Full-scale performance testing of hydrogen combustion mechanisms in a wide range of experimental conditions

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Abstract

To facilitate the transition to new carbonless fuels, an evaluation of currently available detailed combustion mechanisms of hydrogen is made. A data collection of 2190 experimental measurements of laminar burning velocity (LBV) in flames of neat hydrogen was collected from 65 literature publications and encoded in the RKD v2.5 format of the ReSpecTh database. From this collection, 1938 data points were used to test 31 detailed combustion mechanisms published during the last decade. A quantitative evaluation has shown that while some of the mechanisms have shown auspicious results, none of the mechanisms were able to achieve a good performance in more than 90% of all data points. Moreover, an investigation of separate subsets of data related to different experimental conditions has shown that none of the mechanisms can be considered the best in all of the studied conditions, and therefore, the possibilities of further improvement could be found by performing a sensitivity analysis. The largest discrepancies between experimental and simulation results have been found for measurements of LBV in the presence of CO_2 as a bath gas. Thus, the corresponding kinetic parameters require a targeted study.

Keywords: Hydrogen combustion; Laminar burning velocity; Detailed kinetic mechanism; Mechanism testing.

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1. Introduction

The rising demand for a reduction of CO_2 emissions inspires different studies in energy generation and transportation areas. The possible way to achieve this goal is by using alternative fuels with zero or low-carbon content, including pure hydrogen (H_2) and its blends with ammonia (NH_3) or other fuels. One of the aims of our studies is to create a new, reliable hydrogen combustion mechanism with a good performance in different conditions, including those relevant for practical applications.

While detailed combustion chemistry of H_2 has been studied for a long time, continued publications of new experimental data have shown that available mechanisms are still far from perfect. Moreover, the hydrogen combustion scheme serves as a foundation for all high-temperature combustion mechanisms of hydrocarbons and oxygenates. Therefore, its improvement would also be beneficial for other areas of combustion chemistry.

As a first step on the path of mechanism development, it is important to analyze already existing detailed H_2 combustion mechanisms and identify the most reliable and efficient of them. For this purpose, it is necessary to perform testing of mechanisms with the same validation data set, using as many different experimental conditions as possible. Such a task was performed approximately a decade ago by Olm et al. [1] and led to the creation of an optimized H_2 combustion mechanism by Varga et al. [2]. However, several recent studies have proposed new additions and modifications to the well-known H_2 oxidation scheme, and detailed mechanisms that have adopted them have shown a better performance in certain conditions. Moreover, there are several new publications presenting H_2 mechanisms optimized using different methods, strategies, and experimental test sets [3–5]. Analyzing all this information is important to create a hydrogen combustion mechanism of a new generation.

This study aims to investigate the efficiency of recently developed, detailed H_2 kinetic models using all available experimental data, including the latest publications in the field. However, due to the very high amount of data and information, the first step of this investigation includes only laminar burning velocity (LBV) measurements.

2. Experimental data selection

In this work, great attention was paid to the preparation of the data collection for the evaluation of the combustion mechanisms. As mentioned in the previous section, in this stage of the study, only laminar burning velocities measurements were used where H_2 was the only fuel.

Experimental measurements were gathered from literature publications and encoded in data files of RKD (ReSpecTh Kinetics Data) v2.5 format [6]. Each series of measurements (also called data series) is stored in a separate data file of XML (Extensible Markup Language) format, and each file has a unique identifier. For each data series, the standard deviation (σ) was evaluated according to the common procedure:

$$\sigma^2 = \sigma_{sys}^2 + \sigma_{scat}^2 , \quad (1)$$

where σ_{sys} is defined by the experimental article authors' uncertainty estimation, if it is reported in the paper, or by the type of experimental method as proposed by Zhang et al. [7], and σ_{scat} is an estimation of the experimental scatter performed with the *Minimal Spline Fit* computer program [8].

During the previous optimization of the H_2 mechanism [2] a collection of experimental data was gathered and stored in the ReSpecTh database [9]. It included 73 XML files containing 636 measurements of LBV, from 22 publications. These files were updated to the latest RKD version and had the standard deviation reevaluated according to the novel procedure. Experimental data from new research articles published after the initial study was finished was also gathered and encoded. A total of 210 new XLS files were created, containing 1554 LBV measurements from 43 publications.

This collection encompassed a broad range of experimental conditions: initial temperatures from 100 K to 915 K, pressures from 0.2 to 25 atm, equivalence ratios from 0.15 to 7.14, and different diluent gases (N_2, Ar, He, CO_2, H_2O). However, some experimental points were excluded from the mechanism testing procedure for two reasons:

(i) Thermodynamic parameters of species provided in most detailed mechanisms in the form of polynomial fitting (NASA polynomials) are not verified for temperatures below 200 K and can provide unrealistic results at very low temperatures, causing the simulations to fail. Therefore, simulations of datapoints with initial temperatures below 200 K have shown a very high failure rate and were excluded from the mechanism comparison.

(ii) In some cases, multiple experimental datasets have the same initial conditions (or very close ones). If one of such datasets contradicts several others, it is considered an outlier and excluded from the procedure. An example of such a comparison has been shown by Konnov et al. [10].

3. Simulation details

Simulations were carried out with the Optima++ simulation framework code [11], developed at the ELTE Chemical Kinetics Laboratory. Optima++ reads the RKD format data files, sets up simulation tasks based on their content, and invokes a simulation package to perform the requested simulations. In this work, all flame simulations were performed using the Cantera package [12], taking into consideration multicomponent diffusion and the Soret effect (thermal diffusion). Then, Optima++ generates

Table 1
List of detailed kinetic mechanisms tested in the current work and results of an averaged error function calculation.

Mechanism ID	Mechanism size: used (orig.)		Reference	$E_{average}$			
	Species	Reactions		H_2O	CO_2	High-P	**All data**
Mei-2021	17 (40)	53 (257)	[13]	**11.4**	**28.7**	18.0	**12.5**
Glarborg-2018	18 (151)	72 (1397)	[14]	16.5	37.6	**12.1**	**12.5**
HP-2017	17 (92)	57 (612)	[15]	32.6	35.7	**12.0**	**13.9**
FFCM-1-2016	16 (38)	58 (291)	[16]	36.9	40.1	**11.5**	**14.0**
Konnov-2023	25 (498)	150 (5719)	[17]	31.0	52.2	13.5	**14.3**
AramcoMech(3.0)-2018	20 (581)	73 (3037)	[18]	24.1	35.6	**13.1**	14.4
NUIGMech(1.1)-2021	19 (2746)	79 (11279)	[19]	33.1	34.1	**12.4**	14.5
GDFkin-2016	15 (123)	40 (934)	[20]	21.0	38.6	15.5	14.8
Sun-2022	15 (44)	51 (266)	[21]	30.4	**29.8**	16.0	15.5
Konnov-2019	16 (15)	75	[22]	31.0	67.6	31.4	16.0
Burke-2012	13	27	[23]	26.0	66.4	29.2	17.1
CRECK(H2/CO)-2020	21	62	[24]	**10.8**	**26.9**	23.0	18.4
ELTE-2016	15	44	[25]	54.5	53.2	14.4	20.0
ELTE-2015	13 (12)	30	[2]	44.0	76.8	35.9	20.1
Sharipov-2024	14 (35)	47 (256)	[26]	43.9	77.0	36.0	20.1
Hashemi-2015	13	29	[27]	**13.5**	87.6	41.4	20.2
Wang-2024	13 (12)	38	[28]	40.3	91.1	38.6	20.3
SanDiego-2016	16 (59)	40 (271)	[29]	27.0	53.0	31.1	21.4
Konnov-2015	16 (15)	74	[30]	20.0	75.5	44.0	21.8
Keromnes-2013	14	29	[31]	**10.1**	42.3	28.5	21.9
USC-II-2007	15 (111)	48 (784)	[32]	47.6	52.2	14.1	21.9
Wang-2023	16	41	[33]	37.4	**17.2**	34.8	22.0
JetSurF(2.0)-2010	16 (348)	55 (2163)	[34]	53.6	52.7	14.7	23.6
Zhang-2021	12 (11)	32	[35]	29.7	132.5	56.8	24.0
Wang-2022	12 (11)	19	[3]	35.0	102.1	53.1	24.8
Li-2015	14	37	[36]	64.6	56.7	14.1	26.5
Shrestha-2021	16 (125)	65 (1099)	[37]	107.3	42.2	32.0	27.5
Alekseev-2015	12 (11)	30	[38]	**13.9**	99.8	57.4	29.0
Cao-2024	12 (11)	9	[4]	57.8	**27.1**	27.1	29.5
GRI-Mech(3.0)-1999	15 (53)	48 (325)	[39]	124.0	77.1	71.9	54.2
Vlasov-2016	13 (12)	30	[40]	37.5	512.7	223.8	73.1

figures that compare the experimental data with the simulation results and compute various metrics about the quality of the reproduction of the experimental data.

For this study, we selected mostly mechanisms that were developed for flames of hydrogen or its mixtures with other fuels and published during the last decade because H_2 mechanisms released before 2014 were already evaluated during the previous study [1]. This list was expanded to include mechanisms that showed the best performance in the previous study, as well as several popular and frequently used mechanisms for comparison. However, some of the latest mechanisms were skipped because they inherited their hydrogen submechanism from one of the previous mechanisms without any modification, and therefore, their simulation results of hydrogen flames were almost identical. A list of 31 mechanisms selected for participation in the current testing is presented in Table 1.

There were two types of adjustments which had to be made:

(i) Some of the mechanisms don't include He and/or CO_2. To be able to simulate all of the datasets, these molecules were added with necessary thermodynamic and transport parameters as a non-reactive species. This is not the best solution, as most researchers consider it necessary to add 3rd body coefficients for these gases in several important reactions of hydrogen combustion. This issue will be discussed further in the text.

(ii) Mechanisms that included hydrocarbons or NO_x chemistry were truncated, removing all hydrocarbons, except for syngas chemistry, and all nitrogen-containing species, except for N_2, and their corresponding reactions. This was mainly done to reduce computational time, as these species and reactions should not have any considerable impact on this study. CO chemistry, however, was kept to check if it plays any considerable role in studied conditions when CO_2 is used as a bath gas.

Modification in the number of species and reactions in each of the tested mechanisms is shown in Table 1.

4. Quantitative mechanism comparison

In most publications in literature, the performances of different mechanisms are assessed by the visual inspection of figures in which the experimentally measured results are plotted together with model predictions. However, when validation is made against a large set of experimental measurements, it is preferable to use a suitable quantitative method. In this work, we continue to use the method suggested by Turányi et al. [41], which was successfully applied in several studies (for example, [1,7,42]).

Let us have N experimental data series, each stored in a separate data file, in the data collection utilized in the mechanism comparison. Let N_f denote the number of data points in the f-th data series. The averaged error of the mechanism predictions relative to the experimental results is described by the averaged error function as follows [43]:

$$E = \frac{1}{N}\sum_{f=1}^{N}\frac{1}{N_f}\sum_{d=1}^{N_f}\left(\frac{Y_{fd}^{\mathrm{sim}} - Y_{fd}^{\mathrm{exp}}}{\sigma\left(Y_{fd}^{\mathrm{exp}}\right)}\right)^2, \qquad (2)$$

where index f goes through all data series in the data collection, and index d goes through all data points in the f-th data series. Y_{fd}^{exp} and $\sigma\left(Y_{fd}^{exp}\right)$ are the optionally transformed experimentally measured result (data point) and its standard deviation, respectively. The corresponding Y_{fd}^{sim} value is the optionally transformed simulation result for that data point. For LBV measurements, an absolute error was calculated for each data point and provided in the XLS files. Thus, no transformation was needed.

It is assumed that the experimental data follow a normal (Gaussian) distribution; therefore, the function E follows a reduced chi-square distribution. $E = 1$ means that the average deviation between the model predictions and experimental data is equal to the standard deviation of the experimental data. In principle, the value of E can be smaller than 1, but in practice when a large number of data points is investigated, it rarely happens. A smaller E value means better mechanism performance. From this, it also follows that if $E \leq 4$ or ≤ 9, then the model can reproduce the measurement results within their 2σ or 3σ uncertainty limits, on average, respectively.

5. Results and discussion

After all simulations were finished, it was found that some data points could not be reproduced within their 4σ uncertainty limits with any of the investigated mechanisms. These data points may have very large systematic errors that were not considered, or they are related to experimental conditions none of the mechanisms can describe satisfactorily yet. We could not identify which one was the real reason, but these data points were excluded from the quantitative comparison for all models to ensure that the conclusions were unbiased.

All in all, considering the abovementioned reasons and cases described in section 2, a set of 1938 data points was used for mechanism evaluation. For additional analysis, 3 subsets were selected: experiments with the addition of water vapor to the unburnt gas flow (H_2O – 140 data points); measurements with a partial or complete replacement of dilutant gas with carbon dioxide (CO_2 – 136 data points); and measurements obtained at elevated pressures, from 2 bar and higher (High-P – 409 data points). Values of averaged E function, calculated for the full set of data and each of the subsets, are presented for all 31 tested mechanisms in Table 1.

The best overall performance was observed for mechanisms by Mei et al. [13] and Glarborg et al. [14], both of which were initially developed for the combustion of ammonia and ammonia/hydrogen flames, and therefore, considerable attention was paid to the core hydrogen parts of these mechanisms. A good overall score was also shown by several "large hydrocarbon" mechanisms.

Using an averaged value of error function for mechanism evaluation has one flaw that should always be kept in mind. If a mechanism performs very badly only in certain experimental conditions, for which it wasn't designed in the first place, this will heavily affect an overall score. Therefore, it is possible to represent testing results differently. In Figure 1, all tested mechanisms are sorted according to the amount of data points for which the mechanism's simulation result lies beyond the 4σ from experimental data. It is interesting to notice that while the top positions are still kept by mechanisms of Glarborg et al. and Mei et al., they are followed by several mechanisms developed earlier specifically for hydrogen combustion.

It is important to mention that during the previous H_2 mechanism optimization study [2], no datasets which used CO_2 as a diluent gas were considered. Thereby, no 3rd body efficiency coefficients for CO_2 were included in our previous mechanism and some of the other H_2 mechanisms, while mechanisms developed for hydrocarbon combustions usually include this type of information. A very poor performance in this subset is the main reason why H_2 mechanisms by Burke et al. [23], Konnov et al. [22], and Hashemi et al. [27] achieved a lower overall score than more recent hydrocarbon mechanisms, being more reliable at the same time in hydrogen flames.

It is interesting, that the best performance in the CO_2 subset is achieved by the mechanism of Wang et al. [33], which is a recent mechanism optimized for syngas combustion and was finely tuned for this kind of conditions. However, averaged error functions in this subset are generally higher than for a full set of data points, leading to the conclusion that CO_2 as a bath gas for hydrogen flames should receive additional attention in the future.

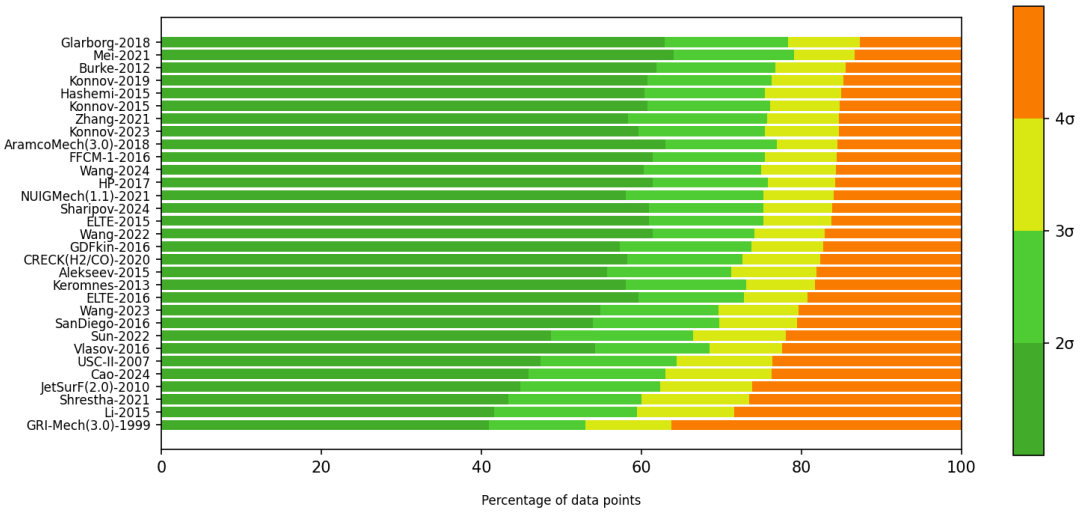

Fig. 1. Stacked bar plot of the ratio that a mechanism can reproduce the LBV data points within a given threshold compared to the estimated standard deviation. The full experimental data set was considered.

H_2O is always produced during H_2 combustion, but its effects on combustion kinetics become much more important if it is added directly to the unburned mixture because, otherwise, its concentration achieves considerable values only in the high-temperature post-flame area, and impact on the kinetic scheme remains negligible. For this subset 3rd body efficiency coefficients are also very important, however, several mechanisms achieved relatively low values of averaged error function in the current study. Surprisingly, the best agreement with experimental data here was achieved by mechanisms developed for syngas combustion: Keromnes et al. [31] and CRECK [24].

The last subset selected for a separate investigation is the measurements at elevated pressures, and it is considered important because in many practical applications, combustion or oxidation is performed in a high-pressure environment. The best mechanisms for this subset are mostly the same as in the overall performance rating. However, hydrocarbon mechanisms provided somewhat better results, and the mechanism by Mei et al. [13] is lagging behind.

To summarize the results, it can be said that the best averaged error values achieved by the tested mechanisms are more than 12, which corresponds to the simulation results being in the interval between 3σ and 4σ of experimental uncertainty on average. This result can be improved by a stricter thinning out of the data collection and exclusion of a larger amount of less reliable data points from testing or by reducing their statistical weight during averaging. However, because none of the mechanisms was able to outclass all the other mechanisms in all of the data subsets at the same time, it is clear that better results can be achieved, and further studies in hydrogen combustion kinetics would be beneficial.

6. Conclusions

A comprehensive quantitative comparison of 31 detailed reaction mechanisms was performed using a large number of experimental measurements of laminar burning velocity for the pure hydrogen flames. The investigated data collection contained 2190 data points from 65 literature publications, which were encoded in RKD format XML files.

Detailed combustion mechanisms by Glarborg et al. and Mei et al. have shown the best performance, but these mechanisms also cannot reproduce the experimental data within their 3σ uncertainty limits, on average, even after the exclusion of less reliable data points from the testing procedure.

It was also found that the best performance in different experimental conditions is achieved by different detailed mechanisms; in particular, the presence of H_2O and CO_2 in the combustible mixture greatly affects the performance of most mechanisms. These results highlight the need for the cross analysis of the mechanisms via sensitivity analysis to identify the possibilities for further improvement.

Current results will be combined with the testing results obtained for other types of experiments, i.e., ignition delay times and specification measurements, to outline the imperfect elements in the current combustion kinetics and develop a strategy for the creation of a hydrogen combustion mechanism of a new generation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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