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# Chemical kinetics calculation of H<sub>2</sub> Laminar Flame Speed: assessment of the performance of public available mechanisms at engine relevant conditions

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**Abstract.** The laminar flame speed (LFS) of actual fuels is a critical property to consider when approaching the computational fluid dynamics (CFD) simulation of turbulent flame propagation in internal combustion engines. A significant gap persists between the conditions under which LFS can be measured and the engine conditions, particularly in terms of pressure and temperature, at high loads in high-specific power engines. Chemical kinetics simulations can be employed to calculate LFS at high pressures and temperatures by using mechanisms that cannot, however, be validated under such conditions due to the unavailability of experimental data. In this study, a literature review was conducted to identify measured values of H<sub>2</sub> LFS to be compared with calculated ones through chemical kinetics simulations, using various published chemical schemes. A methodology is developed to assess the reliability of the tested mechanisms for CFD engine simulations, considering more relevant experimental data at higher pressures and temperatures, low dilution, and near-stoichiometric conditions. At low pressures and temperatures (i.e. at part-load engine conditions), all the considered chemical mechanisms yield similar results consistent with those of the Verhelst correlation. However, as the physical conditions move toward a high-load representative one, the choice of chemical scheme for LFS calculation can significantly impact the prediction of turbulent flame speed in actual engines, leading to non-negligible discrepancies.

## 1. Introduction

Hydrogen as a fuel for internal combustion engines is one of the possible viable options to contain tailpipe emissions of vehicles in a short to medium term period. Fuelling internal combustion engines with hydrocarbons leads to issues related to emissions of greenhouse gases, unburnt hydrocarbons, soot and NO<sub>x</sub>, while, with hydrogen only NO<sub>x</sub> emissions are possible. Moreover, the strong know-how on internal combustion engines design combined with the ability to retrofit existing power units, can significantly accelerate the decarbonization of the transportation sector (1). Engine design is currently even more driven by the outcomes of detailed 3D-CFD studies of in-cylinder processes that, with traditional fuels, have been proven effective in accurately replicating experimental evidence regarding fuel/air mixing, combustion, and emissions



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formation in both research and production engines (2–4). Well-established models and methodologies are available to deeply characterize and optimize in-cylinder processes. Focusing on engine combustion, the accuracy of the simulation relies on the ability of the “flamelet” model to capture the correct burn rate by estimating the flame front propagation in a highly turbulent environment. In such “flamelet” conditions the wrinkling effect of turbulence enhances the laminar flame speed by increasing the flame surface. In 3D CFD simulations of engine combustion, as the flame structure deviates from the 1D unstretched laminar premixed one, the combustion model, to account for the effect of turbulence, plays a crucial role in the correct prediction of the burn rate. Many correlations and approaches are available to account for flame speed enhancement due to turbulence. The tuning of model/correlations parameter is common to improve the simulation reliability especially moving outside the model’s validation ranges. In some cases, the model tuning effort could be related to under/over prediction of the LFS that is an input for the combustion model. However, the reduction of the uncertainties on the applied LFS of the actual fuel plays an important role in reducing the weakness of the overall simulation framework. In the past, the most widely employed approach for the estimation of the LFS at engine relevant conditions was based on the extrapolation of empirical correlations obtained by fitting experimental measurements at temperature/pressure levels far from the target ones (5,6). More recent works are performed to improve the reliability of such correlations fitting LFS values calculated at high pressure/temperature, through chemical kinetics simulations, instead of experimental data (7–9). The need to rely on chemical mechanisms that cannot, however, be validated under such engine conditions is therefore mandatory. In recent years, the increase of the available computational power, has allowed to build wide databases of chemistry-based LFS at engine relevant conditions avoiding issues related to the definition of fitting functions.

As for carbon-containing fuels, the same “flamelet” modelling approach can be effectively applied for the simulation of hydrogen combustion in both research and production engines (10,11); the definition of a reliable LFS is still pivotal especially when high pressure/temperature conditions are met. The Verhelst correlation (12,13) is widely adopted to prescribe LFS among a wide range of equivalence ratios; however, the correlation is valid up to 40 bar and this makes it unusable when approaching full load engine operations. As for fossil fuels, that issue can be overcome using detailed chemistry to calculate LFS through 1-D chemical kinetics simulations. Focusing on hydrogen, the difficulty in measuring LFS at high pressure/temperature due to thermo-diffusive instabilities, make chemical kinetics based study, that for their nature cannot consider instability effects (13), very important in understanding the hydrogen flame characteristics such as LFS and laminar flame thickness (LFT).

The current work aims to identify the most reliable published mechanisms to simulate hydrogen laminar flame speed and thickness. A methodology to compare experiments and simulations is therefore developed to define the best performing schemes when moving towards engine-like conditions. At first mechanism validation is performed by comparing simulation results with experimental data, and after, an assessment of the performance of the mechanisms at uprising thermodynamic conditions is performed emphasizing as the adoption of different schemes for the calculation of the LFS could strongly affect the predicted burn rate in an actual engine case.

## 2. Chemical kinetics mechanisms

Many detailed chemistry mechanisms to model molecular hydrogen oxidation pathway are available in literature. However, the reactions, thermodynamic and transport files necessary to perform simulations are not always freely available for all the published ones.

Furthermore, most of the chemical kinetics mechanisms are validated and adopted to model syngas (a blend of H<sub>2</sub> and CO) (14,15) or ammonia/hydrogen combustion (16,17). Considering that the presence of CO stabilizes the flame, a mechanism created to model syngas could not be as reliable when simulating hydrogen only.

**Table 1.** Tested chemical schemes available online.

Ref.	Year	Mechanism	Species	Reactions	Weighted mean error without He dilution [%]	Weighted mean error [%]
(20)	2020	CRECK	21	62	10.8	18.4
(21)	2020	NUIG 1.1	34	236	4.6	11.4
(22)	2019	KONNOV	15	75	5.8	11.9
(23)	2004	LLNL <sup>a</sup>	10	21	6.8	-
(24)	2021	XJTUNO-2021	44	266	4.3	10.1
(25)	2021	ZHANG	11	32	4.9	11.7
(15)	2005	DAVIS	13	38	5.0	10.5
(26)	1999	GRI 3.0 <sup>a</sup>	53	325	7.8	-
(27)	2022	C3 v3.3	34	245	3.8	12.4
(28)	2016	UCSD	68	311	8.1	18.9
(14)	2014	WANG	14	43	4.1	12.1

<sup>a</sup> Unable to simulate mixture with helium dilution.

In Table 1 the eleven considered schemes in the present study are listed: NUIG 1.1, DAVIS (USC), GRI 3.0, ZHANG, KONNOV, LLNL (O'CONNOR), XJTUNO-2021, CRECK (PoliMi), UCSD, WANG and C3 v3.3. It is noteworthy to underline that the reaction mechanism of NUIG 1.1 has a modular structure: reactions are stored in subgroups, from C0 to C7, among which only C0 group regards hydrogen oxidation: to reduce computational cost, the subgroups from C1 to C7 are not considered. As well in C3 v3.3 mechanism, the reactions including carbon-based molecules were removed to easily simulate hydrogen oxidation, without altering the consistency of the results. Some chemical schemes, such as GRI 3.0 and UCSD, are characterized by a higher number of reactions because they model also CO chemistry. In others, such as NUIG 1.1 and XJTUNO-2021, the modelling of NO<sub>x</sub> chemistry, which increases the number of reaction and computational cost as well, has beneficial effects on the overall accuracy of the mechanism. The transport files employed with different kinetics schemes are the ones provided by the authors of the mechanisms.

### 3. Laminar flame speed data collection

Literature research was carried out to find hydrogen laminar flame speed (LFS) experimental measurements at conditions as similar as possible to engine ones.

**Table 2.** Experimental datasets reporting hydrogen-air laminar flame speed measurements and the weight assigned to each one of them following the relevance criteria.

Ref.	Paper	Dataset	Eq. ratio range	Diluter & Dilution	Temp. [K]	Pressure [MPa]	Weight assigned
(29)	Tse et al. (2000)	1A	0.8 to 2.0	He:O <sub>2</sub> =11.5:1	298	1	5
		1B	0.8 to 2.0	He:O <sub>2</sub> =11.5:1	298	1.5	7
		1C	0.8 to 2.0	He:O <sub>2</sub> =11.5:1	298	2	10
(30)	Hu et al. (2009)	2A	0.5 to 2.5	-	303	0.1	5
		2B	0.5 to 2.5	-	373	0.1	7
		2C	0.5 to 2.5	-	443	0.1	10
(31)	Krejci et al. (2013)	3A	0.5 to 2.5	He:O <sub>2</sub> =7:1	298	0.5	3
		3B	0.5 to 2.5	He:O <sub>2</sub> =7:1	373	0.5	5
		3C	0.5 to 2.5	He:O <sub>2</sub> =7:1	443	0.5	7
(18)	Grosseuvre et al. (2019)	4A	0.8 to 2.5	-	296	0.1	1
		4B	0.5 to 2.5	-	363	0.1	1
		4C	0.5 to 2.5	-	413	0.1	1
(18)	Grosseuvre et al. (2019)	5A	0.8 to 2.5	N <sub>2</sub> :O <sub>2</sub> =5.67:1	296	0.1	3
		5B	0.5 to 2.5	N <sub>2</sub> :O <sub>2</sub> =5.67:1	363	0.1	3
		5C	0.5 to 2.5	N <sub>2</sub> :O <sub>2</sub> =5.67:1	413	0.1	5
(18)	Grosseuvre et al. (2019)	6A	0.8 to 2.5	N <sub>2</sub> :O <sub>2</sub> =9:1	296	0.1	1
		6B	0.8 to 2.5	N <sub>2</sub> :O <sub>2</sub> =9:1	363	0.1	1
		6C	0.8 to 2.5	N <sub>2</sub> :O <sub>2</sub> =9:1	413	0.1	3
(18)	Grosseuvre et al. (2019)	7A	0.8 to 2.5	20% H <sub>2</sub> O	363	0.1	5
		7B	0.8 to 2.5	20% H <sub>2</sub> O	413	0.1	7
(18)	Grosseuvre et al. (2019)	8A	0.8 to 2.5	30% H <sub>2</sub> O	363	0.1	3
		8B	0.8 to 2.5	30% H <sub>2</sub> O	413	0.1	5

Due to the physicochemical properties of H<sub>2</sub>-air flames it is difficult to experimentally track a well-defined flame front at engine relevant conditions. This is the reason why in most of the literature LFS measurements with undiluted mixtures at NTP (Normal Temperature and Pressure) condition only (T=298 K and p=1 bar) are reported. However, some experimental data are available at higher temperatures (443K) or pressures (20 bar) but accepting massive dilutions with inert gases such as helium.

In Table 2 the source of collected data adopted for mechanisms validation are reported. The equivalence ratio range is similar for all the datasets while different pressure/temperature and dilution/diluter are considered. The collected data are organized in datasets as the following: for each mixture composition (equivalence ratio and dilution) three or two different levels of

pressure/temperature are considered for a total of 22 datasets. The dataset nomenclature follows the criteria where the same number indicates the same composition (1, 2, ... up to 8): for each fixed number, i.e. fixed composition, different letters (A, B, C) identify different temperature/pressure levels (e.g 1A, 1B, 1C).

Among the datasets obtained with diluted mixtures, there are groups (7 and 8) that analyse LFS trends by considering water dilution (18). These data are particularly attractive for validation due to the possible interest in diluting hydrogen/air mixture by injecting water in the engine combustion chamber to avoid the risk of pre-ignition especially in high performance H<sub>2</sub>-ICEs.

#### 4. Methodology

The performed activity is organized in two steps to better understand the behaviour and evaluate the accuracy of the different mechanisms:

- in the first step each mechanism is tested performing simulations at the thermodynamic and mixture conditions experimentally tested to perform a direct comparison between measures and calculated data. The best-performing mechanisms are defined applying different weights to each experimental dataset as detailed in the next section.
- in the second step the mechanisms previously identified are employed to calculate laminar flame speed values at engine-relevant conditions targeting high-performance DI-H<sub>2</sub>-engines operated at stoichiometry. This step is crucial to assess how the adoption of different chemical schemes could affect the burn rate prediction in a 3D-CFD framework.

##### 4.1 Experimental validation method

To evaluate the accuracy of the mechanisms, each experimental point was simulated with the CONVERGE 1-D Freely Propagating chemistry tool (version 3.0.28). The accuracy of the mechanisms is strongly affected by the mixture composition, i.e. a best-performing mechanism in lean conditions could be less accurate in stoichiometric or rich conditions and vice versa. For this reason, a target equivalence ratio range should be set searching for the mechanism that performs well in the selected target conditions. The initial target for the activity is to define a LFS database to be used for the combustion simulation of a high-performance DI hydrogen engine operated at stoichiometric conditions. Considering direct injection and reduced time available for ideal (complete) charge homogenization, the attention is focused on the range of equivalence ratio near to stoichiometric conditions including as a target also slightly rich and lean mixtures ( $0.8 \leq \phi \leq 1.2$ ). To quantify the mismatch between each experimental point ( $S_{L,i}^{exp}$ ) and the calculated ones ( $S_{L,i}^{sim}$ ), the absolute value of the relative error ( $err_i$ ) is calculated as follows:

$$err_i = \left| \frac{S_{L,i}^{sim} - S_{L,i}^{exp}}{S_{L,i}^{exp}} \right| \cdot 100 \quad [\%] \quad (1.1)$$

The arithmetic mean error for each dataset i.e. for various equivalence ratio ( $err_m^k$ ) was determined as follows:

$$err_m^k = \frac{\sum_{i=1}^n err_i}{n} \quad [\%] \quad (1.2)$$

Where n is the number of points in the range  $0.8 \leq \phi \leq 1.2$  of the k-th dataset. Once the mean error for each chemical scheme and dataset is estimated, a weighted mean error is calculated assigning different weights to each experimental dataset as in the following equation:

$$\overline{err}_{mech} = \frac{\sum_N err_m^k \cdot w_k}{\sum_N w_k} \quad [\%] \quad (1.3)$$

Where  $N$  is the total number of considered datasets ( $N=22$ ) and  $w_k$  is the weight assigned to each of them as reported in last column of Table 2. The pivotal point of this procedure is the assignment of the appropriate relevance to each set of data to give higher importance to the data obtained at thermodynamic and mixture conditions closer to engine ones. Starting from a maximum weight of 10, which identifies the stronger link between the experimental condition and the engine one, to the minimum weight of 1, that identifies a very weak link, the intermediate values (7, 5 and 3) are assigned to the remaining sets as follows. The maximum weight is assigned to the datasets of the group 1 and 2 that include the experimental data collected at the highest pressure (2 MPa), accepting some helium dilution, and at the highest temperature (443 K) without dilution. For the sake of clarity, to the other sets in the same group a decreasing weight is applied going towards less severe conditions.

High relevance (7) is reserved for the set (7B) with an intermediate water dilution (20%), possible for a high-performance hydrogen H<sub>2</sub>-ICE with water injection, at the highest temperature available (413 K). The minimum weight is employed to avoid overweighting data collected under almost identical conditions (see group 4 almost superimposed to 2) and to almost neglect data measured at extreme diluted conditions and low temperatures (see group 6).

The performance of mechanisms with the lowest weighted mean error at engine relevant conditions will be deeply analysed in the next sections.

#### 4.2 Laminar flame speed at engine relevant conditions

**Table 3.** Pressure, temperature, equivalence ratio and EGR ranges adopted to create laminar flame speed datasets applying the most promising mechanisms.

	Min.	Max	Step
Equivalence ratio [-]	0.2	2.5	0.05
Temperature [K]	550	1250	20
Pressure [bar]	10	150	5
EGR <sup>a</sup> [%]	0	10	5

<sup>a</sup>EGR percentage is evaluated considering only N<sub>2</sub> as residual gas.

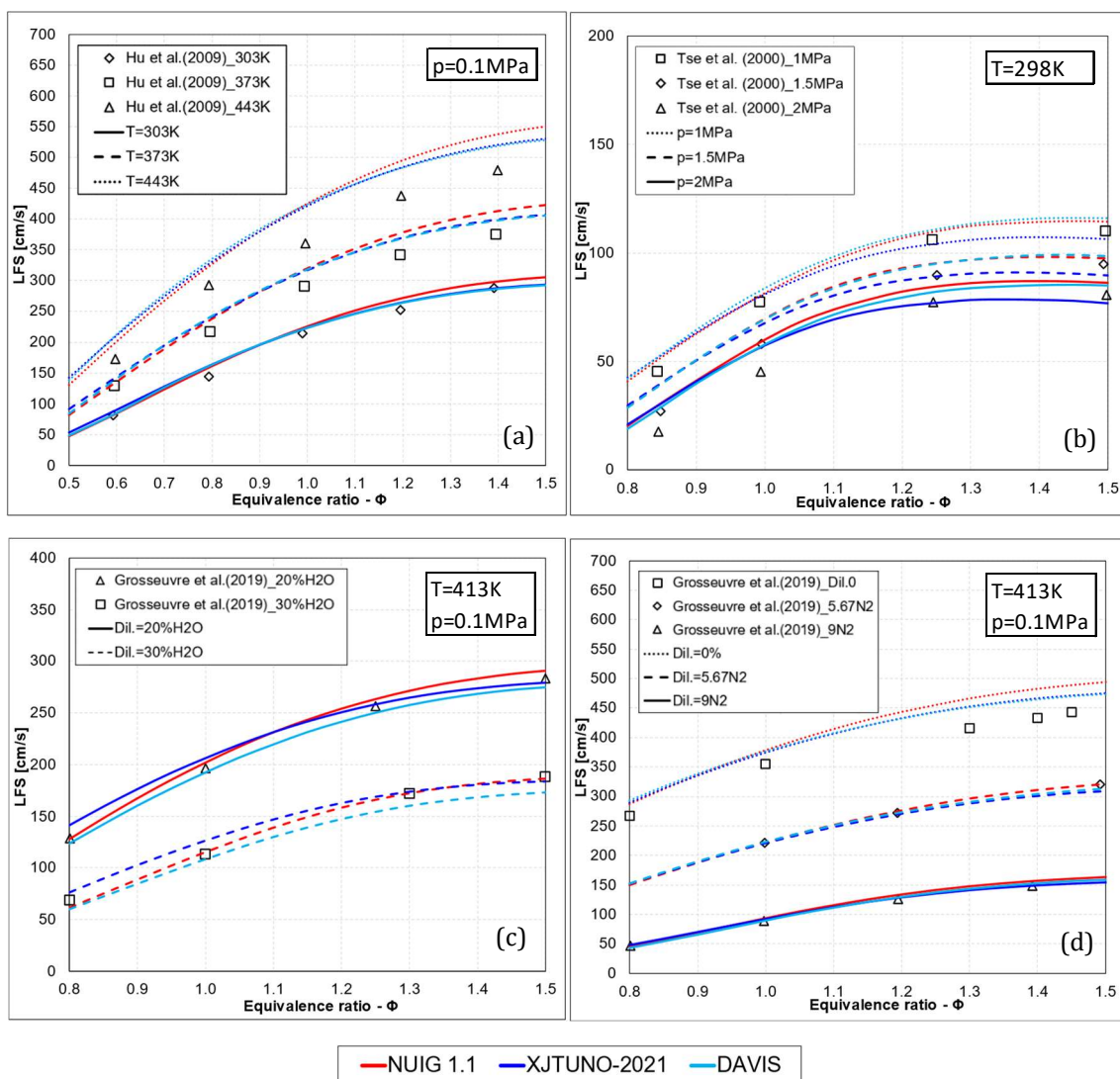
Engine relevant conditions are identified in terms of pressure, temperature, equivalence ratio and EGR dilution as listed in Table 3. The best performing mechanisms are used to generate databases using as stepping for each variable the ones reported in the table. The solver takes advantage of the previously calculated points as starting condition of the ones not already simulated. For sake of clarity each point is identified by a fixed value of pressure, temperature, equivalence ratio and EGR. For this reason, the choice of the interval (step) between consecutive points is crucial to improve simulation stability allowing to reach the convergence in most of the simulated points. To deeply assess the differences among the chemical schemes, some comparisons were carried out between the simulated values obtained with the mechanisms chosen during the validation process.

Some temperature sweeps of the laminar flame speed as function of equivalence ratio are reported at different pressures: these conditions are representative of possible pair of temperature/pressure that can be experienced by the mixture in the combustion chamber of an

actual H2 engine. To better assess the results, the data are compared with the LFS predicted by the GRI 3.0 mechanism, which is one of the widely adopted freely available mechanisms. The behaviour of hydrogen-air flames changes with dilution, leading to an LFS that is dependent not only on the dilution amount but also on the diluter composition. To have reasonably predictive CFD-3D combustion models the applied LFS must be as correct as possible also with diluted mixtures. For this reason, the LFS values calculated by the most reliable chemical schemes will be analysed also in the presence of some dilution.

## 5. Results

### 5.1 Weighted mean error



**Figure 1.** Points represent experimental measurements and lines simulated laminar flame speed with the best mechanisms identified. (a) Group 2. (b) Group 1. (c) Datasets 7B and 8B. (d) Datasets 4C, 5C and 6C.

Applying the procedures detailed in paragraph 4.1, the mean weighted errors are calculated. Some mechanisms such as GRI 3.0 and O'Connaire (LLNL) do not include Helium as a species. For this reason, the weighted mean error is calculated both considering or not the experimental datasets with helium dilution. The results using both methods are reported in Table 1. Despite considering a narrower experimental target, GRI 3.0 and LNL do not show the lowest weighted mean error. This result, coupled with the impossibility of comparing the calculated points with the highest pressure/temperature experimental data (obtained with He dilution), excludes them from the final mechanism choice. According to the results in the rightmost column of Table 1, three mechanisms show the highest accuracy: XJTUNO-2021, NUIG 1.1 and DAVIS. The first is the most reliable considering a weighted mean error of 10.1%.

Representative sample of laminar flame speed results are provided in Figure 1. The mechanisms identified show almost the same trends: slight difference with rich mixtures can be found using XJTUNO-2021. Simulated data with water and N<sub>2</sub> dilution fit very well the experimental target (Fig. 1, c and d) as well as at lower temperatures, while an overestimation of the calculated flame speed is noticeable when temperature increases (Fig. 1, a). The experimental trend increasing pressure for a fixed temperature is well captured as well (Fig. 1, b).

### 5.2 Comparisons at engine like conditions

Some comparisons of the flame speed calculated with the three previously defined chemical schemes (NUIG 1.1, XJTUNO-2021 and DAVIS) at engine relevant conditions are reported. The results are compared to the one obtained with GRI 3.0 mechanism.

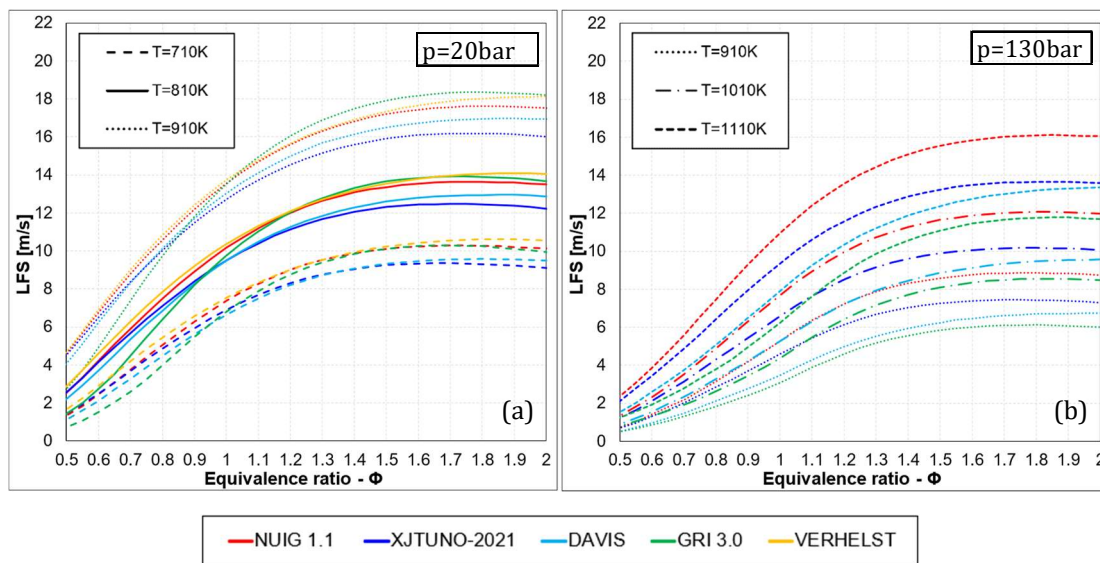
**Table 4.** Representative thermodynamic conditions of high-performance H<sub>2</sub>-DI-ICE.

Pressure [bar]	Temperature [K]	Equivalence ratio range
20	710 - 810 - 910	0.5 - 2.0
130	910 - 1010 - 1110	0.5 - 2.0

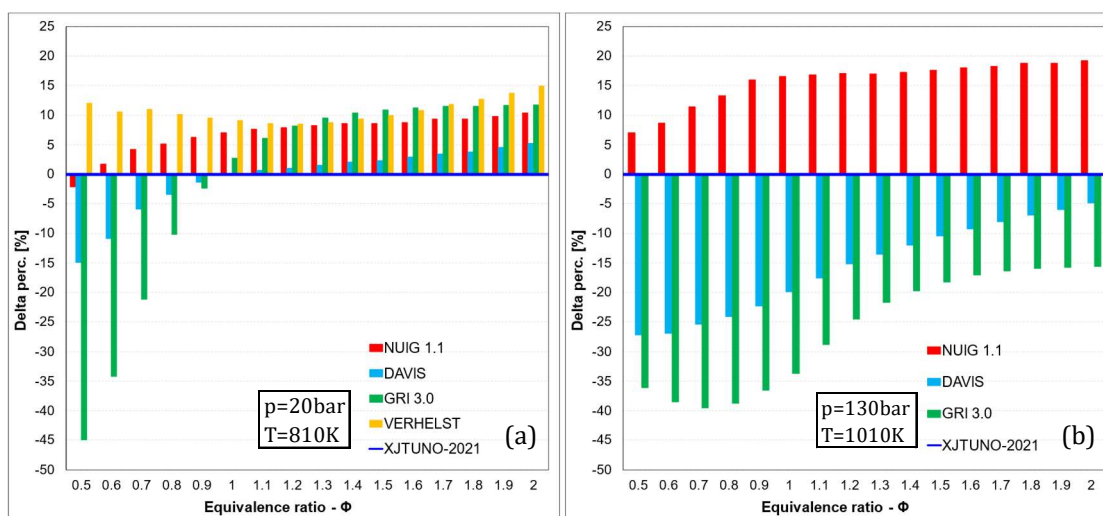
In Table 4 thermodynamic and mixture conditions considered for the analysis are listed. They are relevant for a high-performance DI-ICEs fuelled with a stoichiometric hydrogen/air mixture; the range of equivalence ratio is widened to consider the presence of stratified mixture inside the combustion chamber.

The sweeps of temperature at fixed pressures in Figure 2 show that the differences between the laminar flame speed simulated by different mechanisms increase with rising pressure and temperature. This attitude is underlined by the graphs in Figure 3 that report on the percentage difference between LFS predicted by the mechanisms analysed and XJTUNO-2021, as a reference, at two representative thermodynamic points (20 bar and 810 K; 130 bar and 1010 K).

At lower pressure and with lean mixture DAVIS and GRI 3.0 predict LFS values lower than the others; this trend changes going towards rich mixtures. DAVIS was created by tuning the reaction rates of GRI 3.0: it simulates LFS slightly higher than the latter, but with the same trend as GRI 3.0. In all the simulated conditions, the most reliable mechanisms identified predict different laminar flame speeds: those discrepancies increase with rising pressure and temperatures. In these conditions GRI 3.0 calculates the slowest flame speed, while NUIG 1.1 the highest one.



**Figure 2.** Hydrogen-air laminar flame speed sweeps of temperature at different pressures: (a) 20 bar; (b) 130 bar.



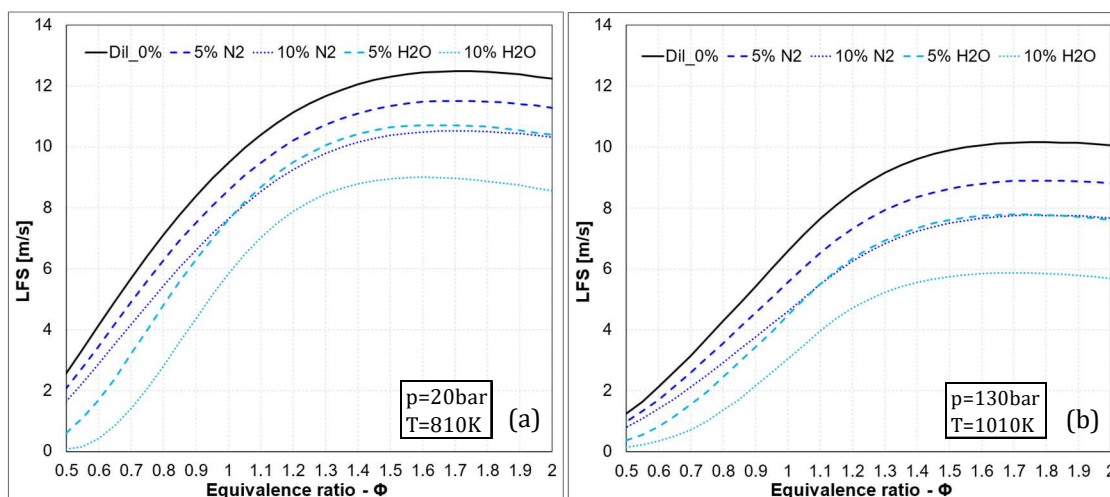
**Figure 3.** Percentage difference between LFS predicted by the mechanisms analysed and XJTUNO-2021 at: (a) p=20 bar and T=810 K; (b) p=130 bar and T=1010 K. At 20 bar is also reported the LFS calculated with Verhelst correlation.

Considering that the GRI 3.0 has been proven to be one of the less reliable in reproducing the experimental data among the validated mechanisms, the usage of a LFS calculated with it in a 3D CFD simulation of engine combustion is expected to produce non accurate results and a general underestimation of the burn rate. A similar but improved result can be obtained with DAVIS mechanism, whereas a too fast combustion is expected using NUIG 1.1.

At lower pressure (20 bar) the Verhelst correlation flame speed is almost superimposable with NUIG 1.1; moreover, with lean mixtures the correlation calculates LFS almost 40% higher than that predicted using GRI 3.0. At the same pressure condition, the Verhelst correlation has a quite similar trend to the XJTUNO-2021 inferred one: varying equivalence ratio, the correlation

overestimates the LFS of an almost constant 10% value with respect to the best performing mechanism.

More in details, at high pressure and temperature, comparing the three most reliable mechanisms identified, with respect to the reference XJTUNO-2021, a 15% overestimation of the LFS is expected with NUIG 1.1 mechanism (at stoichiometry), while a 20% underestimation is found with DAVIS in the same condition. NUIG 1.1 chemical scheme is more reliable when moving towards leaner mixture, while the DAVIS one performs better towards richer condition.



**Figure 4.** LFS simulated by XJTUNO-2021 with N<sub>2</sub> (blue) and H<sub>2</sub>O (light blue) dilution at: (a) p=20 bar and T=810 K; (b) p=130 bar and T=1010 K.

To deepen the analysis, in Figure 4 is reported the assessment of the behaviour of the most reliable mechanism (XJTUNO-2021) working with diluted mixtures: nitrogen and water. The introduction of water into the combustion environment subtract heat to the reactants. This heat reduction decreases the reaction rates and consequently laminar flame speed reduces. Furthermore, water is more effective than nitrogen in lowering LFS, especially with lean mixtures, influencing the hydrogen oxidation pathway by shifting the termination reaction towards higher temperature, similar to an increase in pressure (19).

## 6. Conclusions

In this work the accuracy of eleven chemical kinetics models to simulate laminar flame speed of hydrogen-air mixture focusing on the equivalence ratio range  $0.8 \leq \phi \leq 1.2$  is assessed. Literature research was conducted to collect experimental measurements of the LFS of H<sub>2</sub>-air mixtures. The data found were analysed and higher importance is assigned to the ones which are closer to the thermodynamic and mixture conditions representative of the ones experienceable by the hydrogen-air mixture in a high-performance DI-ICE fuelled with a globally stoichiometric charge. The simulations are performed by employing the 1-D Freely Propagating CONVERGE chemistry tool and the results are compared with their experimental counterpart. By means of a developed methodology based on the mean weighted average of global errors, the three most reliable mechanisms are defined. XJTUNO-2021, DAVIS and NUIG 1.1 are the best-performing ones and, more in detail, the lowest error (10.1%) is found with the first one.

A comparative analysis was carried out to examine the trends of the flame speed calculated by these chemical schemes at engine relevant conditions. GRI 3.0 mechanism, because of its widespread use, and Verhelst correlation are also considered in the comparative analysis. At low pressure and intermediate temperature (representative of ignition or part load engine conditions) the differences, in terms of predicted LFS calculated by the different mechanisms, are generally lower. The Verhelst correlation is reliable in that condition: varying the equivalence ratio, it has an almost constant overestimation (10%) of the flame speed with respect to XJTUNO-2021 mechanism. For lean mixtures NUIG 1.1 performs better than DAVIS that strongly underestimates the LFS similarly to GRI 3.0. In rich conditions, all the mechanisms overestimate the flame speed, but the relative difference is lower than 15%. At higher pressure/temperature (representative of the main combustion phase in a high-performance ICE) relative differences between the three best performing mechanisms are significantly higher: NUIG 1.1 overestimates the LFS, while DAVIS underestimation becomes higher moving toward lean mixtures.

To sum up, the XJTUNO-2021 mechanism is found to be the most reliable in predicting LFS at engine relevant conditions. With respect to that, the following conclusions can be drawn:

- Verhelst correlation is reliable for the LFS prediction at low pressure levels (up to 40 bar) with both lean and rich mixtures. A slight LFS overestimation, in the order of 10%, is experienced.
- NUIG 1.1 mechanism is reliable in a wide range of equivalence ratio and, generally, overestimates the flame speed at both low and high pressure/temperature levels.
- DAVIS mechanism is more reliable for rich mixtures, while a strong underestimation of the flame speed is expected in lean conditions.
- GRI 3.0 mechanism has a very similar behaviour compared to DAVIS one, but the underestimation of the flame speed is even more pronounced.

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## References

1. Kalghatgi GT. Developments in internal combustion engines and implications for combustion science and future transport fuels. *Proceedings of the Combustion Institute*. 2015;35(1):101–15.
2. Giovannoni N, Breda S, Paltrinieri S, D’Adamo A, Fontanesi S, Pulvirenti F. CFD Analysis of the Effects of Fuel Composition and Injection Strategy on Mixture Preparation and Fuel Deposit Formation in a GDI Engine. In 2015.
3. Iaccarino S, Breda S, D’Adamo A, Fontanesi S, Irimescu A, Merola S. Numerical Simulation and Flame Analysis of Combustion and Knock in a DISI Optically Accessible Research Engine. *SAE Int J Engines*. 2017 Mar 28;10(2):2017-01-0555.
4. Breda S, D’Adamo A, Fontanesi S, D’Orrico F, Irimescu A, Merola S, et al. Numerical Simulation of Gasoline and n-Butanol Combustion in an Optically Accessible Research Engine. *SAE Int J Fuels Lubr*. 2017 Mar 28;10(1):2017-01-0546.

5. Metghalchi M, Keck JC. Burning velocities of mixtures of air with methanol, isooctane, and indolene at high pressure and temperature. *Combust Flame*. 1982 Jan;48:191–210.
6. Gülder ÖL. Laminar burning velocities of methanol, ethanol and isooctane-air mixtures. Symposium (International) on Combustion. 1982 Jan;19(1):275–81.
7. D’Adamo A, Del Pecchia M, Breda S, Berni F, Fontanesi S, Prager J. Chemistry-Based Laminar Flame Speed Correlations for a Wide Range of Engine Conditions for Iso-Octane, n-Heptane, Toluene and Gasoline Surrogate Fuels. In 2017.
8. Del Pecchia M, Breda S, D’Adamo A, Fontanesi S, Irimescu A, Merola S. Development of Chemistry-Based Laminar Flame Speed Correlation for Part-Load SI Conditions and Validation in a GDI Research Engine. *SAE Int J Engines*. 2018 Apr 3;11(6):2018-01–0174.
9. Pessina V, Berni F, Fontanesi S, Stagni A, Mehl M. Laminar flame speed correlations of ammonia/hydrogen mixtures at high pressure and temperature for combustion modeling applications. *Int J Hydrogen Energy*. 2022 Jul;47(61):25780–94.
10. Sfriso S, Berni F, Breda S, Fontanesi S, Ramalho Leite C, Brequigny P, et al. Proposal and Validation of 3D-CFD Framework for Ultra-Lean Hydrogen Combustion in ICEs. In 2024.
11. Sfriso S, Berni F, Fontanesi S, d’Adamo A, Frigo S, Antonelli M, et al. Proposal and validation of a numerical framework for 3D-CFD in-cylinder simulations of hydrogen spark-ignition internal combustion engines. *Int J Hydrogen Energy*. 2024 Jan;53:114–30.
12. Verhelst S, T’Joel C, Vancoillie J, Demuynck J. A correlation for the laminar burning velocity for use in hydrogen spark ignition engine simulation. *Int J Hydrogen Energy*. 2011 Jan;36(1):957–74.
13. Verhelst S, Wallner T. Hydrogen-fueled internal combustion engines. *Prog Energy Combust Sci*. 2009 Dec;35(6):490–527.
14. Wang QD. An updated detailed reaction mechanism for syngas combustion. *RSC Adv*. 2014;4(9):4564–85.
15. Davis SG, Joshi A V, Wang H, Egolfopoulos F. An optimized kinetic model of H<sub>2</sub>/CO combustion. *Proceedings of the Combustion Institute*. 2005 Jan;30(1):1283–92.
16. Shrestha KP, Seidel L, Zeuch T, Mauss F. Detailed Kinetic Mechanism for the Oxidation of Ammonia Including the Formation and Reduction of Nitrogen Oxides. *Energy & Fuels*. 2018 Oct 18;32(10):10202–17.
17. Zhang X, Moosakutty SP, Rajan RP, Younes M, Sarathy SM. Combustion chemistry of ammonia/hydrogen mixtures: Jet-stirred reactor measurements and comprehensive kinetic modeling. *Combust Flame*. 2021 Dec;234:111653.
18. Grosseuvres R, Comandini A, Bentaib A, Chaumeix N. Combustion properties of H<sub>2</sub>/N<sub>2</sub>/O<sub>2</sub>/steam mixtures. *Proceedings of the Combustion Institute*. 2019;37(2):1537–46.
19. Santner J, Dryer FL, Ju Y. The effects of water dilution on hydrogen, syngas, and ethylene flames at elevated pressure. *Proceedings of the Combustion Institute*. 2013;34(1):719–26.
20. CRECK Modeling Group. CRECK\_2003\_SYNGAS [Internet]. Available from: <https://creckmodeling.chem.polimi.it/menu-kinetics/menu-kinetics-detailed-mechanisms/107-category-kinetic-mechanisms/401-mechanisms-1911-syngas/>
21. University of Galway. NUIG 1.1 [Internet]. [cited 2024 May 22]. Available from: <https://www.universityofgalway.ie/combustionchemistrycentre/mechanismdownloads/>
22. Konnov AA. Yet another kinetic mechanism for hydrogen combustion. *Combust Flame*. 2019 May;203:14–22.
23. LLNL. Hydrogen mechanism [Internet]. [cited 2024 May 22]. Available from: <https://combustion.llnl.gov/archived-mechanisms/hydrogen>

24. Sun W, Zhao Q, Curran HJ, Deng F, Zhao N, Zheng H, et al. Further insights into the core mechanism of H<sub>2</sub>/CO/NO<sub>x</sub> reaction system. *Combust Flame*. 2022 Nov;245:112308.
25. Zhang Y, Fu J, Xie M, Liu J. Improvement of H<sub>2</sub>/O<sub>2</sub> chemical kinetic mechanism for high pressure combustion. *Int J Hydrogen Energy*. 2021 Jan;46(7):5799–811.
26. Gregory P. Smith, David M. Golden, Michael Frenklach, Nigel W. Moriarty, Boris Eiteneer, Mikhail Goldenberg, et al. GRI 3.0 [Internet]. [cited 2024 May 22]. Available from: [http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/)
27. Dong S, Wagnon SW, Pratali Maffei L, Kukkadapu G, Nobili A, Mao Q, et al. A new detailed kinetic model for surrogate fuels: C3MechV3.3. *Applications in Energy and Combustion Science*. 2022 Mar;9:100043.
28. UC San Diego Combustion Research Group. San Diego Mechanism [Internet]. 2016 [cited 2024 May 22]. Available from: <https://web.eng.ucsd.edu/mae/groups/combustion/mechanism.html>
29. Tse SD, Zhu DL, Law CK. Morphology and burning rates of expanding spherical flames in H<sub>2</sub>/O<sub>2</sub>/inert mixtures up to 60 atmospheres. *Proceedings of the Combustion Institute*. 2000 Jan;28(2):1793–800.
30. Hu E, Huang Z, He J, Miao H. Experimental and numerical study on laminar burning velocities and flame instabilities of hydrogen–air mixtures at elevated pressures and temperatures. *Int J Hydrogen Energy*. 2009 Oct;34(20):8741–55.
31. Krejci MC, Mathieu O, Vissotski AJ, Ravi S, Sikes TG, Petersen EL, et al. Laminar Flame Speed and Ignition Delay Time Data for the Kinetic Modeling of Hydrogen and Syngas Fuel Blends. *J Eng Gas Turbine Power*. 2013 Feb 1;135(2).