Uncertainty Evaluation of the Indirectly Produced Data for the Melting Point and Specific Heat of Uranium Dioxide

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1. Introduction

Uncertainty assessment plays an essential role in a measurement in order to obtain reliable data which affects the soundness and safety of nuclear fuel materials, and the process of an uncertainty evaluation are explained in the standard international guide[1]. In this study, uncertainty evaluations of the specific heat at 1000 $^{\circ}C$ and melting point of uranium dioxide(UO_2) are performed via the method of an uncertainty evaluation using indirectly produced data. The indirect production of data means that the data has been collected from previous documents such as scientific treatises, academic accounts, and authorized database etc., not from direct experiments or measurements. The case in which uncertainties are stated in documents and the case otherwise are considered by applying statistical analyses to each case according to the means presented by ICTP[2]. In respect to the case of no uncertainty values, there has been no established procedure for the uncertainty evaluation. Our research is thus new and meaningful to estimate the uncertainty for the thermophysical properties of a nuclear fuel.

2. Methods and Results

In this section uncertainty evaluations are carried out separately for two cases: uncertainty stated and uncertainty not stated. Their procedures are illustrated concisely using flowcharts in Fig. 1.

2.1 Uncertainty Evaluation of the Melting Point of UO_2

The melting point of UO_2 varies greatly by measurers and measuring methods, which is attributed to the fact that the O/U ratio or impurities affect the melting point of UO_2 and a high vapor pressure above 2450 $^{\circ}C$ makes it difficult to measure the melting point accurately[3]. Fig. 2 shows the melting points of UO_2 with uncertainties.

The procedure of case I in Fig. 1 is applied to evaluate the uncertainty excluding the Lyon datum which does not present an uncertainty value. To avoid the effect of an outlier and consider the effect of the uncertainty values differently, the weight(w_i) is defined by the reciprocity of each squared uncertainty value, enabling small uncertainty values to contribute largely. The weighted mean($\bar{x}_w$) and the standard deviation of $\bar{x}_w$ (σ_w) are given as follows:

$$\bar{x}_w = \sum_{i=1}^{N} w_i x_i \Big/ \sum_{i=1}^{N} w_i \ , \ w_i = 1/\sigma_i^2 \qquad (1)$$

The drawback of the above method is the possibility of too great effect of one datum which is not preferable especially when data are not consistent. In that sense, it is necessary to adjust the relative weight to yield a rather conservative uncertainty value. This process, called the Limitation of Relative Statistical Weight(LRSW), is widely used to evaluate an uncertainty.

As an overall result of the above method, the melting point of UO_2 is represented as:

$$T_{mt} = 2841.52 \pm 20.76 \ (^{\circ}C) \qquad (2)$$

2.2 Uncertainty Evaluation of the Specific Heat of UO_2

Specific heat data samples at 1000 $^{\circ}C$ from numerous experimental papers are taken to evaluate the uncertainty of the specific heat. Table I. shows the data.

Table I: Specific Heats of UO_2 at 1000 $^{\circ}C$

Authors[4]	Specific heat (J/mol K)
Moore(1947)	85.3736
Hein(1968)	85.7820
Fredrickson(1970)	84.0598
Kerrisk(1972)	84.7053
Takahash(1993)	85.9144
Fink(1997)	84.2200
Fink(2000)	84.2000

We follow the procedure of an uncertainty assessment applicable to the case containing no information of the uncertainties, obtaining the arithmetic mean($\bar{x}_u$) and the standard deviation of the mean(σ_u):

$$\bar{x}_u = \sum_{i=1}^{N} x_i \Big/ N \ , \ \sigma_u = \sqrt{\sum_{i=1}^{N} (x_i - \bar{x}_u)^2 \Big/ N(N-1)} \qquad (3)$$

where x_i is a sample value and N is the number of data. Provided that the data is all consistent, i.e., any datum is not too far from mean, we choose σ_u as the uncertainty. In order to judge whether there are an outlier to be eliminated, we have to pass through some steps which are briefed in case II of Fig. 1. It is noticeable that the standard deviation used for the chi square calculation about N data is obtained with N-1 data, i.e., without datum farthest from mean:

$$\chi^2 = \sum_{i=1}^{N} \chi_i^2 \text{ , } \chi_i^2 = (x_i - \bar{x}_u)^2 / \sigma_i^2 \qquad (4)$$

where $\sigma_i = s_{N-1} = \sqrt{\sum_{i=1}^{N-1} (x_i - \bar{x}_u) / (N-2)}$ which is the standard deviation of N-1 data. This process enables the standard deviation to become smaller when we calculate the chi square, thus making it more reasonable. Then the chi square value is compared with the following:

$$\chi^2 < \chi^2_{0.05, N-1} \text{ , } \chi_R^2 = \chi^2 / (N-1) \approx 1 \qquad (5)$$

where $\chi^2_{0.05,N-1}$ denotes the number on the measurements axis such that 0.05 of the area under the chi-squared curve with N-1 degrees of freedom lies to the right of [5]. If Eq. (5) is satisfied, the consistency of the collected data is ascertained, so the standard deviation of the mean(σ_u) can be used as the uncertainty value. Otherwise, the above process is iterated until the Eq. (5) is satisfied by removing an outlier datum to avoid the effect of the outlier datum in determining an uncertainty. The final result is given as follows:

$$T_{c_p} = 84.89 \pm 0.30 \text{ (J/mol K)} \qquad (6)$$

3. Conclusions

In the preceding sections the uncertainties of the melting point and specific heat of UO_2 have been evaluated based on the described procedure. Irrespective of the two cases, it is necessary to confirm the consistency of collected data to acquire reasonable uncertainties. The uncertainty value of the melting point has been produced through the LRSW method which prevents a specific datum from contributing to the determination of an uncertainty too much by tuning the relative weights. In case of the specific heat data containing no uncertainty values, however, the iteration process has been introduced to reduce the effect of an outlier by excluding an inconsistent datum via the chi square test. As a conclusion, the uncertainty expressions of the specific heat and melting point of UO_2 are expected to be helpful in the research for a standard establishment for the thermophysical properties of nuclear fuel materials.

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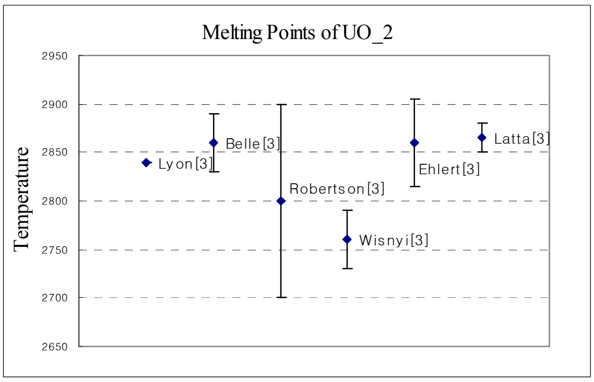

Fig. 2. Melting points of UO_2 from several documents.

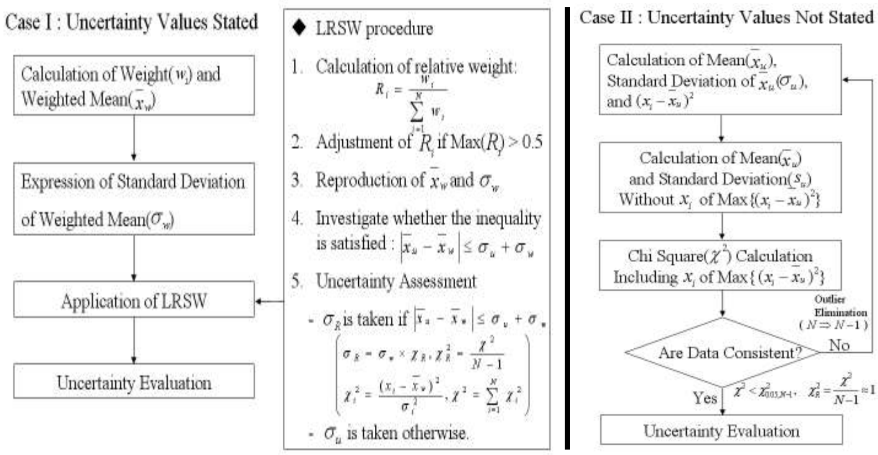

Fig. 1. Flowcharts of the uncertainty evaluation for two different cases.