Application of the Kragten method in order to evaluate the uncertainty of the heat release rate determination using of the cone calorimeter

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ABSTRACT

Assigning uncertainties to measurement results is primordial in a certification framework using fire benches as the cone calorimeter [1] developed by NIST [2]. Indeed, this process allows in the first place to validate the measurement method accuracy and in second place to provide proper results to compare obtained between different labs (reproducibility).

However, even if numerous methods enable uncertainties determination, some can become complex when the data of interest is mathematical formulation powered by many measured parameters aimed to use in a model such as the Heat Release Rate (HRR).

This article aims to propose an intermediate uncertainty calculation method whose difficulty of application is sized between the GUM method [3] and the Monte Carlo method [4]: the Kragten one [5]. In order to validate the opportunity of using such a method, the three approaches were used to assess the measurement uncertainty on the HRR parameter in the specific case of small scale fire tests using cone calorimeter.

The results obtained show that the Kragten method allows to evaluate more easily and faster the HRR uncertainties measured at the Cone Calorimeter than the Monte Carlo method. Furthermore, the Kragten method is more reliable and reduces the risk of miscalculations than the GUM approach.

KEYWORDS

Suggested Keywords: Cone Calorimeter, Heat Release Rate, numerical method of Monte Carlo, GUM approach, Kragten approach, uncertainty.
INTRODUCTION

Uncertainty measurement is often an important issue dealing with experimental data processing. Although a proper uncertainties measurement is primordial to present reliable results in taking into account the factors affecting the outcome of the measurement as means, reliability and external parameters (i.e. ambient conditions).

Evaluation of experimental data uncertainty depends strongly on the mathematical model of the measurand or of the measurement system considered. Indeed, the measurand can be determined by direct or by multivariable measurements (equation of calculation). The measurement system corresponds itself to the integration of the input (i.e. sensor) at the output of the system (i.e. data processor or readout device) including the intermediate modules (i.e. amplifier, A/D converter, multiple interfaces). NASA [6] proposes procedures to evaluate uncertainty according to the measurement system considered (single or multi-variable and complete system). For the case of a direct measurement (mono variable), the uncertainty depends only on the Type A (statistical analysis) and Type B (resolution of instrumentation, calibration certificates, manufacturers’ specifications, previous measurement data and other relevant information) uncertainty components of the measuring device [7]. When using multiple variables to determine the data of interest (i.e. HRR), the definition of the mathematical relationship between the measurand and its component variables is important [6], especially considering the notion of linearity and dependence between variables, in particular when the different terms of the mathematical model contain the same variables [5].

Linearity and variable dependences are the parameters allowing to choose the most adapted uncertainties quantification method. Past study [8] highlighted characterization of HRR uncertainty, but at large scale. At small scale however, there is no available studies that explores different method to determine uncertainties on the HRR measurement (commonly evaluated with cone calorimeter [11]). The present study thus proposes to apply GUM, Monte Carlo Simulation and Kragten methods in order to determine the heat release rate measurement uncertainties. Besides in this study, are considered the parameters which are meant to be used for the HRR calculation and not the direct measurements from the sensors as in [8]. Thus, the proposed method also takes into account the uncertainties associated with transposition of measured data (signal conversion). The results obtained allows to highlight the advantages of the Kragten method comparing to other aforementioned approaches.

PRESENTATION OF THE 3 METHODS

Our study focuses on 3 main methods. The first is the law of propagation of variances or GUM (the most used) [3]. The uncertainty of the result \( u(Y) \) is evaluated by combining the uncertainties of each variable \( x_i \) and the covariance \( \text{cov}(x_i, x_j) \) between each correlated variable, according to Eq. 1 [3]. When all the variables are independent, the covariance term is zero \( (\text{cov}(x_i, x_j) = 0) \). Nevertheless, the GUM approach encounters some limitations, detailed by [7] and [8]: especially the non-linearity of the mathematical relation. Furthermore, if the mathematical formulation is complex and that the variables are correlated, the partial derivations of \( Y \) according to \( x_i \) (or \( \partial Y/\partial x_i \)) requires advanced mathematical skills and generate a risk of calculation errors.

\[
\begin{align*}
\sum_{i=1}^{n} \left( \frac{\partial Y}{\partial x_i} \right)^2 u^2(x_i) + 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \frac{\partial Y}{\partial x_i} \frac{\partial Y}{\partial x_j} \text{cov}(x_i, x_j) 
\end{align*}
\]  

\( u^2(Y) \) = \( \sum_{i=1}^{n} \left( \frac{\partial Y}{\partial x_i} \right)^2 u^2(x_i) + 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \frac{\partial Y}{\partial x_i} \frac{\partial Y}{\partial x_j} \text{cov}(x_i, x_j) \) (1)

The second is the Monte Carlo method (MCS) [4]. It is a numerical approach for solving mathematical problems by means of the simulation of random variable [8]. The principle is to calculate a result \( Y \) from the generation of a random number \( i \) for each input variables according to the assigned probability distribution function. Each simulation must generate at least 100,000 random numbers and this simulation must be repeated at least 10 times [9]. The uncertainty is then determined by the average of the uncertainties of these \( n \) simulations, described by Eq. 2. This approach is favoured for complex models (correlated variables, significant uncertainties of the input variable or model involving many variables) or non-linear models [7, 9, 10]. Nevertheless, the calculation times can be long in complex cases [9]. Another difficulty consists in selecting the probability distribution functions of input variables [9, 11].

\[
\sum_{i=1}^{n} \left( \frac{1}{i-1} \sum_{k=1}^{i} (Y^{(k)} - Y) \right) / n
\]

\( u^2(Y) = \sum_{i=1}^{n} \left( \frac{1}{i-1} \sum_{k=1}^{i} (Y^{(k)} - Y) \right) / n \) (2)
The third is the Kragten numerical method (KM) [5, 11]. This approach implies a modification of the propagation law of uncertainties concerning the sensitivity coefficient \( c \) [11]. Thus, each uncertainty contribution is calculated between two values of \( Y \): one corresponding to the measured value and the other corresponding to the measured value corrected by a term which is the uncertainty of this variable. So, this approach represents a gradient method similar to the first order finite difference approach. Instead of having Eq. 1 to determine the uncertainty of the measurand, Eq. 3 is used. Besides using an approximative numerical method of differentiation, the advantage of this method is that it only requires the mathematical formula used to obtain the measurand and the numerical values of the various variables and their uncertainties [11]. Moreover, according to Kragten [5], this method takes into account dependences of the variables within the mathematical formulation, reduces the risks of calculation errors and allows the calculation of uncertainty very quickly. Indeed, Kragten has developed a spreadsheet method that is adaptable to all error propagation calculations. The design of this sheet is clearly explained by [5] and an example of its use is presented in Table 1.

\[
\begin{align*}
 u^2(Y) &= \sum_{i=1}^{n} u^2(Y, x_i) + 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} (u(Y, x_i) \cdot u(Y, x_j)) \cdot \text{cov}(x_i, x_j) \\
 \end{align*}
\]  

The Heat Release Rate (HRR) produced during the combustion of materials subjected to a radiative heat flux can be determined in different ways depending on the variables taken into account (i.e. with additional gas analysers, such as \( \text{CO}_2 \), \( \text{CO} \) and \( \text{H}_2\text{O} \)) [12]. The most used mathematical formulation of HRR is the one given in the ISO 5660-1 standard [1]. It is expressed by Eq. 4 and depends on 6 variables.

\[
\dot{q}(t) = \left( \frac{\Delta H_c}{\rho_o} \right) \cdot (1.10) \cdot C \cdot \sqrt{\frac{\Delta P}{T_e}} \cdot \frac{x_{O_2}^0 - x_{O_2}}{\alpha - 1.5x_{O_2}} \quad (kW)
\]

With \( \Delta H_c \) the heat of combustion (MJ/kg), \( \rho_o \) the stoichiometric demand in oxygen, \( C \) the orifice flow meter calibration constant (named hereafter C-factor), \( \Delta P \) the orifice meter pressure differential (Pa), \( T_e \) the absolute temperature of gas at the orifice meter (K), \( x_{O_2}^0 \) and \( x_{O_2} \) respectively the initial concentration of oxygen and actual oxygen analyser reading (mol/mol), and \( \alpha \) the expansion factor equal to 1.105.

Several studies deal with calculating HRR uncertainties [13, 14, 15] or one of the variables of the HRR [16] according to the GUM method. Enright et al. [14] highlight that the HRR calculation variables are dependent of each other. This especially true for the gas-analysis terms and flow rate term both associated with the oxygen depletion factor [14] and for the C-factor which is calculated using variables also used to determine HRR (especially the temperature of the exhaust duct) [13, 14]. Nevertheless, Guillaum et al. [13] and Enright et al. [14] consider the effect insignificant. The results of the partial derivatives are detailed in [13] and [14].

Since the mathematical formulation is a combination of division and multiplications, Guillaum et al. [13] express the relative uncertainty of the HRR in order to simplify the calculation (Eq. 5).

\[
\begin{align*}
 u^2(\dot{q}(t)) &= \left( \frac{\dot{q}(t)}{C} \right)^2 \cdot \left( \frac{u^2(C)}{C^2} + \frac{u^2(\Delta P)}{\Delta P^2} + \frac{u^2(T_e)}{T_e^2} + \frac{u^2(x_{O_2})}{x_{O_2}^2} + \frac{u^2(x_{O_2}^0)}{x_{O_2}^0} + \frac{u^2(\Delta H_c)}{(\Delta H_c/\rho_o)^2} \right) \quad (kW^2)
\end{align*}
\]

Given the number of variables involved, the complexity of the partial derivatives that can lead to calculation errors and the presence of dependence between variables, it seems interesting to use alternative methods to the GUM to estimate the uncertainties of the HRR: those of Kragten and Monte Carlo. 

**HRR UNCERTAINTY WITH KRAGTEN’S METHOD**

Bryant and Mulholland [8] have already shown that the Kragten method allows to calculate the HRR uncertainty for full-scale fire tests with the same precision as the GUM method. However, in order to avoid dependencies between variables, the calculation of the uncertainties mainly concerns the basic measurement inputs such as instrument voltages, thermocouple temperatures and constant parameters. In our study, we use output data from measuring devices. So, the uncertainties of the variables (\( \Delta P \), \( T_e \), \( C \), \( x_{O_2} \) and \( x_{O_2}^0 \)) are determined according to the evaluation methods proposed by [13]. Finally, we also choose the uncertainty proposed by [14] for the effective heat of combustion (\( \Delta H_c/\rho_o \) or \( \text{EHC} \)) and we neglect the uncertainty expansion factor as proposed by Brohez [15].
The HRR data for this sensibility study are related to a pine tar which have been tested in a standard cone calorimeter under a radiant flux of 40 kW/m² [17]. The calculated HRR curve (according to Eq. 4) is illustrated in Fig. 1, which shows the maximum, the average and low (between 0.07 and 0.40 kW) values of HRR taken into account for this study (red squares).

Table 1 presents the spreadsheet to compute the maximum HRR value. In the first column, each parameter \( x_i \), measured, equivalent to the maximum HRR, is entered (i.e. 391.05 K for the temperature). Then, is entered the absolute uncertainties of each variable \( u(x_i) \) in the second row (i.e. 1.44 K for the temperature). These uncertainties are added to each corresponding \( x_i \) along the diagonal. For example (second column), the temperature uncertainty is added only at the temperature. Thus, the measured temperature of 391.05 K becomes 392.49 K and the values of the other parameters remain unchanged. For the third column, only the pressure differential is corrected. In the 9th line, the mathematical formulation for \( \dot{q}(t) \) is entered and copied to all right columns on the same line. We can observe a difference between the measured result equal to 11.143 kW (first column) and the corrected result (second to 7th column). The sum of the differences observed between the corrected HRR value and the measured HRR value make it possible to calculate the uncertainty of 0.647 kW (penultimate row). The expanded uncertainty of the HRR, equal to 1.294 kW, is obtained by applying the enlargement factor \( k \) (last line).

**Fig. 1. Evolution of HRR as a function of time - Pine tar - 40 kW/m².**

| Base computation of \( \dot{q}(t) \) | Numerical differentiation by change of the diagonal elements with the absolute uncertainty |
|---------------------------------------|-----------------------------------------------------------------------------------------|
| \( T_p \) (K) = 391.05                | \( u(T_p) = 1.44 \) \( u(\Delta P) = 0.60 \) \( u(x_{O_2}^0) = 0.002 \) \( u(x_{H_2}) = 0.007 \) \( u(C\text{-factor}) = 0.00126 \) \( u(EHC) = 655 \) |
| \( \Delta P \) (Pa) = 99.77            | 392.49 391.05 391.05 391.05 391.05 391.05 391.05 |
| \( x_{O_2}^0 \) (mol/mol) = 20.954    | 99.77 100.37 99.77 99.77 99.77 99.77 99.77 |
| \( x_{H_2} \) (mol/mol) = 17.986      | 20.954 20.954 20.954 20.954 20.954 20.954 20.954 |
| \( C\text{-factor} \) (-) = 0.04308   | 17.986 17.986 17.986 17.993 17.986 17.986 17.986 |
| \( EHC \) (kJ/kg) = 13 100           | 0.04308 0.04308 0.04308 0.04308 0.04308 0.0434 0.04308 |
| \( \dot{q}(t) \) (kW) = 11.143        | 0.04308 0.04308 0.04308 0.04308 0.04308 0.04308 0.04308 |
| \( \dot{u}(\dot{q}(t)) \) = \( \sqrt{(11.143 - 11.122)^2 + (11.143 - 11.1176)^2 + \cdots + (11.143 - 11.700)^2} = 0.647 kW \) |
| \( \dot{U}(\dot{q}(t)) \) = \( \dot{u}(\dot{q}(t)) \cdot k = 0.647 \cdot 2 = 1.294 kW \) |

Like the GUM method, the Kragten one can take into account the uncertainties of measuring devices, but also those related to ambient conditions, operators, materials or other sources of influence. In order to, introduce these parameters a parameter representing a global source of error (repeatability, accuracy and reproducibility) have to be added in Table 1, whose value is always equal to 1 and whose value of its uncertainty corresponds to the influence of the parameter (i.e. the standard deviation for a repeatability).
COMPARISON WITH OTHERS METHODS

Table 2 compares the results obtained with the GUM, the Kragten and the Monte Carlo approach. Results obtained with Kragten method are very close to the ones obtained with Monte Carlo approach. However, the calculation time of the Monte Carlo method is close to 2h for each value of HRR (20 runs of 1e6 random number) whereas the results are obtained several minutes using Kragten’s approach.

| Value of HRR (kW) | Uncertainty of HRR (kW) | GUM | Kragten | MCS |
|-------------------|-------------------------|-----|---------|-----|
| 11.143            | 0.650                   | 0.647| 0.642   |     |
| 0.610             | 0.036                   | 0.047| 0.047   |     |
| 0.404             | 0.024                   | 0.039| 0.035   |     |
| 0.151             | 0.009                   | 0.034| 0.033   |     |
| 0.066             | 0.004                   | 0.033| 0.032   |     |

Table 2. Uncertainty of HRR according to the GUM, Kragten and Monte Carlo (MCS) method.

Figure 2 shows that of the relative contribution of each variable of the uncertainty calculated using Kragten’s method or GUM (Guillaume et al. [13]) are in accordance. For HHR less than 2 kW, the variable of oxygen concentration pilots the uncertainty while above it is the C-factor. These observations had already been proven for full-scale fire tests [8]. In this specific case, the GUM method does not capture the influence of the oxygen concentration as the two other approaches. The error is caused by the covariance of several parameters and the non-linearity because the term $xO_2$ appears twice in the Eq. 4.

| Value of HRR (kW) | Relative Uncertainty of HRR with k=2 (%) |
|-------------------|----------------------------------------|
| 11.143            | 11.7                                   |
| 0.610             | 11.6                                   |
| 0.404             | 11.6                                   |
| 0.151             | 11.6                                   |
| 0.066             | 11.6                                   |

Fig. 2. Relative evolution of the different components uncertainty according to the HRR. Left: this study – Right: Guillaume et al. [13].

Then, the relative uncertainty changes as a function of the HRR decay for the Kragten and Monte Carlo methods, whereas it remains constant using the GUM approach (Table 2). This last point is contrary to the observations of Guillaume et al. [13] which specifies that above a 2 kW HRR, the relative uncertainty (according to the GUM method) increases very rapidly. Above 12 kW, the relative uncertainty of HRR remains constant and slightly less than 10% for the Kragten and the Monte Carlo methods, as shown in Table 2.

CONCLUSION

When the mathematical formulation of the measurand becomes complex or involves many parameters, it is shown that the Kragten method is a good alternative to the GUM or the Monte Carlo approaches. The calculation of the uncertainty is easier because of the absence of the coefficients of sensitivity. Besides Kragten method is simple and fast to use (a few minutes of treatment), because only the uncertainty of each variables, the value of the variables and the mathematical formulation to determine the HRR has to be specified (Eq. 4).
In the end, the precision of the uncertainties is very close to the Monte Carlo method whereas the computation time is extremely fast. The Kragten method is thus the most accurate when variables are interdependent and when covariance is unknown or poorly controlled, which is exactly the case concerning the heat release rate determination.

Moreover, the Kragten method is applicable to all results of the cone calorimeter determined by a multivariable measure. This concerns the mass loss rate, specific mass loss rate and total heat release rate.

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