of the result with a weight of 1 being fully black and a weight of 0

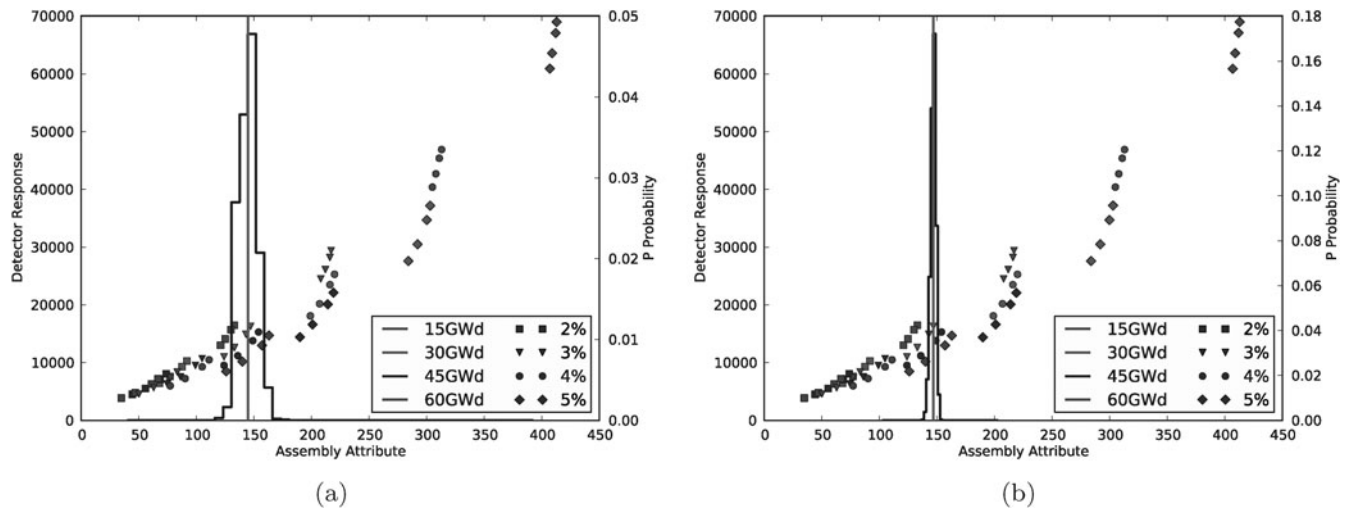


Fig. 5. Results of estimating the assembly attribute measured by the DN instrument. (a) Full parameter range sampling. (b) Limited parameter range sampling.

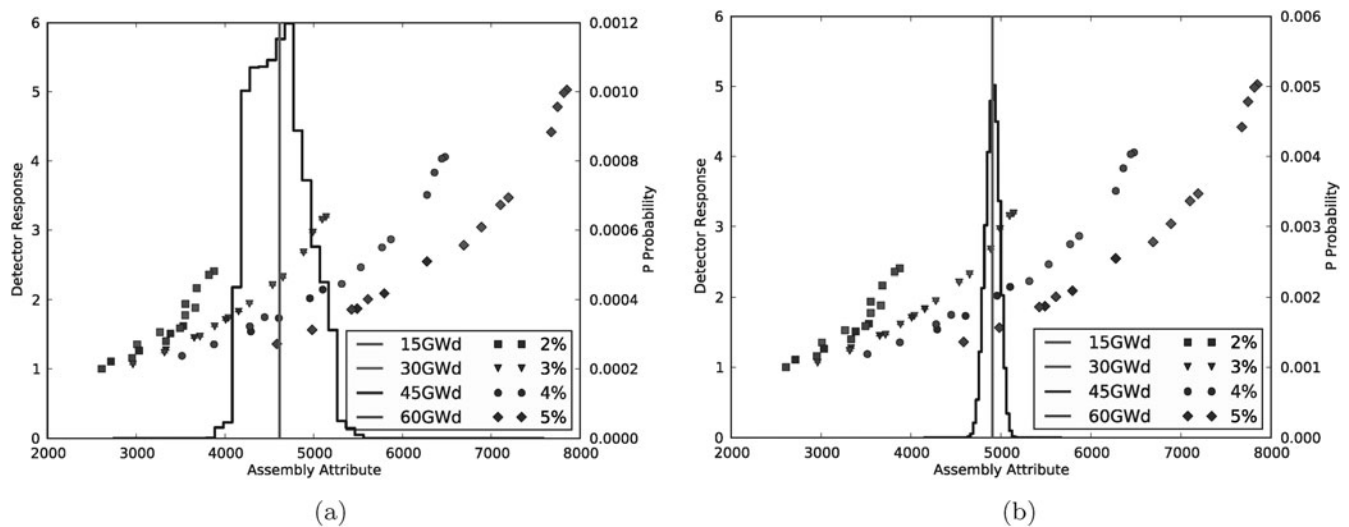


Fig. 6. Results of estimating the assembly attribute measured by the DDSI instrument. (a) Full parameter range sampling. (b) Limited parameter range sampling.

being fully white. The randomly sampled results span a range much larger than the smudge indicates; the other results are simply not visible because of their white color. The individual results are not plotted for the other instruments as they only distract from the information, but they are similar to the individual results of the PNAR-FC calculations.

The Monte Carlo estimation of the mean and distribution of the assembly attribute requires only a few seconds to perform 1×10^5 samples, including calculating the interpolated mapping functions. In contrast, a single MCNPX simulation of one of the spent fuel library models can require more than 200 CPU hours to complete

and cannot estimate the distribution of possible values. The difference in the computational expense is ten orders of magnitude and is due to emulating MCNPX simulations using $M_D(B, E, C)$ and $M_P(B, E, C)$ rather than performing explicit MCNPX simulations.

The results from the SINRD (Fig. 7) instrument are different from the other instruments because all 64 models from the spent fuel library have not yet been simulated; only those assembly models with a 5-yr cooling time have been simulated. Nevertheless, the Monte Carlo-based method is still capable of accurately predicting the assembly attribute well within 1σ . The asymmetry of the distribution of assembly attributes is due

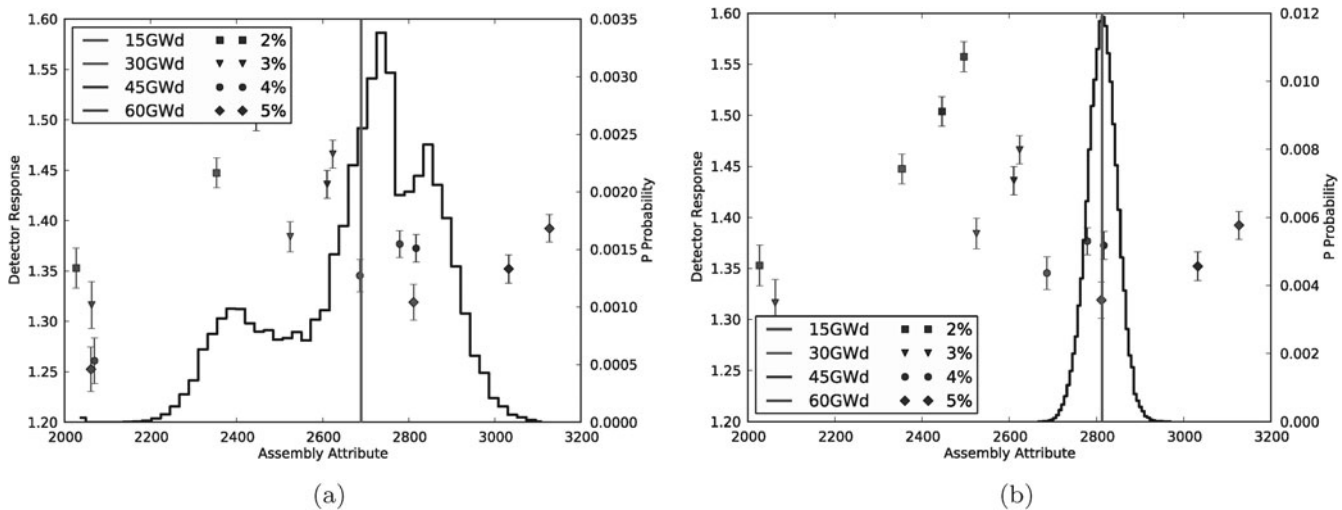


Fig. 7. Results of estimating the assembly attribute measured by the SINRD instrument. (a) Full parameter range sampling. (b) Limited parameter range sampling.

to the asymmetry of the explicitly simulated assemblies that provide the data for the interpolation; i.e., the 15 GWd/t U results tend to stretch the distribution to lower values of the assembly parameter. Furthermore, in the limited sampling result (Fig. 7b), we see a symmetric distribution of assembly attributes because the 15 GWd/t U results are never chosen.

IV. VALIDATION OF THE MONTE CARLO-BASED METHOD

We now turn our attention to validating the Monte Carlo-based method described in Sec. II. Validating a method is necessary to know the limits of the method as well as ensuring the results are unbiased and accurate. In this section, we will show four different simulations assessing the validity of this Monte Carlo-based method of analysis.

To begin, we repeat the above Monte Carlo estimations without the explicitly simulated MCNPX results for the assemblies with 45 GWd/t U burnup parameter values. This cross-validation¹⁶ assessment shows how accurately the method can predict the assembly attribute for an assembly that has not been explicitly modeled. To perform this check, we repeated the simulation from Sec. III for the PNAR-FC technique but have excluded the 45 GWd/t U results when the mapping functions M_D and M_P are defined. By excluding some results from the data that define the mapping functions, we can still define the mapping functions, but we also have data to which we can compare the Monte Carlo simulation results.

The results are shown in Fig. 8, where in Fig. 8a a full range of parameter values is used for sampling and in Fig. 8b a limited range of parameter values is used.

The limited ranges from which the assembly parameters were sampled are the same as before: 45.00 ± 2.25 GWd/t U, 4.0 ± 0.2 wt% ^{235}U , and 5 ± 1 yr. Figures 8a and 8b are directly comparable with Figs. 2a and 2b. Note the absence of the 45 GWd/t U markers in Fig. 8, indicating that the simulation results from assemblies with 45 GWd/t U burnup were not included in the interpolation. The mean assembly attribute was estimated as 5586 ± 359 for the simulation with a full range of parameter sampling and 5621 ± 122 for the simulation with a limited range of parameter sampling. There is no difference graphically or statistically between these results and the simulations that include the 45 GWd/t U simulation results, giving confidence in the accuracy and usability of this analysis method.

The second assessment we have attempted is to know how sensitive the Monte Carlo-based method is to a change in the uncertainty in the “measured” detector response. Remember that we have assumed an uncertainty of 1%. We have repeated the simulations, but with measured detector uncertainties of 1%, 5%, and 10%. The results are summarized in Table II and shown graphically in Fig. 9. Figure 9a shows the results when a full range of parameter values is used for sampling, and Fig. 9b shows a limited range of sampling values.

The results show that as the measured uncertainty increases, the uncertainty in the Monte Carlo results increases (as expected) but that the results are all within 1σ of each other. This gives confidence that there is no bias introduced when the measured uncertainty increases. Perhaps more interesting is that when independent information is known about the assembly parameters allowing a more limited range of sampling, the measured uncertainty is much less important. Figure 9b shows that the three simulations have nearly the same

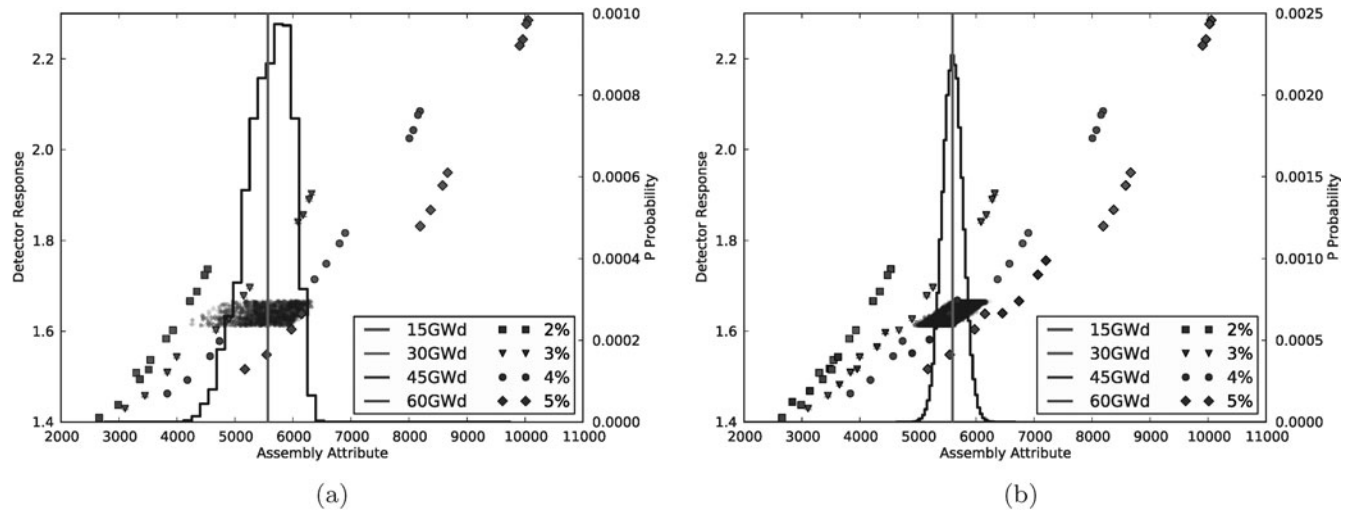


Fig. 8. Results of estimating the assembly attribute measured by the PNAR-FC instrument without using the MCNPX simulation results for assembly models with 45 GWd/t U burnup values. (a) Full parameter range sampling. (b) Limited parameter range sampling.

TABLE II

Results Obtained by Changing the “Measured”
Uncertainty from 10% to 1% of the Detector Response*

Measured Uncertainty	Full	Limited
10%	5265 ± 877	5619 ± 260
5%	5405 ± 652	5615 ± 255
1%	5568 ± 382	5597 ± 176

*The underlying data came from the PNAR-FC instrument.

result—well within 1σ —and that the uncertainty in the assembly attribute is similar regardless of the measured uncertainty.

We now show another set of three simulations where we investigate the sensitivity of the estimated assembly attribute to the number of Monte Carlo trials. The results of these simulations are given in Table III and shown in Fig. 10. The number of Monte Carlo trials for these simulations ranged from 1×10^2 to 1×10^6 .

It is easy to see in Fig. 10 that changing the number of Monte Carlo trials has a big effect on the noise of an individual bin of an assembly attribute but that the distribution of the assembly attribute remains the same. Table III shows that the results of all the simulations are well within 1σ of each other, indicating once again that no bias is introduced for a different number of Monte Carlo trials. As before, we can see by comparing Figs. 10a and 10b that limiting the range of sampled parameter values greatly improves the estimate of the assembly attribute, in this case by reducing the noise of the indi-

vidual assembly attribute bins in addition to reducing the uncertainty of the assembly attribute distribution.

In all of the simulations shown in this paper, we have chosen to estimate the assembly attribute for a reference assembly with the parameters 45 GWd/t U burnup, 4 wt% ^{235}U initial enrichment, and 5-yr cooling time. Our final validation assessment looks at the ability of the Monte Carlo-based method to accurately predict the assembly attribute for assemblies with parameters that differ from our reference assembly. It would be impossible to explore all the possible combinations of assembly parameters in this paper, so we have limited our assessment to four additional assemblies. These four assemblies all have 4 wt% ^{235}U initial enrichment and 5-yr cooling time; they differ in their burnup with a range of 15 to 60 GWd/t U.

As with all of our simulations in this paper, we have done two simulations for each assembly: one with a full range of parameter values to sample and the other with a limited range of parameters. The results of all the simulations are given in Table IV, the results with the full

TABLE III

Results Obtained by Changing the Number of
Monte Carlo Trials N from 1×10^2 to 1×10^6 *

N	Full	Limited
1×10^2	5430 ± 752	5612 ± 283
1×10^4	5405 ± 645	5614 ± 254
1×10^6	5404 ± 651	5616 ± 255

*The underlying data came from the PNAR-FC instrument.

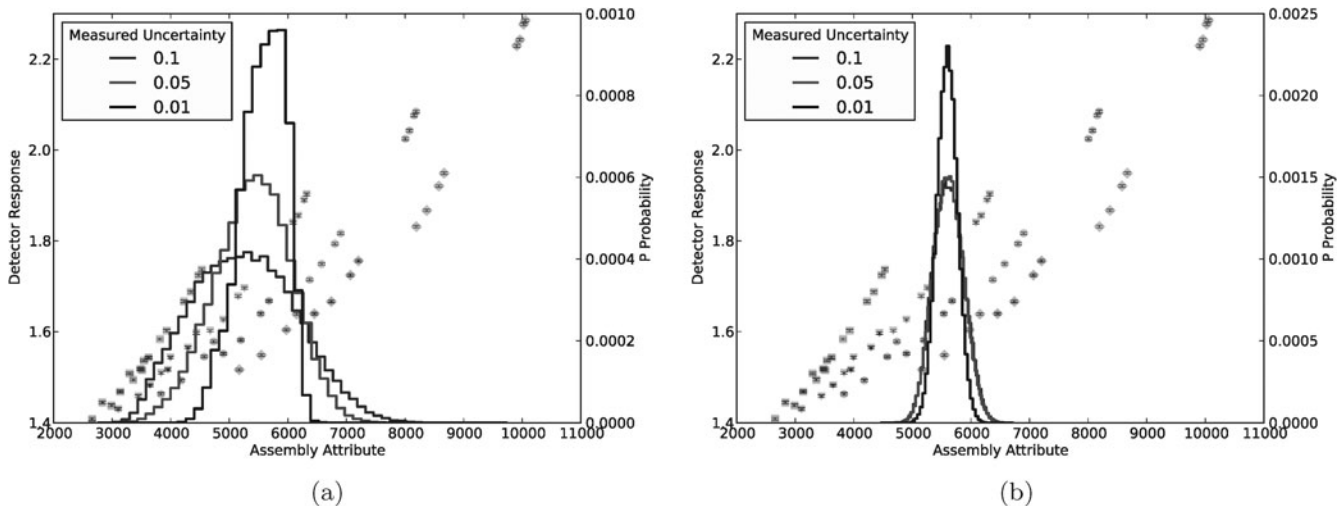


Fig. 9. Demonstration of the change in assembly attribute distribution with changing measured uncertainty. The measured uncertainty shown is 10%, 5%, and 1%; the 1% uncertainty is the same as for the previous simulations. The underlying data came from the PNAR-FC instrument. (a) Full parameter range sampling. (b) Limited parameter range sampling.

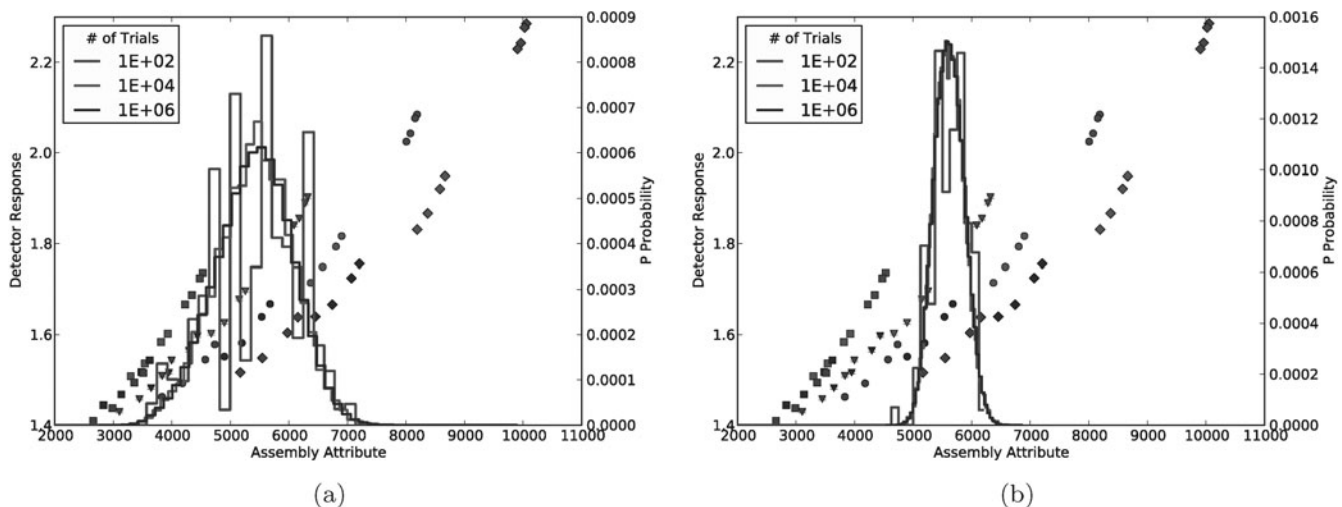


Fig. 10. Demonstration of the change in assembly attribute distribution with changing measured uncertainty. The measured uncertainty shown is 10%, 5%, and 1%; the 1% uncertainty is the same as for the previous simulations. The underlying data came from the PNAR-FC instrument. (a) Full parameter range sampling. (b) Limited parameter range sampling.

range of parameter sampling are shown in Fig. 11, and the results with the limited range of parameter sampling are shown in Fig. 12. These results again show the validity of the Monte Carlo–based method for estimating the assembly attribute. With the exception of the assembly with 15 GWd/t U burnup, all of the simulations utilizing the full range of parameter sampling fall within 1σ of the reference value; the assembly with 15 GWd/t U is easily within 2σ . All of the simulations utilizing a limited range of parameter sampling are well within the 1σ of the reference assembly. Again, we see the impor-

tance of using information on assembly parameters from independent measurements.

The fact that the estimate of the assembly attribute of the assembly with 15 GWd/t U burnup falls slightly outside 1σ of the reference value is not too surprising. Note that the estimate from the assembly with 60 GWd/t U is almost outside 1σ . Both of these assemblies lie on the edge of the mapped parameter space, and we expect the quality of the mapping to be less certain on the edges of the parameter space. Nevertheless, the Monte Carlo–based technique was able to accurately (within 2σ or

TABLE IV
Estimated Assembly Attribute for
Four Reference Assemblies*

Burnup	Simulation	Full	Limited
15	8155	8407 ± 215	8100 ± 183
30	6803	6407 ± 449	6778 ± 192
45	5535	5567 ± 386	5597 ± 177
60	4571	4898 ± 386	4789 ± 170

*All assemblies have 4 wt% ^{235}U initial enrichment and 5-yr cooling time; they differ in their burnup with a range of 15 to 60 GWd/t U. The underlying data came from the PNAR-FC instrument.

better) estimate the assembly attribute even at the extremes of the parameter space.

V. CONCLUSIONS

This paper introduced a Monte Carlo–based method of estimating attributes of spent fuel assemblies, such as the fissile content of the assembly. The method utilizes results from MCNPX simulations of a variety of spent fuel assembly models and interpolates between these results to construct functions that map assembly parameters (e.g., burnup, initial enrichment, and cooling time) to either a detector response or an assembly attribute. We

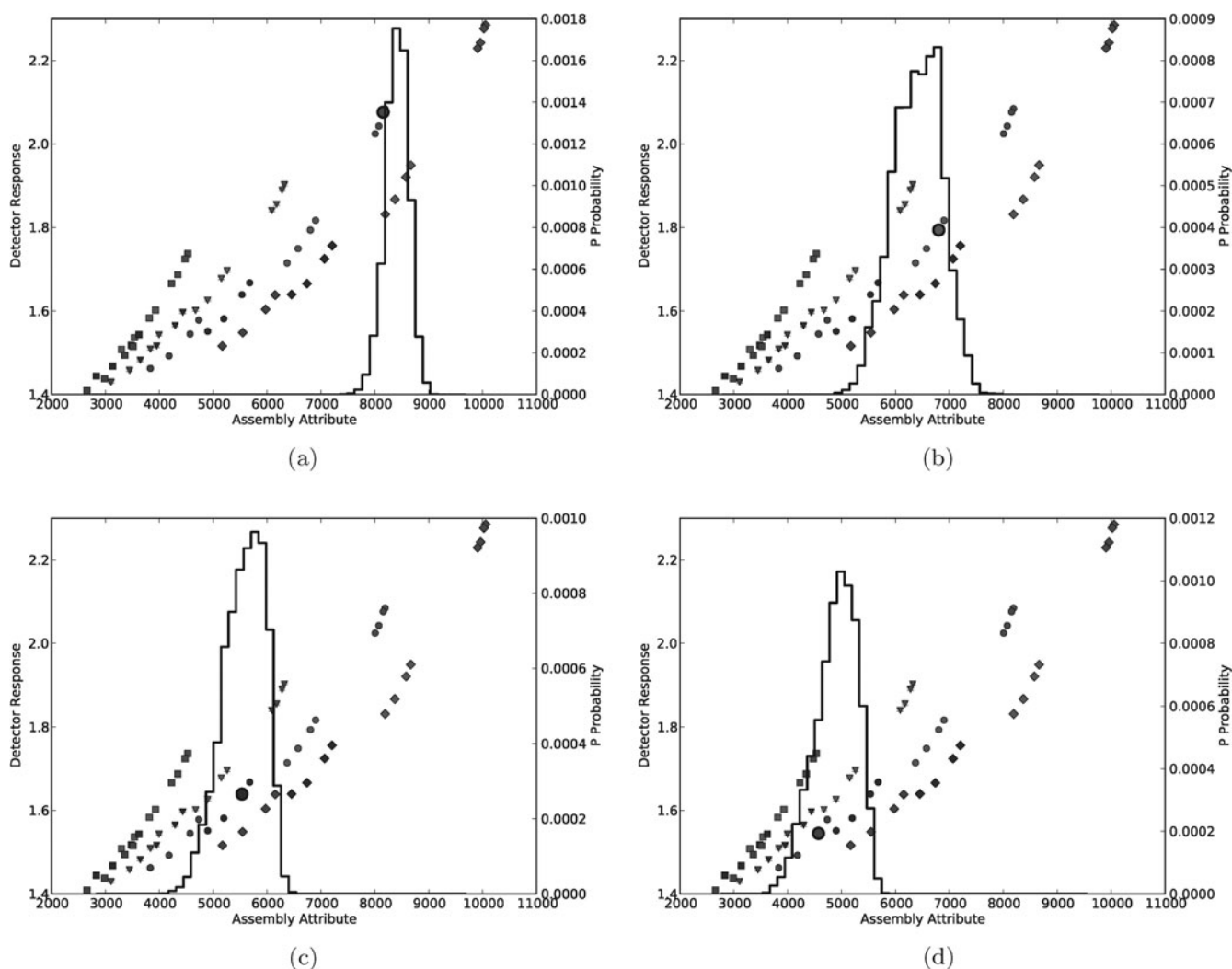


Fig. 11. Results from estimating the assembly attribute for an assembly with 4 wt% ^{235}U initial enrichment and 5-yr cooling time and a burnup of (a) 15 GWd/t U, (b) 30 GWd/t U, (c) 45 GWd/t U, and (d) 60 GWd/t U. The sampling range of parameters in the Monte Carlo estimation is the full range of possible assembly parameters. The underlying data come from the PNAR-FC instrument.

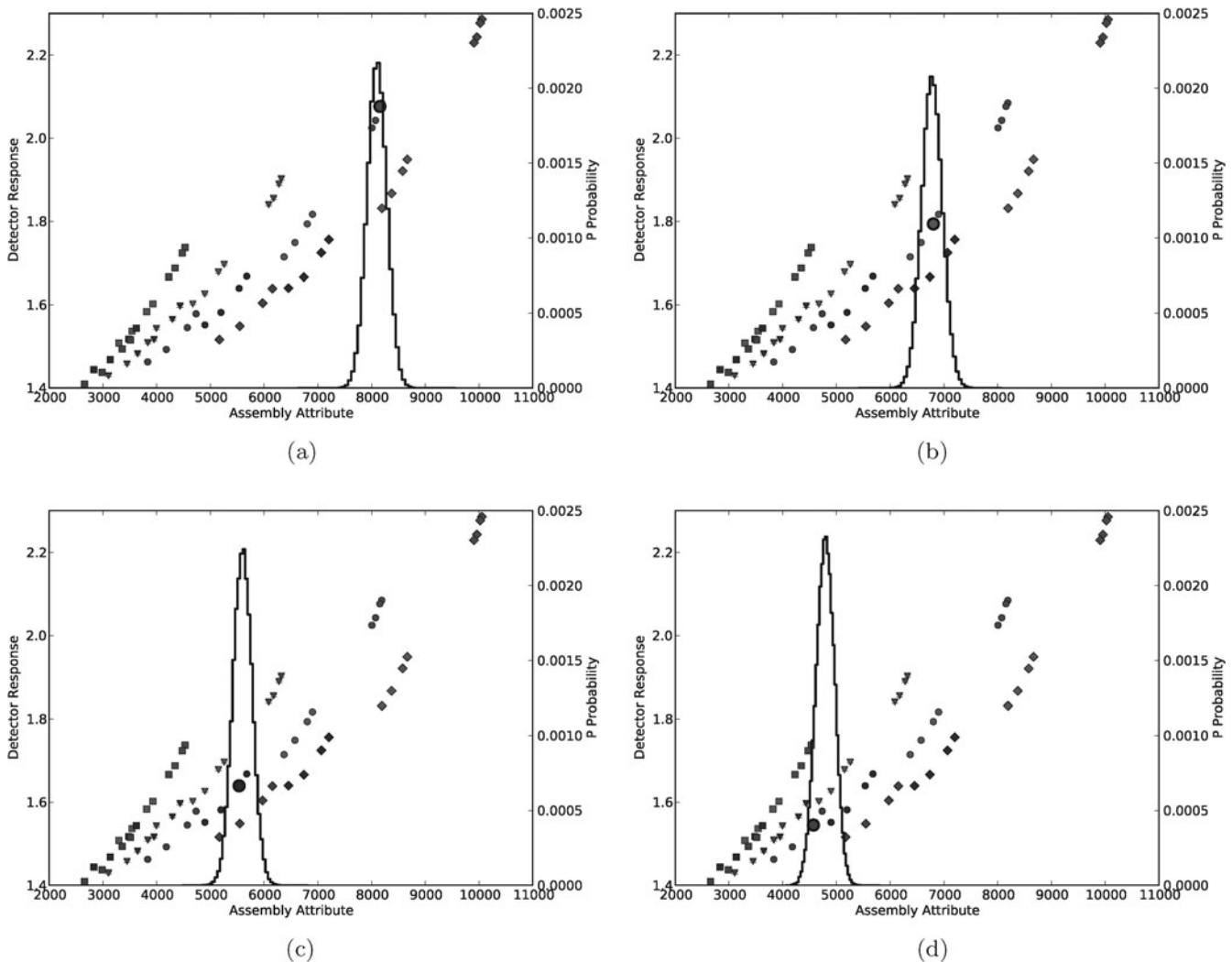


Fig. 12. Results from estimating the assembly attribute for an assembly with 4 wt% ^{235}U initial enrichment and 5-yr cooling time and a burnup of (a) 15 GWd/t U, (b) 30 GWd/t U, (c) 45 GWd/t U, and (d) 60 GWd/t U. The sampling range of parameters in the Monte Carlo estimation is 4.0 ± 0.2 wt% ^{235}U , 5 ± 1 yr with the burnup sampled from a Gaussian centered at the burnup value (15, 30, 45, or 60 GWd/t U) with a 5% standard deviation. The underlying data come from the PNAR-FC instrument.

have chosen to use radial basis functions to perform our interpolation since they can interpolate in many dimensions. The use of the mapping functions is a method of emulating MCNPX simulations and reduces the computational expense by ten orders of magnitude.

This analysis was developed to estimate the mean and distribution of values for a specific assembly attribute and is applicable to all of the 14 NDA instruments we are currently investigating. This Monte Carlo-based method is independent of the detector response and assembly attribute. While all the results from the instruments shown in this paper detect neutrons in some fashion, the quantified assembly attributes include the fissile content of the assembly as well as the ^{239}Pu mass.

We have demonstrated this method for six different NDA instruments whose responses and assembly attributes were simulated for 64 different spent fuel assembly models. For each instrument, we performed this Monte Carlo-based analysis and compared the result to one of the individually simulated spent fuel assembly model results. Two simulations were performed: one using the full range of possible assembly parameter values and the other using a limited range of assembly parameter values. In both cases, the estimated mean was well within 2σ of the original MCNPX simulation and for some instruments within 1σ .

We have made a few additional simulations (in Sec. IV) to assess the validity and sensitivity of this

technique. All of the simulations indicate that the Monte Carlo-based method is appropriate for estimating the assembly attribute of an unknown assembly, based upon a measured detector response. One must be careful when estimating the assembly attribute for assemblies on the periphery of the mapped parameter space.

We would like to emphasize the importance of using independent measurements of the assembly parameters of burnup, initial enrichment, and cooling time. When independent measurements of these parameters are used, the estimate of the assembly attribute is always better (i.e., a smaller uncertainty) compared to when independent measurements are not available. In addition to reducing the uncertainty of the estimated assembly attribute, using independent measurements to estimate the assembly parameters reduces the number of Monte Carlo trials needed, improves the assembly attribute estimate at the periphery of the parameter space, and reduces the dependence on the measured detector response.

The Monte Carlo-based method introduced in this paper is a promising approach for estimating assembly attributes using emulated data based upon results from explicit simulation. In creating the mapping functions, we have assumed that the results from explicit MCNPX modeling had no uncertainty. To accurately quantify the uncertainty in the estimated assembly attribute, the uncertainty in the simulations that provide the framework for the mapping functions must be propagated to the uncertainty in the distribution of the assembly attribute.

We intend to use the Monte Carlo-based method to assist in measuring the plutonium content in spent nuclear fuel assemblies as part of the NGSF effort. A calibration is needed so that the modeled assemblies match the real-world assemblies. A calibration of this sort would require an assembly with well-known parameters. The detector response from the NDA techniques would be calibrated to this known assembly, and the modeled assemblies could alter the mapping of assembly attributes and detector responses to make the Monte Carlo-based estimate of the assembly attribute accurate to the specific system being measured. One goal of such a calibration is to allow us to include an MCNPX model-error component of uncertainty, which is currently ignored.

Once the calibration has been performed, measurements of the spent fuel assembly would be made with a variety of NDA techniques. Inevitably, the assemblies measured would not have the same parameters as the assemblies that have been explicitly modeled. The Monte Carlo-based method for estimating the assembly attribute would be used, and the detector responses would be used as inputs to the method. The estimated assembly attribute from the Monte Carlo-based method would be the best estimate based upon the measured detector response and the independent measurements of the assembly attributes.

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