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Experimental Error Assessment of Laminar Flame Speed Measurements for Digital Chemical Kinetics Databases

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Abstract

This paper focuses on the uncertainty sources in experimental techniques applied for laminar flame speed measurements. The work was motivated due to the necessity to develop flexible standard sets of the key experimental parameters and descriptors to be included in the machine-readable files of digitalized data repositories such as ReSpeTh, PriMe, CloudFlame, etc. Besides identifying and making the data findable through the associated parameterized descriptions, available information should be interoperable with numerical codes evaluating uncertainty of experimental data. These uncertainty boundaries are very important for interpreters of the data and for development of statistical methods applied for

the kinetic model optimization. On this way, four most common used techniques—Heat Flux Method (HFM), Bunsen Flame Method (BFM), Spherical Flame Method (SFM) and CounterFlow Method (CFM) were analyzed. The possible sources of experimental uncertainties have been investigated using data published by different research groups. Respective principles and structures of the experimental uncertainty sources for each studied method have been described. The uncertainty sources, their parameters and descriptors have been classified and systematically summarized in a universal data set to be used in the XML files of digitalized data repositories.

Keywords:

laminar flame speed; error assessment; model optimization; machine-readable files

1. Introduction

Laminar flame speed (LFS) is one of the most important characteristics for combustion investigation. Accurate measurement and prediction of LFS is important for development and validation of kinetic models [1, 2]. The main problem is that the different measuring methods exhibit large scatters for results. Moreover, even measurements performed with the same method but obtained employing different approaches and/or in different laboratories yield different results. In the past decades, great attention has been paid to the development of experimental techniques for measuring of LFS [3-10] and a number of excellent reviews on LFS measurements have been published over the years [10-14]. These reviews summarize remaining problems and challenges in the LFS measurements. The source of inaccuracy of LFS data, which unfortunately could not be avoided, follows from the equipment, experimental procedures, and data processing. Thus, one can classify two groups of uncertainty sources in flame speed measurements: equipment or "hardware" uncertainties and numerical interpretation of measured data, data processing (software) uncertainties. The human factor might be assessed only by the experimentalists themselves.

To establish the numerical methods for objective evaluating the uncertainty of measured data, it is necessary to fix the different error sources and evaluate them quantitatively. That helps by expanding growth of the amount of experimental data to develop the advanced technologies for digitalized collecting data and making them

findable, interoperable and interpretable (data mining). The machine-readable files should content all necessary information for that. In this paper we try to collect it for the LFS measurements. Therefore, our aim is not to establish an error assessment methodology for any particular measurement system, but to collect all basic uncertainty sources, their criteria and parameters and summarize them all together. The past decades have seen a renewed improvement in uncertainty quantification and error assessment [15-18]. Gas phase reaction experimental database such as NIST Chemical Kinetic Database [19], ATcT database [20], ReSpecTh [21], CloudFlame [22, 23] and PrIMe [24] increased rapidly. PrIMe [23-25] has received much attention as the prototype for ReSpecTh CloudFlame [22, 23] and of the most promising cyber systems offering kinetic database platforms, calculations and data analysis tools. In the Warehouse, data is stored in form of Extensible Markup Language (XML) files. This format and its modifications are mostly used in digital databases and are easily compatible with numerical tolls implemented for statistical data analysis [24-28]. The main fields, which should be included in such files for data submission, storage and analysis are analyzed and described in the presented paper concerning the four most common methods for LSF measurement - Heat Flux Method (HFM), Bunsen Flame Method (BFM), Spherical Flame Method (SFM) and CounterFlow Method (CFM). The section 2 shortly describes these experimental technologies for the determination of LFS. The sources of experimental uncertainty for each method are analyzed and summarized in the section 3. The summary and conclusions are drawn in the final section. Open questions and future investigation are discussed in this section as well. We hope this work can promote and initiate the active discussion in kinetic community to find an optimal and objective form for presentation of the studied data in the digital form.

2. Experimental methods

In this part, an overview of four methods for LFS measurement is presented. Since a growing body of literature has examined the described experimental methods, only brief descriptions will be given here. However, as the numerical interpretation of measured data have less attention in then literature, we described those with same details. Details of designs of experimental installations are given in Supplement 1.

2.1 Bunsen Flame Method

Bunsen flame method is a traditional method used for laminar flame characteristic study [29-31]. A schematic of a Bunsen flame experiment system from He et al. [30] is shown in Fig. S1-1.

In this method, a conical flame under laminar flow condition is generated with a Bunsen burner. Once the conical flame has stabilized on the burner, it is then evaluated by optical methods such as streak photography or OH chemiluminescence. [29]. A distinction can be made between two methods for determining the laminar flame velocity [30]. In the first case, it is assumed that the burning velocity is the same everywhere on the flame surface. The laminar flame velocity can then be

calculated using the mass conservation rate:

$$\rho_u S_L A = \rho_u \dot{Q} \to S_L = \frac{\dot{Q}}{A},$$

where ρ_u is a density of unburned gas mixture;

 \dot{Q} -volume flow of the unburned gas mixture;

 S_L – laminar flame speed;

A – a size of the flame surface.

In order to use this method, an area A is required. This area is determined by analyzing the recordings of the flame using various programs (Figure 1). In the Fig. 1, the Abel-inverted recording is illustrated. The Abel inversion is a reconstruction of a circular, axisymmetric and two-dimensional function based on their mapping. This sets 2-D limits of the flames based on the maximum OH emission.

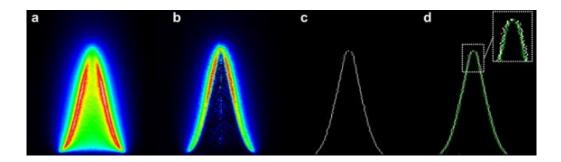


Figure 1. Processing of OH chemiluminescence recording: (a) original recording; (b)

Abel inverted image; (c) maximum intensified contour after Abel inversion; (d)

superimposed outlines of the images with / without Abel inversion (adopted from [30]).

In the second case, the angle of the conical flame is determined and used to calculate the flame velocity (Figure 2). The determination of the angle is carried out as in the

flame surface method by evaluating the recordings of the flame. This method is very convenient for straight-sided flames and requires aerodynamically contoured nozzles. Here, the speed of the gas mixture at the nozzle exit is assumed to be uniform and the laminar flame speed is then calculated:

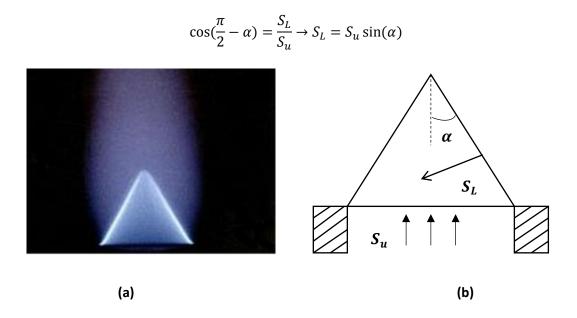


Figure 2. Bunsen flame: (a) photography of stoichiometric methane flame at 10 bar (DLR, Institute of Combustion Technology, Stuttgart); (b) schematic diagram of the conical Bunsen flame.

2.2 Heat Flux Method

In 1993, de Goey and coworkers introduced the heat flux method for stabilizing adiabatic flat flames and measuring laminar flame speed [3]. Since then many studies on this method have been performed [32-34]. The principle of the heat flux method is to use the heat flow to determine the flame speed. **Error! Reference source not found.** shows a schematic of a flat flame burner and its top view. The burner consists

of a burner head, a burner plate and a plenum chamber [32]. The gas mixture absorbs heat from the burner plate, causing an increase of the local burning rate of the adiabatic flame as compared to the local burning rate of non-preheated gas mixture at the exit of the burner plate. That causes thereby a stabilizing of the flame: if the velocity of the unburned gas mixture, S_u , equal to the laminar flame velocity, S_L , $(S_u=S_L)$, then the stabilized state is reached. In this state, the heat loss of the flame q_f equals the heat gain of the gas mixture q_g , $(q_f=q_g)$, which causes the net heat flux $\Delta q_{(f-g)}$ is equal zero.

From this result the relation with the laminar flame speed can be deduced:

$$\lambda_f \frac{T_{ad} - T_{in}}{\delta_{rz}} = \dot{m}c_p (T_{in} - T_0) = \rho_u S_u c_p (T_{in} - T_0),$$

$$S_u = \lambda_f \frac{T_{ad} - T_{in}}{\delta_{rz} \rho_u c_p (T_{in} - T_0)} = S_L,$$

where δ_{rz} -width of the reaction zone; δ_{vz} -width of preheating zone; λ_f -thermal conductivity coefficient in the reaction zone; T_{ad} -adiabatic temperature of the flame; T_{in} -temperature at the boundary between the reaction and preheating zone; T_0 -initial temperature or surface temperature of the burner plate; \dot{m} -mass flow of the unburned gas mixture; ρ_u -density of unburned gas mixture; c_p -specific heat capacity of the gas mixture.

In order to stabilize an adiabatic flame, a heating jacket with hot water to heat up the unburnt gas flowing through the burner plate, which can compensate the heat loss of the flame [3]. Thermocouples are attached on the burner plate radially to measure the

upstream surface temperature of the burner plate, as shown in Figure 3.

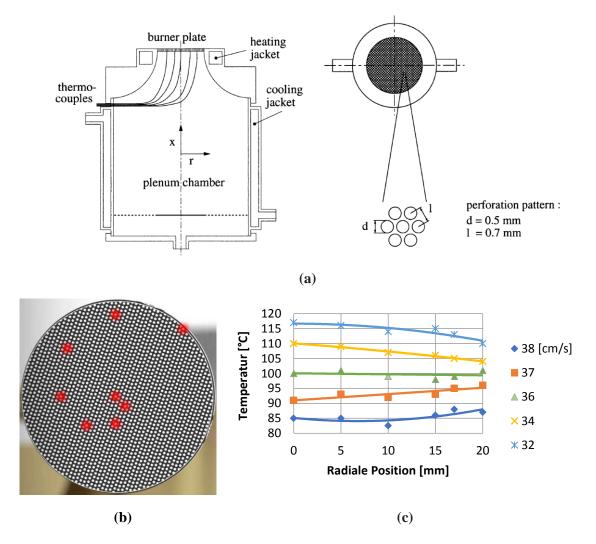


Figure 3. (b) A schematic of a flat flame burner and its top view (b) Flat flame burner and the $T_p(r)$ measurements points; (c) typical $T_p(r)$ vor different S_u

The objective here is to determine the inflow velocity at which the temperature profile over the entire surface of the burner plate is constant and corresponds to the temperature in the middle of the burner plate, where no heat losses occur. The measurements needed to determine are the temperature profile through the surface, $T_p(r)$, and velocity of unburned gas mixture, S_u . The measured temperature profile through the surface of the burner plate was analytically explained by De Goey et al.

[3]. Later, K. Bosschaart and L. De Goey [34, 35] simplified this temperature curve to the following equation:

$$T_p(r) = T_p(0) - \frac{\Delta q_{f-g}}{4\lambda_p b} r^2 \to T_p(r) = T_p(0) + \gamma r^2$$

where $\gamma=-\frac{\Delta q_{f-g}}{4\lambda_p b}$ is a parabolic coefficient and $T_p(r)$ -radial temperature profile of the burner plate; $T_p(0)$ -temperature in the middle of the burner plate; b-width of the burner plate; λ_p -thermal conductivity of the burner plate in the radial direction; Δq_{f-g} -net heat flow. The adiabatic state is reached when the temperature profile is even or constant $T_p(r_i)=T_p(0)$. This is the case when $\gamma=0$ and thus, $\Delta q_{f-g}=0$, which describes the state where the heat losses in the burner plate are zero and can be neglected. The speed of the gas mixture S_u is varied and the respective radial temperature profiles are measured. Thereafter, the respective temperature profile is adjusted to the parabolic curve using the least squares method, with γ_i as the parabolic coefficient, Fig. 3b. The individual γ_i are adapted to a function $\gamma(S_u)$ using the method of least squares and then plotted as a function of corresponding incident velocities, Figure 4.

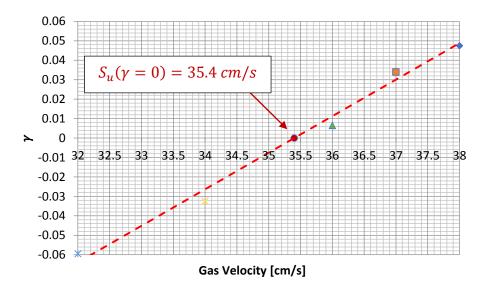


Figure 4. An example of graphic for determining $\gamma = 0$ and thus $S_u = S_L$

It can be seen from the Fig. 4 that the velocity S_u equals $\gamma = 0$ (with $S_u = 35.4$ cm/s) and thus one also finds the laminar flame velocity S_L .

2.3 Spherical Flame Method

In the spherically symmetric flame, the radial propagation velocity of the spherically symmetric flame front is measured to derive the laminar flame velocity. Unlike other methods, which operational ranges are limited to a few atmospheres due to flame stability problems; this technic is applicable at elevated pressures and temperatures. Two methods can be used to measure flame speed in this methodology: recording the flame front-constant pressure method [36, 37] and recording the pressure rise history constant volume [8, 9, 38] method.

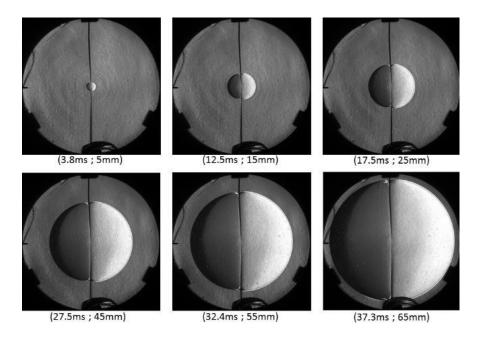


Figure 5. Flame front propagation in the combustion chamber (adopted from [39]).

In this method, the premixed fuel and air mixture are filled in the chamber with known initial temperature and pressure conditions. The mixture is centrally ignited and the propagation of the spherical flame front can be recorded with a high-speed camera, as shown in Fig [39]. Before the ignition, a vacuum state is established in the combustion chamber by a pumping system. The flame front to be examined is subject to a stretch or curvature. First, the radial propagation velocity of the flame, S_n , is calculated following $S_n = \frac{dr}{dt}$. The propagation velocity of the unstretched flame, S_b , is then obtained from Markstein length and stretch rate. After determining S_b , the laminar flame velocity, $S_{L,u}$, with respect to unburned mixture, is calculated from the following continuity equation:

$$\rho_u S_{L,u} = \rho_b S_b \rightarrow S_{L,u} = S_b \frac{\rho_b}{\rho_u},$$

where ρ_b and ρ_u are the densities of the burned or unburned gas mixture.

2.4 Counterflow Flame Method

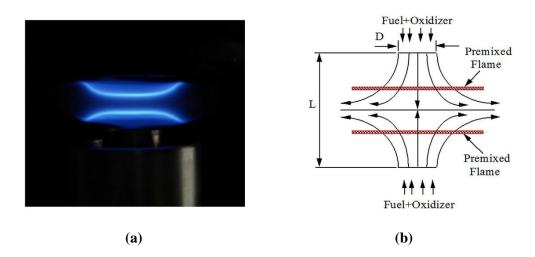


Figure 6. Counterflow flame: a) image b) schematic [12].

As described in [5, 40-45], the basic principle of this method is to create a plane of stagnation by directing two identical gas mixture streams against each other. Ignition creates two flames, one on each side of the plane, as shown in Fig. 6. The objective here is to stabilize a flat as possible one-dimensional flame, which is necessary to investigate the structure, stability and extinction of pre-mixed and non-premixed flames [46-48].

The counterflow flames have a stretch effect, it makes the velocity vary with the nozzle radius [49, 50]. The scale of stretch depends on the ratio of the nozzle distance to the nozzle diameter. Therefore, in this method, the axial velocities, $S_{u,ax}$, measured by Digital Particle Image Velocimetry (DPIV) technology as a function of the distance from the nozzle exit and the associated scale rates, K, are used to determine the laminar flame velocities, Fig. 7, [12, 51]. The minimum of the

measured axial velocity directly in front of the flame front is defined as the reference flame velocity, $S_{u,ref}$, and is plotted as a function of the associated scale rates defined as the slope. The ascertain data is then extrapolated either linearly or non-linearly to determine the strain-free reference flame velocity for K = 0, which is defined as the laminar flame velocity. The difference between linear and non-linear extrapolation is quite large, as the linear method tends to overestimate the laminar flame velocity.

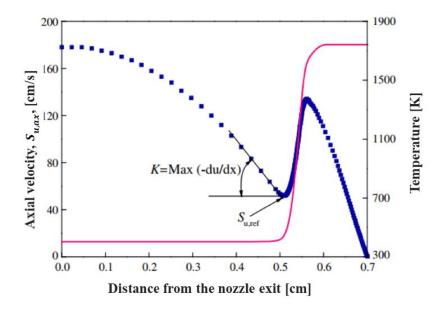


Figure 7. Line: Temperature profile; Symbol: axial velocity profile (counterflow)

(adopted from [6])

3. Uncertainty Sources Analysis

How it was be already noted, the systematical uncertainty of LFS measurements follow from factors related to the experimental design ("hardware") and procedure ("software"). In this part, the section 3.1 lists the uncertainty sources shared by four studied methods. Section 3.2-3.5 analyzes the characteristics that are related to each individual analyzed method of the LFS determination.

3.1 Common Uncertainty Sources

Some systematical uncertainty sources related to manufacture, experimental condition deviations, measurement facilities, premixed mixture preparation, heat loss, etc. can be assumed as common for the studied methods. Unfortunately, we could not find the exact quantitative evaluations of these errors in the literature. The different estimations of individual factors were done in some studies [3, 12, 37, 49, 52-58]. The uncertainty boundaries for experimental devices are mostly given by manufacturers. The inaccuracy of thermocouple, pressure sensor and mass flow controller can be directly evaluated from recommendations of manufacturers. It is assumed that there is no independent (re)calibration. This characteristic can be replaced if a calibration is carried out. It is useful to note, that the calibration of the measuring instruments must be replicated with certain time intervals to obtain over time deviations.

The **specific material properties** of the burner may can cause to inaccuracy in the LFS measuring [59, 60] through unsmooth surface of the burner plate. It may have active sites with bound radicals, which can react with the fuel. These centers can also operate as catalysts, which can accelerate the reaction. This uncertainty source is considered to contribute 0.2% to the total uncertainty of LFS.

The uncertainty of the **mixture preparation** can follow from the composition of air, specific properties of the fuel and the premixed mixture stoichiometry [61, 62]. There are three main sources of the air: compressed atmospheric air, factory made premixed O_2/N_2 gas in cylinders and O_2/N_2 mixture produced during the experiment. The

inaccuracy of the dilution ratio is considered as 0.2%. The impurity in liquid fuel can result in inaccuracies of equivalence ratio. Some fuels leave vestiges in the evaporator or in the line, which may have unknown chemical reactions and change the composition of the fuel.

The chemical and physical properties of fuel influence the measurements uncertainties through possible reactions with devices and phase change. If the fuel is CO, the interaction of CO and the material of the gas cylinder wall can produce nickel carbonyl or iron carbonyl [63, 64]. Considering that the flowing oscillation can lead to undesired changes in equivalence ratio and liquid fuels face a stronger oscillation than gaseous fuels due to the difference of supply system, there is a higher inaccuracy for liquid fuels than gaseous fuels, which are 0.5% and 0.2% for liquid and gaseous fuels respectively [61, 62]. If the fuel is liquid, a heating tube will be used to prevent the condensation of the vaporized mixture on the way from the evaporator to the chamber, and a long heating tube will increase the error [32, 65]. From the available database, it is deduced that the fluctuation of the flame velocities increases for quite lean and quite rich combustion, which can contribute 0.5% [5] to the uncertainty of LFS The experimental conditions, pressure and temperature are also sources for uncertainty of LFS determination [3, 66-71]. The real pressure and temperature of the test may not be the desired ones. It has been observed that in high-pressure experiments, the flame becomes unstable at pressures higher than 4 atm due to the fact that the diffusion of the radicals is slowed down and thus the velocity decreases,

so an uncertainty of 0.5% is added when the pressure is higher than 4 atm [5]. The influence of temperature can be evaluated following Alekseev et al.[11]:

$$S_{L,set} = S_{L,m} \left(\frac{T_{g,set}}{T_{g,set} + \Delta T_g} \right)^{\alpha}$$

where $\Delta T_{\rm g}$ is the temperature deviation, $S_{\rm L,set}$ is the LFS at the chosen temperature $T_{\rm g,set}$, $S_{\rm L,m}$ is the LFS at the measured temperature $T_{\rm g,set} + \Delta T_{\rm g}$, and α is the temperature exponent. The flame velocity $S_{\rm L,set}$ is proportional to $(T_{\rm g,set} + \Delta T_{\rm g})^{1-\alpha}$. Thus, applies to the error in the flame speed:

$$\frac{\Delta S_L}{S_L} = \frac{(1-\alpha)\Delta T_g}{T_{g,set}}$$

For a small α , the inaccuracy of the LFS is negligibly small. However, for gas mixtures at the explosive limit, α is large enough and the inaccuracy of LFS can increase up to 2%.

The **heat loss** of the flame caused by radiation has an influence on the downstream temperature. According to study of Yu et al. [72], the radiation-induced uncertainty in the spherical flames is within 2%. Chen's work [73] indicated that the difference caused by radiation re-absorption is within 1%. So here we give a limitation of 2% for the uncertainty caused by radiation in the LFS measuring.

The **numerical interpretation of measured data** involves some inaccuracies that cannot be eliminated. For the extrapolation, a linear method of approximation tends to overestimate the laminar flame velocity, so an uncertainty of 0.5% is added when a linear method is used [32, 74]. Moreover, every numerical method contribute 0.05% [58].

Table 1. Common uncertainty sources for LFS measurement.

| Source | Uncertainty (%) |
|--|-----------------|
| specific material properties of the burner | +0.2% |
| mass flow controller | Λ* |
| pressure sensor | Λ* |
| thermocouple | Λ* |
| composition of the air | +0.2% |
| | liquid: +0.5% |
| specific properties of the fuel | gaseous: +0.2% |
| length of the heating tube | L > 2 m: +0.2% |
| atai ahi amatuu | φ < 0.8: +0.5% |
| stoichiometry | φ > 1.4: +0.5% |
| | up to 1.5% |
| pressure | p > 4atm +0.5% |
| temperature | up to 2% |
| radiation | up to 2% |
| numerical method | basic: +0.05% |
| numericai method | linear: +0.5% |

 $^{*\}Lambda$ is the measuring error self-calibrated or specified by the manufacturer.

The common uncertainty sources for LFS measurement analyzed in this section are listed in Table 1. These uncertainty sources are very common in experimental works and are shared by the following four methods, so that they will not be discussed repeatedly. Except the measuring error determined by manufacturers, the errors of temperature and the heat loss caused by radiation contribute the two highest values to the total uncertainty. The error sources of properties of the reactants, the length of

heating tube and numerical method can be reduced by making a better experiment design or choosing a good source of fuel and air. It is difficult to give exact quantitative evaluations of these errors, especially for some extreme conditions like high temperature and fuel lean cases. The values here, also in the following sections, are generally estimated based on the references and help with identification of different uncertainty sources.

3.2 Uncertainty sources for Bunsen flame method

The factors that influence the LFS determination in the Bunsen flame method are as follow:

- (a) Nozzle geometry: A large nozzle contraction ratio is beneficial for keeping a steady laminar flow at the nozzle outlet [29].
- (b) Length of the line burner: A ratio of line burner length and burner tube diameter higher than 50 can ensure a laminar flow [60].
- (c) Diameter of the burner tube: A diameter of the burner tube between 4mm and 12mm is beneficial for the flame stability [29].
- (d) Placement of the thermocouple: A thermocouple can be placed in the center of the burner to measure the temperature of the gas mixture. This thermocouple can interact with the laminar flow, which will lead to inaccuracy in the LFS [75].
- (e) Height of the flame: A short flame will lead to an increase of the heat loss at the burner edge. On the contrary, a high flame will contribute to the expansion effect.

Both of too short or too high flames can generate high uncertainty in the determination of LFS [76].

- (f) Pilot flame: Without a pilot flame, it is difficult to stabilize the jet flame because of the heat loss at the burner edge. However, the thermal effect of the pilot flame on the main flow cannot be neglected [76].
- (g) H₂ proportion (Syngas): The LFS shows a linear development for H₂ content between 10% and 70%. Outside this range, the LFS shows an obvious non-linear variation and increasing fluctuation. In addition, a large H₂ proportion can lead to a rapid burning and make it difficult to stabilize the flame, and a low H₂ proportion with a higher CO fraction will cause poor burning [29].

Considering the above described factors, the uncertainty sources for LSF measurement in the Bunsen flame method are listed in Table 2.

Table 2. Uncertainty sources for LFS measurement in Bunsen flame method.

| Source | Uncertainty (%) |
|-------------------------------|----------------------------|
| Nozzle geometry | +0.2% |
| Length of the line burner | L/d< 50: +0.2% |
| Diameter of the burner tube | d > 12 mm: +0.5% |
| | d < 4 mm: +0.5% |
| Placement of the thermocouple | yes: +0.5% |
| Pilot flame | with pilot flame: +0.2% |
| | without pilot flame: +0.5% |
| Height of the flame | h <10mm: +0.5% |
| | h >30mm: +0.5% |

| H2 proportion (Syngas) | [H ₂] <10%: +0.5% |
|------------------------|-------------------------------|
| | [H ₂] >70%: +0.5% |

3.3 Uncertainty sources for heat flux method

The factors that influence the LFS determination in the heat flux method are as follow:

- (a) Diameter of the burner plate: Due to the interactions with ambient air, the edge effect can cause nonuniform distributions in the heat flux and radial diffusion. However, a quasi-one-dimensional laminar flame assumption can be applied to the central part of the flame surface. Its size is influenced by the stoichiometry, the speed of the gas mixture and the diameter of the burner plate. A burner plate with a larger diameter can lead to a larger central flame surface. On the contrary, a small burner plate diameter, especially in low-pressure conditions, makes the inaccuracy non-negligible because of the nonuniform effect on the laminar flame velocity [77, 78].
- (b) Cooling / Heating system: The temperature difference between the heated burner plate and the gas mixture has no direct influence on the flame speed, but affects the stabilization of the flame. A small temperature difference may cause a premature extinction to the flame. Therefore, it is important to keep the temperature difference large enough to ensure a stabilized laminar flame [11, 79].
- (c) Number of thermocouples: Blocking of the holes in the burner plate for thermocouples can affect the flame by interfering the uniformity of the gas mixture

flow [12, 32]. The error can be estimated by:

$$error = \frac{nA_{TE}}{A_{Br}},$$

with n – number of thermocouples; $A_{TE}=4\pi r_{TE}^2$ – area of the holes, and $A_{Br}=4\pi r_{Br}^2$ – surface of the burner.

Considering the above factors, the uncertainty sources for LSF measurement in the heat flux method are listed in Table 3.

Table 3. Uncertainty sources for LFS measurement in heat flux method.

| Source | Uncertainty (%) | |
|------------------------------|---|--|
| Diameter of the burner plate | d < 16 mm: +0.5% | |
| Cooling / Heating system | dT < 30 K: +0.2% | |
| North of Assessed | The percentage of blocked holes is then the gross | |
| Number of thermocouples | error in LFS: e.g. 0.5% (of the 30 mm burner) | |

3.4 Uncertainty sources for Spherical Flame Method

The factors that influence the LFS determination in the spherical flame method are as follow:

- (a) Product residues: Before each test, the chamber is rinsed several times with dry air to remove the residual products of the previous test, but it is possible that these products are not completely eliminated, which can affect the results of the new test [36, 80].
- (b) Time to set a homogeneous condition: It takes time to reach the homogeneous state in the chamber, so that the condition may not be 100% homogeneous state when

the mixture is ignited [7].

- (c) Ignition delay: The ignition delay can affect the recording time and make a source of error [81, 82].
- (d) Measuring radius: For a small radius, the flame is influenced by the ignition and electrodes. For a large radius, the flame can be influenced by the wall effects (premature extinguishing of the flame, the assumption of constant pressure is no longer valid for the large radius) [58, 83].
- (e) Thinning agent: The thermal-diffuse instability of the flame increases with increasing proportion of diluent, for example CO2 diluent, since this reduces the H2 content [38].

Considering the above factors, the uncertainty sources for LSF measurement in the spherical flame method are listed in Table 4.

Table 4 Uncertainty sources for LFS measurement in spherical flame method

| Source | Uncertainty (%) |
|-------------------------------------|--|
| product residues | 0.2% |
| time to set a homogeneous condition | 0.5% |
| ignition delay | 0.5% |
| measuring radius | r < 7 mm: 0.5% |
| | $r > \frac{r_{in,VK}}{2}$: 0.5% |
| | $(r_{in,VK})$ is the inner radius of the |
| | combustion chamber) |
| thinning agent | used: 0.5% |

3.5 Uncertainty sources for Counterflow Method

The factors that influence the LFS determination in the spherical flame method are as follow:

- (a) Nozzle geometry: The same as the Bunsen flame method, a large nozzle contraction ratio is beneficial for keeping a steady laminar flow at the nozzle outlet [45].
- (b) Nozzle distance-relationship: The ratio of nozzle pitch to nozzle diameter L/D has an influence on the rate of elongation and the one-dimensional flame assumption [43].
- (c) Silicone fluid particles: Silicone fluid articles can affect the composition of the fuel and its behavior [41, 42, 84].
- (d) Co-flow: A N_2 -CO flow can be used to shield the counterflow flame from the environment, otherwise the interaction between the flame and ambient air or radial diffusion can lead to the flame instability [41].

Considering the factors described above, the uncertainty sources for LSF measurement in the spherical flame method are listed in.

Table 5. Uncertainty sources for LFS measurement in counterflow flame method.

| Source | Uncertainty (%) |
|------------------------------|------------------------|
| Nozzle geometry | +0.2% |
| Name distance relationship | L/D < 1: +0.2% |
| Nozzle distance-relationship | L/D > 1: +0.2% |
| Silicone fluid particles | +0.2% |
| Co-flow | without co-flow: +0.5% |

3.6 Optimization of XML-data

Based on the identified possible sources of uncertainty for the different methods for determining the laminar flame speed, the XML files, earlier used in PrIMe, were extended with additive fields and indicators which describe the sources of the measured data uncertainty. Table 6 contains the information collected in the performed data error analysis. It is a universal list containing all possible uncertainty sources appearing in four studied laminar flame speed techniques of measurements described above. The methods are abbreviated as follows: heat flux method (HFM), Bunsen flame method (BF), spherical flame method (SF) and counterflow method (CF). The first column, Category, contains the categories of the error sources. The second column, Error Source, contains the error sources. The third column contents related methods. The column Property Name contains parameters that determine uncertainty sources. The last column Label contains the indicators of the error prescribed to parameters used in the developed XML file.

Table 6. Summary of error parameters.

| Category | Error Source | Method | Property Name | Label |
|----------|-------------------------|--------|-----------------------|-------|
| Design | Burner plate diameter | HFM | BurnerDiameter | D |
| | Heating/Cooling System | HFM | BurnerHeadTemperature | T_B |
| | | | ChamberTemperature | T_C |
| | Number of thermocouples | HFM | BurnerDiameter | D |
| | | | PerforationDiameter | D_P |

| | | | NumberTC | N_TC |
|-------------|--------------------------|------------|-------------------------|--------|
| | Heating tube length | HFM, BF | TubeLength | L_T |
| | Burner tube length | BF | TubeLength | L_B |
| | Burner tube diameter | BF | BurnerTubeDiameter | D_B |
| | thermocouple in the flow | BF | TCPresence | TC |
| | Pilot flame | BF | PilotFlame | PF |
| | Measuring radius | SF | RadiusMin | R_m |
| | wicasuring radius | 51 | RadiusChamber | R_ch |
| | Nozzle distance ratio | CF | NozzleDistance | L |
| | Nozzie distance rano | Cr | NozzleDiameter | D_N |
| | Co-Flow | CF | CoFlow | CF |
| | Calibrations | HFM, BF, | OwnCalibration | OC |
| | Calibrations | SF, CF | ManufactureCalibrations | MC |
| | Mass flow controller | HFM, BF, | MassFlowController | MFC |
| | Mass flow controller | SF, CF | | MITC |
| | Pressure controller | HFM, BF, | PressureController | PC |
| G-lile ti | Tressure controller | SF, CF | | 10 |
| Calibration | Coriolis mass flow | HFM, BF, | CoriolisMassFlow | CMFC |
| | controller | SF, CF | Controller | CIVITC |
| | Thermocouples | HFM, BF, | TCScatter | TCS |
| | | SF, CF | UnburntGasTemperature | T |
| | | 51, C1 | | 1 |
| | Temperature controller | BF, SF, CF | TemperatureController | TempC |
| Process | Fuel properties | HFM, BF, | | - |
| | | SF, CF | FuelProperties | F |
| | H2 matio (Symmass) | HFM, BF, | H2-Ratio | H2-R |
| | H2-ratio (Syngas) | SF, CF | 112-Nau0 | 112-K |

| | Pressure | HFM, BF, | Pressure | P |
|-----------------------------|------------------|----------|------------------------|------|
| | | SF, CF | | |
| | Equvalence ratio | HFM, BF, | EgivelenceDatio | Phi |
| | | SF, CF | EqivalenceRatio | FIII |
| | Dilution | SF | Dilution | DL |
| Linear or non-linear method | | HFM, SF, | LinearExtrapolation | ExL |
| | | CF | NonLinearExtrapolation | ExNL |

4. Summary and conclusion

Having analyzed a very large set of data [11, 12, 29, 32, 38, 41-43, 45, 60, 75-79, 81-84]. We can conclude that researchers are reluctant to present detailed analyses of the uncertainty of their measured data. Very often, we have to follow from one reference to another one to find the background work, which describes the experimental facilities in detail and, probably, explains sources of possible errors. Very often, two publications are many years apart, so that the background work could be considered only approximatively.

Nevertheless, we analyzed experimental device configurations, diagnostics and experimental methodologies of the four techniques widely applied for the flame speed measurements and defined parameters and indicators, which describe the important sources of the experimental uncertainties. Some parameters are common for all four techniques and their minimal contribution to the error can be estimated to within 5%-6%, as shown in Table1.

It is worth to note that the parameters which we describe are related to the systematical errors only and random errors have to be determined by investigators. Generally, parameters, which we collected in Tables 1-5, can be exactly determined only by each experimental group individually How it follows from our evaluations, in ideal cases, systematic uncertainties, conditioned by peculiarities of each methodology, can reach 3%-4% for the Bunsen flame method, 1.5%-2% for the heat flux method, 3% for the spherical flame method and 1.5%-2% for the counterflow method.

The Table 6 presents the generalized factors, which we propose to include in the corresponding fields of XML files used for submission of experimental data in the digitalized data depositaries. Keywords, specifying the meaning of the properties, are machine and human interpretable and interoperable for further handle in numerical tools applied for uncertainty analysis.

Digitalized, parameterized descriptions of experimental devices and methodologies are today the fundamental processes of data storing and data mining. We would like to emphasize that this work is not a presentation of a final start-of-art in the LFS data uncertainty, but an invitation to discuss this problem with focus on the data structure for machine-readable files. One of the purposes of this work is to initiate the discussion devoted to the reporting studied experimental data. It is very useful and actual to establish the consortia of researchers for developing standards and rules for systematical cataloging data in a machine-readable format and data exchange

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