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Evaluation of uncertainty associated with totalisation of time-sampled data in gas quantity and energy measurements

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ABSTRACT

The measurement uncertainty attributed to gas quantity and energy measurements includes among others a contribution for the calculation of the total/average from time-sampled data. The aim of this paper is to establish a procedure for evaluation of this component of uncertainty, which considers contributions related to deterministic and random variations of the input data. The principal steps of the proposed procedure are (i) separation of deterministic and random components via time-domain filtering, (ii) evaluation of uncertainty associated with deterministic component by the decimation method and (iii) evaluation of uncertainty associated with random component by statistical analysis. The paper presents this evaluation procedure for a test case of time-sampled data of the superior calorific value.

1. Introduction

The introduction of renewable energy gases such as hydrogen, requires an appropriate metrological infrastructure along the entire supply chain, from production to storage and end use. Typical measurands for fiscal metering are quantity, energy and composition [1]. Calculation units convert data from measuring equipment into the required measurands and calculate their total/average over certain periods of time. The overall measurement uncertainty of these results, supplementary to the uncertainty due to the measurement of the particular data points, also includes the measurement uncertainty associated with the calculation of the total/average from time-sampled data. This paper focuses on the evaluation of this contribution to the overall measurement uncertainty.

The discussed uncertainty of totalisation/averaging shows different dependencies on the number of samples for random and deterministic variations in time-sampled data. For random variations, this uncertainty is inversely proportional to the square root of the number of samples [2]. On the other hand, the error of numerical integration of deterministic variations by rectangle rule is inversely proportional to the number of samples [3]. For this reason, random and deterministic components require different methods for uncertainty evaluation. Time-sampled data in gas quantity and energy measurements is generally a combination of random and deterministic variations. In the proposed method, Savitzky-Golay time-domain filtering is used to separate the two components, where the part of the signal that passes the filtering is considered as a deterministic component, whereas the removed part is considered as the random component.

Within the framework of this paper, the analysis of the calculation uncertainty is made for a practical case of determining the average value of time-sampled data for superior calorific value of natural gas. To estimate the uncertainty associated with the deterministic component, the decimation method is used. This method is based on the analysis of changes in calculated values for different decimation factors. The uncertainty associated with the random component is estimated by statistical analysis, both by considering uncorrelated and correlated data [4,5]. The auto-correlation is also introduced into the deterministic component as a result of employing time-domain filtering for its determination.

2. Procedure for evaluation of calculation uncertainty

An outline of the proposed procedure for evaluating uncertainty associated with calculation of total/average from the time-sampled data is presented in Fig. 1.

In the first step, time-domain signal processing is used to separate the deterministic and random components of the time-sampled input data, q_i, $i = 1 \ldots N$. Savitzky-Golay (S-G) filtering, a generalized moving average method based on least squares polynomial fitting across a moving window, is employed in this work. The setting parameters of the S-G filter are the order of the smoothing polynomial (set to 2 in this work) and the size of the smoothing window in terms of the number of samples N_{win} on either side of centre point (smoothing window contains $(2N_{\mathrm{win}} + 1)$ samples). The passed part of the signal is considered as the deterministic component, $q_{\mathrm{det},i}$, $i = 1 + N_{\mathrm{win}} \ldots N - N_{\mathrm{win}}$, and the removed part of the signal is considered as the random component $q_{\mathrm{ran},i} = q_i - q_{\mathrm{det},i}$, $i = 1 + N_{\mathrm{win}} \ldots N - N_{\mathrm{win}}$.

The contribution to the totalisation/averaging uncertainty, which is related to the numerical integration of the deterministic component $q_{\mathrm{det},i}$, is estimated using the decimation method. Decimation or down-sampling with the decimation factor n_{dec} means that only every $n_{\mathrm{dec}}^{\mathrm{th}}$ sample is taken from the observed data $q_{\mathrm{det},i}$. The sought total/average Q is calculated for different decimation factors, $Q(n_{\mathrm{dec}})$, $n_{\mathrm{dec}} = 1 \ldots N_{\mathrm{dec}}$, and its dependence is least square approximated by the function $Q_{\mathrm{fit}}(n_{\mathrm{dec}}) = a\, n_{\mathrm{dec}} + b$. Here, the use of the linear function of n_{dec} is based on the assumption that the rectangle-rule numerical integration error is

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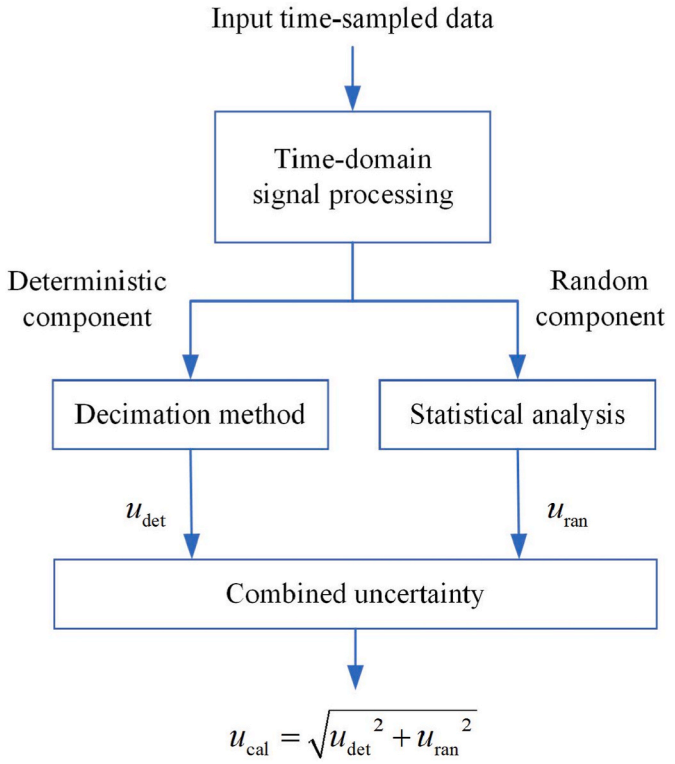

Fig. 1. Schematic diagram of the procedure for evaluating the calculation uncertainty.

inversely proportional to the number of samples. The parameter $b = Q_{fit}(0)$ is used as a prediction of the reference value for the case of infinite sample rate, and thus the numerical integration error is estimated as:

$$e_{det} = Q(1) - Q_{fit}(0), \tag{1}$$

with the standard error of estimate of the parameter b:

$$u(e_{det}) = s\left(Q_{fit}(0)\right). \tag{2}$$

The standard uncertainty of calculation associated with the deterministic component is determined as:

$$u_{det} = \sqrt{\left(\frac{e_{det}}{\sqrt{3}}\right)^2 + u^2(e_{det})}. \tag{3}$$

The contribution to the totalisation/averaging uncertainty, which is related to the averaging of the random component, is estimated by statistical analysis. Without taking correlation effects into account, it is determined as:

$$u_{ran}^{(uncor)} = \frac{s(q_{ran,i})}{\sqrt{N}}, \tag{4}$$

and with consideration of correlation effects as:

$$u_{ran}^{(cor)} = \frac{s(q_{ran,i})}{\sqrt{N}} \sqrt{1 + \frac{2\sum_{k=1}^{N_{cor}} (N_{ran} - k)\rho(k)}{N_{ran}}}, \tag{5}$$

where $\rho(k)$ is the kth auto-correlation coefficient, N_{cor} is the number of considered auto-correlation coefficients and N_{win} is the number of samples of the separated random component. In this paper, N_{cor} is determined by identifying the smallest k for which $\rho(k) > 0$ and $\rho(k+1) < 0$.

Combined totalisation/averaging uncertainty, which considers the contributions related to deterministic and random components, is determined as:

$$u_{cal} = \sqrt{u_{det}^2 + u_{ran}^2}. \tag{6}$$

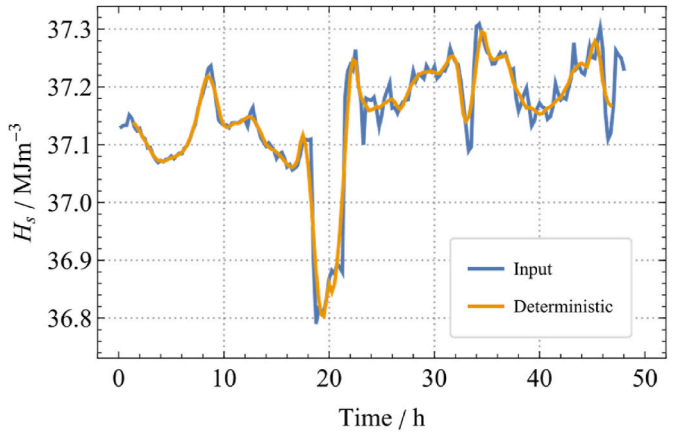

Fig. 2. Input data for the superior calorific value and the separated deterministic component ($N_{win} = 5$).

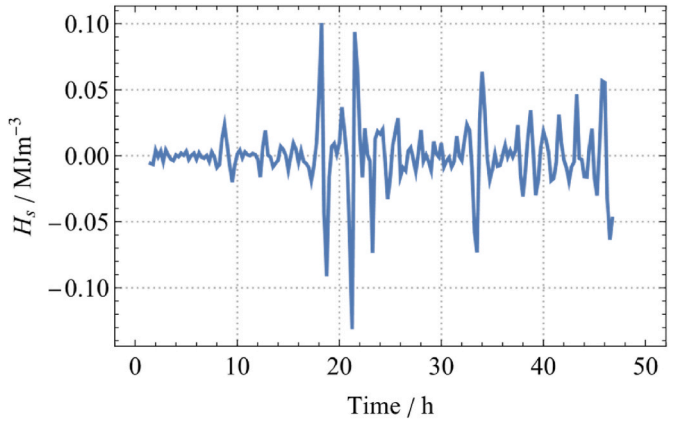

Fig. 3. The separated random component of the superior calorific value ($N_{win} = 5$).

3. Test case results

The evaluation of the calculation uncertainty is carried out for the test case of time-sampled data of the superior calorific value $H_{s,i}$ with the sampling period t_{samp} of 15 min, as presented in Fig. 2 under the label

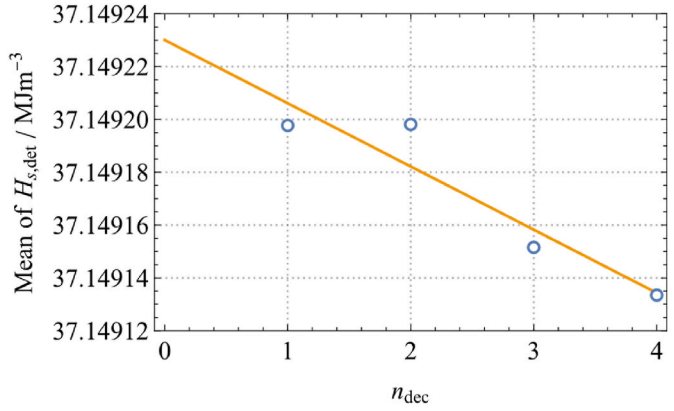

Fig. 4. Approximation of the average values of the decimated deterministic component ($N_{win} = 5$, $N_{dec} = 4$).

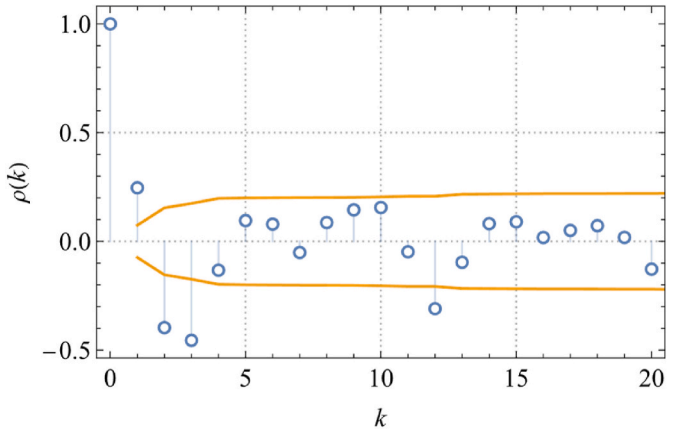

Fig. 5. Auto-correlation coefficients of the random component of the superior calorific value ($N_{win} = 5$); leads to $N_{cor} = 1$.

"Input". The goal was to estimate the standard uncertainty associated with the calculation of its average value using the rectangle-rule numerical integration, which equals the arithmetic mean formula in the case of the constant-period sampled data, $t_{samp,i} = t_{samp}$, $i = 1 \ldots N$:

$$\overline{H_s} = \frac{\sum_{i=1}^{N} H_{s,i} t_{samp,i}}{\sum_{i=1}^{N} t_{samp,i}} = \frac{1}{N} \sum_{i=1}^{N} H_{s,i} = 37.1508 \text{ MJ} \Big/ \text{m}^3. \tag{7}$$

Fig. 2 also presents an example of the deterministic component, which is separated from the input data using the Savitzky-Golay filter of the 2nd order with the window length $N_{win} = 5$. The corresponding random component, which is obtained as the difference between the input data and the deterministic component, is shown in Fig. 3.

Fig. 4 shows the approximation of the average values of the decimated deterministic component of the superior calorific value with n_{dec} up to $N_{dec} = 4$. The given case leads to the following estimate of the standard uncertainty of calculation associated with the deterministic component, u_{det}:

$$\begin{aligned} e_{det} &= \overline{H_{s,det}}(1) - \overline{H_{s,det,fit}}(0) = -0.032 \text{ kJ} \Big/ \text{m}^3, \\ u(e_{det}) &= s\left(\overline{H_{s,det,fit}}(0)\right) = 0.017 \text{ kJ} \Big/ \text{m}^3, \\ u_{det} &= \sqrt{\left(\frac{e_{det}}{\sqrt{3}}\right)^2 + u(e_{det})^2} = 0.025 \text{ kJ} \Big/ \text{m}^3. \end{aligned} \tag{8}$$

Fig. 5 shows the values of the correlation coefficients for the random component of the superior calorific value. The given case leads to the following estimate of the standard uncertainty of calculation associated with the random component, u_{ran}, without and with consideration of the correlation between the samples:

$$u_{ran}^{(uncor)} = \frac{s(H_{s,ran,i})}{\sqrt{N}} = 1.83 \text{ kJ} \Big/ \text{m}^3, \tag{9}$$

$$u_{ran}^{(cor)} = \frac{s(H_{s,ran,i})}{\sqrt{N}} \sqrt{1 + \frac{2 \sum_{k=1}^{N_{cor}} (N_{ran} - k) \rho(k)}{N_{ran}}} = 2.23 \text{ kJ} \Big/ \text{m}^3.$$

Given that in this case the contribution associated with the random component is significantly greater than that of the deterministic component, the estimated combined standard uncertainties of calculation nearly equal the results in Eq. (9).

To show the influence of the window size of the S-G filter (N_{win}) and the number of considered decimation factors (N_{dec}) on the estimated measurement uncertainty, we performed calculations for $N_{win} = (2 \ldots 10)$ and $N_{dec} = (3 \ldots 10)$. The results taking the auto-correlation effects into account are presented in Figs. 6 and 7, respectively. For comparison, the dashed line in both figures represents the value of the standard uncertainty, if it had been (inappropriately!) evaluated as the standard deviation of the mean of the input data:

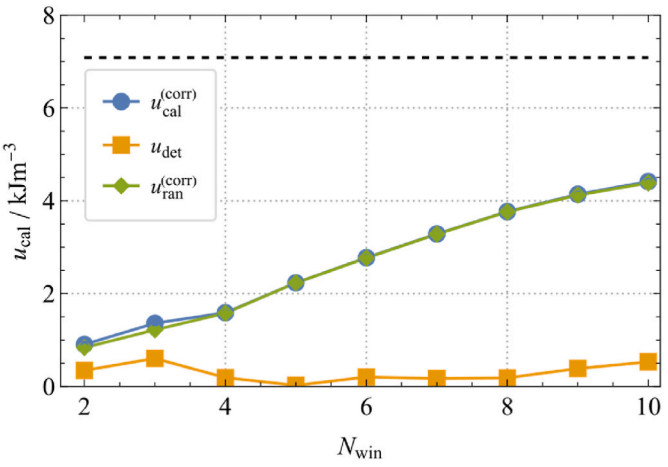

Fig. 6. Standard uncertainty of calculation for different values of the window length N_{win} ($N_{dec} = 4$, considering auto-correlation).

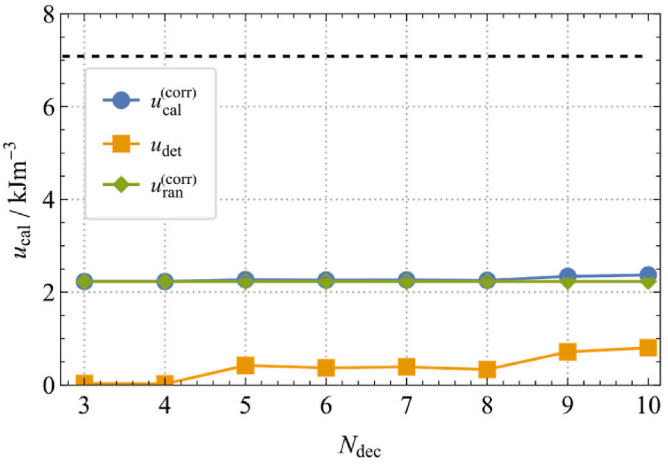

Fig. 7. Standard uncertainty of calculation for different values of the decimation range N_{dec} ($N_{win} = 5$, considering auto-correlation).

$$u_A = \frac{s(H_{s,i})}{\sqrt{N}} = 7.08 \text{ kJ} \Big/ \text{m}^3, \tag{10}$$

i.e., without separate evaluation of the deterministic and random components. With the procedure proposed in this paper, we get a substantially lower value for the totalisation/averaging uncertainty for all observed input parameters.

Fig. 6 shows that with the increase of the filtering window length N_{win}, the estimated value of the calculation uncertainty associated with the random component increases significantly. According to variations of the observed input data, which also contain sudden major changes in the sample values, e.g. as seen in Fig. 2 between 18 h and 22 h, this can be expected; a longer filtering window can cause a certain proportion of deterministic changes to be included in the random component at such parts of the input signal. We claim that for the studied case the calculation uncertainty estimates are more realistic at lower N_{win} values, but it will be necessary to confirm this with additional studies.

Fig. 7 shows that with the increase of the decimation range N_{dec}, the estimated value of the calculation uncertainty associated with the

deterministic component also shows a certain increasing trend. However, if we take into account the variations in the deterministic contribution observed in Fig. 6 at a constant N_{dec}, this is more attributable to the statistical scatter of the method.

4. Conclusions

In the paper, we presented a proposal for a procedure for evaluating uncertainty associated with the calculation of the total/average from time-sampled data in gas quantity and energy measurements, which enables separate treatment of deterministic and random variations. We demonstrated the proposed procedure on the example of evaluation of the calculation uncertainty associated with determination of the average value of the superior calorific value.

The proposed procedure shows a sensitivity to the setting parameters of time-domain filtering, which poses a challenge for future studies: what is the optimal filtering window length for a certain signal and how to determine this value during the procedure of evaluation of the calculation uncertainty.

In the future, we plan to validate the proposed procedure through a systematic analysis of synthesized signals, for which it is known what features were included in the data, so it is possible to define a realistic value of the totalisation/averaging uncertainty and used it in the evaluation of the results.

Finally, we would like to emphasize that it is not necessary to take into account the contributions of both the random and deterministic components in every calculation of totalized/average values from time-sampled data. For example, in further totalisation of the volume readings that are already internally integrated in the flow meter, it makes sense to consider only the random-component uncertainty. A certain open question remains regarding how to properly evaluate calculation uncertainty for energy data, which are products of time-sampled enthalpy values and internally integrated volume readings.

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