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Uncertainty assessment for the thermal expansion of simulated fuel via the Monte Carlo method

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Abstract

The uncertainty of the thermal expansion of simulated fuel was evaluated based on the Monte Carlo method. The uncertainties of the thermal expansion were divided into three components: initial sample length, system calibration factor, and an iterative measurement. For each component, a normal probability distribution function was assumed and the extended uncertainty was evaluated for various samples and batches. The results were compared with an international standard guide. Furthermore, the Shapiro–Wilk test was performed to establish a normality of the estimated sample means.

Keywords: Uncertainty; Thermal expansion; Simulated fuel; Monte Carlo method; Shapiro–Wilk test

1. Introduction

The Monte Carlo method provides approximate solutions to various mathematical and physical problems by performing statistical sampling experiments on a computer. The method applies to problems with no probabilistic content as well as to those with an inherent probabilistic structure [1]. Recently, many researchers have developed new theories for a computational complexity to provide a more precise and persuasive rationale for employing the Monte Carlo method. In particular, the Monte Carlo method was applied to estimate an uncertainty evaluation to obtain more accurate and realistic data [2].

In this study, the Monte Carlo method was newly used to evaluate the uncertainties for the thermal expansion of a simulated fuel [3]. In ref. [3], the uncertainties were evaluated via a standard international guide [4]. The simulated fuel denotes a simulated irradiated fuel. When the fresh uranium fuel has been irradiated in the reactor, the fuel contains various fission products which are very toxic and radioactive [5]. The thermal and mechanical properties of this irradiated fuel are very important for the fuel performance in the reactor. The research for the reuse for the spent fuel have been performed around world and especially, the direct use of spent fuel without reprocessing has been studied [6]. But, a high radioactivity of spent fuel prevents an ease treatment to measure the properties. Thus, some toxic isotopes are replaced with non-toxic and stable isotopes when fabricating a fuel pellet. This is called a simulated fuel. The weights of the impurities or additives are changed by the irradiation period which is called a burnup. The simulated fuel has been widely used to measure the thermophysical and mechanical properties of an irradiated fuel [7].

Thermal expansion as well as thermal conductivity is one of the most important thermophysical properties of a nuclear fuel. Most solid materials expand when heated up and shrink when cooled down [8]. The thermal expansion is defined as a variation of the length with a temperature change, which is expressed as follows:

$$\frac{\Delta l}{l_0} = \frac{l_\mathrm{f} - l_0}{l_0} = \alpha_\mathrm{l}(T_\mathrm{f} - T_0) \quad (1)$$

where l_0 and l_f are length at temperatures T_0 and T_f, respectively, and α_l is the linear coefficient of a thermal expansion.

From the experiments, the linear coefficients of a thermal expansion for UO_2 fuel are distributed from $1.03 \times 10^{-5}\,\mathrm{K}^{-1}$ to $1.08 \times 10^{-5}\,\mathrm{K}^{-1}$ [7].

The objective of this study is to present uncertainty evaluation for thermal expansion with Monte Carlo approach. The Monte Carlo method is not popular in the application of uncertainty evaluation especially for thermal properties of nuclear fuel. Thus, our research is new and valuable to estimate uncertainty for thermophysical properties of nuclear fuel.

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Table 1
Conditions for thermal expansion experiment

Item	Value
Instruments	Dilatometer (DIL402C)
Range of measurement	Room temperature ~2000 °C
Measuring target	Linear thermal expansion
Heating rate	5 K/min
Acquisition rate	2 points/K
Reference material	Al_2O_3 (9.59 mm length)
Environment	Ar 100%
Sample	Simulated fuel (9.40 mm)

In Section 2, a brief description on the uncertainty evaluation for the thermal expansion is given based on an international guide. In Section 3, a detailed procedure from the Monte Carlo method is described to estimate an uncertainty. And it provides some results of the Monte Carlo simulation for three different temperatures. Additionally, the Shapiro–Wilk normality test is discussed. Finally, a conclusion of this study is given in Section 4.

2. Uncertainty of the thermal expansion

An uncertainty is defined as a parameter, associated with the result of a measurement, which characterizes the dispersion of a value that could reasonably be attributed to the measurand [9]. The measurand means a particular quantity subject to measurement and the definition of the measurement can be a major source of uncertainty [4]. An uncertainty is often called an error, deviation, etc., depending on the application areas. There are several ways to determine an uncertainty depending on the models and measurements. A general approach is applicable for one measurement target and one model equation. If the measurement objectives are more than one or there are several model equations, then the matrix method is widely used. This matrix method based on mathematics is also applied to complicated models for a measurement, an output, and an input. Recently, the Monte Carlo simulation method [1] has often been used to simulate a measurement, especially to find the uncertainty for a complicated model where it is not easy to calculate the uncertainty.

Thermal expansions of a simulated fuel are measured by using a horizontal type dilatometer (DIL402C, Netzsch) from room temperature to 1600 °C under an argon environment [10]. There exists an uncertainty in the measurement, which should be quantified based on statistics. Table 1 shows the conditions for the thermal expansion experiments in this study.

The approach for an uncertainty of the thermal expansions of a simulated fuel starts from the following formulation [11]:

$$f_E(T) = \frac{l(T) - l_0}{l_0} \times f_{cal} \quad (2)$$

where $f_E(T)$ is the thermal expansion, or output of the experiments, l_0 the sample length at room temperature (mm), $l(T)$ the sample length at T °C (mm) and f_{cal} is the ratio due to system calibration.

The factor of f_{cal}, which was introduced for a previous approach, has a unit value and its uncertainty comes from a system calibration test with the reference material. If the results of the system calibration lie within a proper criterion, the system (DIL402C) is thought to be a normal state and no other calibration is performed. It contains two kinds of uncertainties: the first one is an uncertainty of iterative experiments with a reference material (u_{fcal1}, type A) and the second one is a reference material uncertainty from a report (u_{fcal2}, type B). The uncertainty of l_0 is composed of three kinds: the first one comes from a resolution (u_{l01}, type B), the second one comes from a calibration report (u_{l02}, type B) and the third one from a variation of the room temperature (u_{l03}, type B). The uncertainty of $l(T)$ is derived from the iterative experiments with a nuclear fuel ($u_{l(T)}$, type A). From the above standard uncertainties, the combined standard uncertainties are calculated and the expanded uncertainty is calculated by the standard procedure for an uncertainty evaluation. Table 2 shows the uncertainty factors for the thermal expansion experiments.

Table 2
Uncertainty parameters for the thermal expansion of a simulated fuel

Parameter	Type of uncertainty	Degree of freedom
Initial length (l_0)		
Resolution (l_{01})	B (rectangular)	Inf.
Calibration (l_{02})	B (normal)	Inf.
Temperature variation (l_{03})	B (rectangular)	Inf.
Length ($l(T)$)		
Iterative measurement	A (normal)	4
System calibration (f_{cal})		
Calibration test (f_{cal1})	A (normal)	4
CRM[a] report (f_{cal2})	B (normal)	Inf.

[a] Certified reference material.

Especially, the standard uncertainty of f_{cal} is obtained as:

$$u_{fcal}^2 = u_{fcal1}^2 + u_{fcal2}^2, \quad (3)$$

and the degree of freedom is derived as:

$$\nu_{fcal} = \frac{u_{fcal}^4}{((u_{fcal1}^4/\nu_{fcal1}) + (u_{fcal2}^4/\nu_{fcal2}))}, \quad (4)$$

where $\nu_{fcal1} = M - 1$, $\nu_{fcal2} = (100/R)^2/2$, R the degree of risk (=100% confidence level), and M is the iterative experiment number.

In this same way, the standard uncertainty and combined uncertainty are obtained by following the ISO guide [4]. The expanded uncertainty is obtained by multiplying the k-value from the student t distribution and the combined uncertainty as shown in Eq. (2). Fig. 1 shows the overall procedure for an uncertainty evaluation of the thermal expansion experiment of a simulated fuel. The approximate confidence level used in this study is 95% and the coverage factors (k) are found from the student t distribution.

In Table 3, the uncertainties of the thermal expansions of the simulated fuel are given at the temperatures of 500 °C, 1000 °C, and 1500 °C, respectively. In this experiment, the thermal expansion data is obtained with a 25 °C step. Three different temperatures from the results are chosen to observe the typical

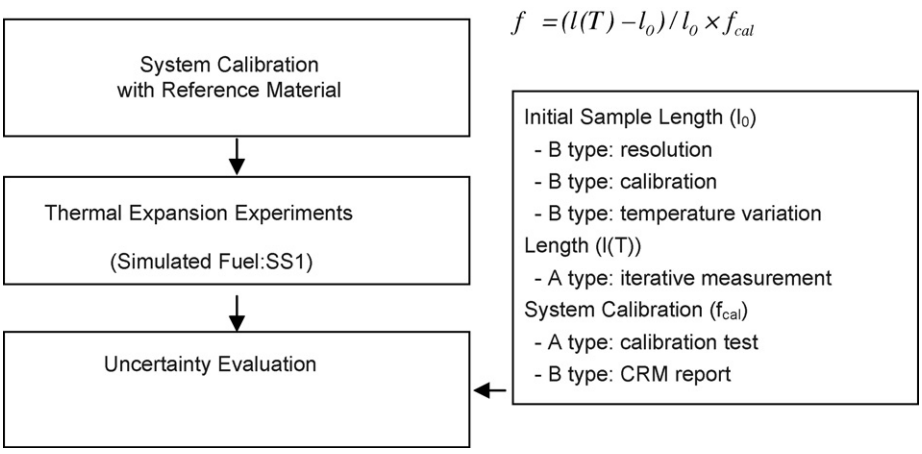

Fig. 1. Flowchart of the uncertainty evaluation for the thermal expansion of simulated fuel.

trend of an uncertainty. The combined standard uncertainty of the initial length is 1.755×10^{-3} mm, which is the same for all the cases. The standard uncertainties of the iterative experiments of the length variation increase as the temperature increases. But the combined standard uncertainties of the calibration decrease as temperature increases due to the behavior of the calibration report. In this table, contribution factors are defined as the ratio of the squares of the combined uncertainties for each factor. From the results, a system calibration is the most important factor which affects the overall combined uncertainty for the temperature ranges. From the table, the expanded uncertainties of the thermal expansion of the simulated fuel increase as the temperature increases.

3. Uncertainty evaluation by the Monte Carlo approach

When obtaining uncertainty of the guide to the expression of uncertainty in measurement (GUM) method [4], a formula for uncertainty is approximated and its partial derivatives are also truncated for simplicity. If variable of uncertainty becomes strongly non-linear or the standard uncertainty is very small compared with the input variable, it may produce significant errors in the standard GUM method. To overcome those weaknesses of the standard method for uncertainty evaluation, a statistical uncertainty approach is proper alternative including Monte Carlo method. The Monte Carlo method only needs the information of the distribution of the input parameters to expand the system uncertainty. Eliminating complications due to decomposition of uncertainty factors in the whole system, the Monte Carlo method provides powerful tool to evaluate system uncertainty. Furthermore, in order to obtain correct and robust uncertainty with respect to the non-linearity of input, not only additional biasing test, but also normality test should be followed in the Monte Carlo method.

To estimate an uncertainty by the Monte Carlo method, the proper numbers of batches and samples are determined first. From the central limit theory, the sample means approach a normal distribution if enough batches are used. That is, a sample

Table 3
Uncertainty budget for the thermal expansion of simulated fuel (95% confidence level)

Parameter	500 °C		1000 °C		1500 °C	
	Standard uncertainty	Combined uncertainty	Standard uncertainty	Combined uncertainty	Standard uncertainty	Combined uncertainty
Initial length (l_0), mm		1.76×10^{-3} (0.27)[a]		1.76×10^{-3} (0.19)		1.76×10^{-3} (0.16)
Resolution (l_{01})	0.001		0.001		0.001	
Calibration (l_{02})	4.37×10^{-4}		4.37×10^{-4}		4.37×10^{-4}	
Temperature variation (l_{03})	1.39×10^{-3}		1.39×10^{-3}		1.39×10^{-3}	
Length ($l(T)$) (mm)		6.50×10^{-4} (0.04)		1.02×10^{-3} (0.06)		1.50×10^{-3} (0.11)
Iterative measurement	6.50×10^{-4}		1.02×10^{-3}		1.50×10^{-3}	
System calibration (f_{cal})		6.58×10^{-2} (0.69)		3.71×10^{-2} (0.75)		2.43×10^{-2} (0.73)
Calibration test (f_{cal1})	6.56×10^{-2}		3.68×10^{-2}		2.40×10^{-2}	
CRM report (f_{cal2})	5.29×10^{-3}		4.68×10^{-3}		3.51×10^{-3}	
Overall combined uncertainty (u_{total})	3.66×10^{-4}		4.38×10^{-4}		4.82×10^{-4}	
Thermal expansion	4.64×10^{-3}		1.02×10^{-2}		1.70×10^{-2}	
Expanded uncertainty	7.34×10^{-4}		8.79×10^{-4}		9.70×10^{-3}	

[a] Contribution factor (or importance factor) = $C_i^2 u_i^2 / u_{total}^2$.

Table 4
Extended uncertainty of the Monte Carlo method

Temperature (°C)	ISO Guide	Monte Carlo	
		Batch and sample #	Extended uncertainty
500	7.34E−04	(25,100)	7.22E−04
		(25,1000)	7.37E−04
		(100,1000)	7.36E−04
		(1000,100)	7.35E−04
1000	8.79E−04	(25,100)	8.57E−04
		(25,1000)	8.78E−04
		(100,1000)	8.78E−04
		(1000,100)	8.78E−04
1500	9.70E−04	(25,100)	9.86E−04
		(25,1000)	9.67E−04
		(100,1000)	9.71E−04
		(1000,100)	9.69E−04

mean ($\tilde{x}$) for a batch is expressed as follows:

$$\tilde{x} = \frac{1}{H}\sum_{h=1}^{H} x_h, \tag{5}$$

where x_h is a sample value and H is the number of samples.

For each batch, the above sample means could be obtained and the unbiased total mean ($\bar{x}$) of the batches is given by averaging the sample means:

$$\bar{x} = \frac{1}{G}\sum_{g=1}^{G}\tilde{x}_g = \frac{1}{G}\frac{1}{H}\sum_{g=1}^{G}\sum_{h=1}^{H} x_{gh}, \tag{6}$$

where $\tilde{x}_g$ is the sample mean of the gth batch, x_{gh} a sample value of the gth batch, and G is a number of batches.

The unbiased variance (S^2) of the sample means are derived as:

$$S^2 = \frac{1}{G}\frac{H}{H-1}\sum_{g=1}^{G} s_g^2 = \frac{1}{G}\frac{H}{H-1}\sum_{g=1}^{G}\left(\frac{1}{H}\sum_{h=1}^{H}(x_{gh}-\tilde{x}_g)^2\right). \tag{7}$$

To determine the unbiased mean and variance is one of important works in the Monte Carlo method. Especially, if neglecting a statistical treatment, it may create a biased result for a complicated system where the exact solution is not known. However, biased results are usually used to reduce the variances of the Monte Carlo methods [1].

Table 4 shows the estimated uncertainties of the Monte Carlo method. The estimation was performed based on Eq. (2) and the uncertainties of each component were used as the standard deviations of the normal probability distribution functions. Three different cases were chosen to establish the sensitivity of the number of batches and samples. From the results, the lower batch number provides poor results when compared to the high batch number.

But nobody knows which batch number is good and it may be vain to perform a simulation with a huge batch number without knowing the confidence interval. For this satisfaction, normality tests are usually performed for the Monte Carlo method. In this study, the Shapiro–Wilk normality test [12] was done for the low batch number. The Shapiro–Wilk test begins by obtaining the following coefficients:

Table 5
Coefficient for the Shapiro–Wilk test ($G = 25$)

g	a_g	g	a_g
1	−0.4450	8	−0.1046
2	−0.3069	9	−0.0823
3	−0.2543	10	−0.0610
4	−0.2148	11	−0.0403
5	−0.1822	12	−0.0200
6	−0.1539	13	0
7	−0.1283		

$a_{26-g} = -a_g, \quad 1 \le i \le 12$

$$b = \sum_{g=1}^{G} a_g y_g, \tag{8}$$

$$S^2 = \sum_{g=1}^{G} y_g^2 - \frac{1}{G}\left(\sum_{g=1}^{G} y_g\right)^2, \tag{9}$$

$$w_G = \frac{b^2}{S^2}, \tag{10}$$

where a_g is a given coefficient, y_g a sorted value of the sample mean of the gth batch ($\tilde{x}_g$), and w_G is a determinant for the normality. Table 5 shows the coefficient of a_g when the number of batches is 25. Table 6 gives the results of the Shapiro–Wilk test for the low batch number simulations. For three different temperatures, the parameters of w_G were calculated by using Eq. (10) and they were also compared with the criterion of the confidence limits. If w_G is less than the criterion of a certain confidence level, it says that the estimated means distributed with a given confidence within a normal distribution. When the sample number is 100, all the values of w_G are less than the criterion of the 50% confidence limit, that is, at most half of the estimates have a normal distribution. Therefore, it needs more batch numbers to have a good enough normality. When the sample number increases as 1000, the values of w_G also increase slightly, but they are still less than the 90% confidence limit. This is a reason why the uncertainties of the low batch numbers exhibit large differences when compared with those

Table 6
Results of the Shapiro–Wilk normality test

Temperature (°C)	w_G	
	$G = 25$, $H = 100$	$G = 25$, $H = 1000$
500	0.9639	0.9805
1000	0.9215	0.9690
1500	0.9470	0.9561

Confidence of 10%: criterion of $w_G = 0.931$
Confidence of 50%: criterion of $w_G = 0.964$
Confidence of 90%: criterion of $w_G = 0.981$

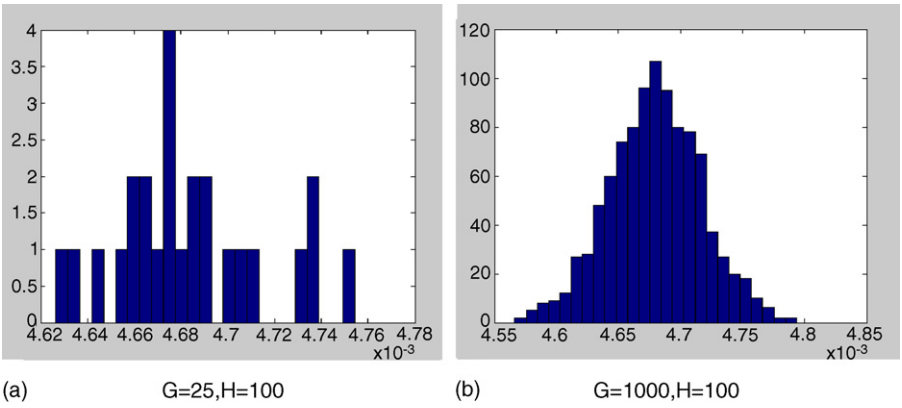

Fig. 2. Distributions of the estimated sample means for the thermal expansion when the temperature is 500 °C: (a) $G = 25$, $H = 100$ and (b) $G = 1000$, $H = 100$.

of the ISO method in Table 4. In this simulation, the minimum batch number can be also estimated from Table 6. For the 50% confidence, in the case of 500 °C, the batch number (H) 100 is enough to satisfy the normality condition. For 1000 °C, the batch number should be given around 1000. However, for 1500 °C, the batch number should be more than 1000 to obtain an enough normality. The exact estimation for the minimum is impossible and useless because every simulation provides different results. Thus, it is proper to adjust simulation number from the results to obtain an enough normality. Fig. 2 shows the distributions of the estimated sample means when the temperature is 500 °C. When the batch number is small, the distribution is considerably random. But for a large batch number, the sample means are distributed normally as expected. From this figure, it shows that the number of batches is important during a sampling to satisfy the central limit theorem.

4. Conclusions

Thermal expansion was measured with a dilatometer for a simulated fuel and its uncertainty was obtained with the Monte Carlo method and an ISO guide. The expanded uncertainties, which increase slightly as the temperature increases, were computed for discrete temperatures and it was found that the Monte Carlo method exhibits a similar behavior the compared to the ISO guide. Additionally, the Shapiro–Wilk normality test was performed to establish the distribution of the estimated means. It was found that both the batch number and sample number should be chosen carefully to obtain a good enough normality. As a conclusion, the Monte Carlo method is a useful tool to evaluate a system uncertainty for various experiments of the thermophysical properties for a nuclear fuel. Furthermore, it would be applied to thermophysical properties of various materials including nuclear fuel.

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