Performance analysis of detailed reaction mechanisms of neat H_2, neat CH_4 and H_2/CH_4 mixtures under oxyfuel combustion conditions

Ákos Veres-Ravai[a,b*], Anna Hasche[c], István Gyula Zsély[a],
Hartmut Krause[c], Tamás Turányi[a], Sven Eckart[c]

[a]Institute of Chemistry, ELTE Eötvös Loránd University, Budapest, Hungary
[b]ELTE Hevesy György PhD School of Chemistry, Budapest, Hungary
[c]Institute of Thermal Engineering, TU Bergakademie Freiberg, Germany

---

Abstract

Reducing CO_2 emissions is a central goal of the energy industry to combat climate change. A promising technology for emission reduction is oxyfuel combustion, which uses pure oxygen instead of air for combustion. This technology is becoming increasingly relevant in the industry, with several large-scale plants already operating on oxyfuel to reduce fuel consumption. Hydrogen/oxygen systems are currently at the pilot and small-scale industrial levels. For the prediction and optimization of such systems, validated detailed reaction mechanisms are necessary. This study extensively reviewed the literature on burning velocity, ignition delay, and species concentration measurements. The reaction mixtures considered may contain water, carbon dioxide and small amounts of noble gases, but not nitrogen. The extracted data (1292 data points in 243 data series) were encoded in ReSpecTh Kinetic Data format XML files. While a good number of measurements are available for neat methane, the literature is much more limited for neat hydrogen. Notably, there is a lack of data for hydrogen-methane mixtures under oxyfuel conditions. The clustered data revealed significant differences in the underlying data for various pressure, temperature, equivalence and diluent ratio ranges. In some cases, the data were inconsistent, and the measurement methods were outdated. Several detailed and optimized mechanisms were employed to predict the experimental data. The performance of these mechanisms was compared in a quantitative way, showing significant differences in lean and rich conditions. This paper highlights the strengths and weaknesses of the mechanisms and provides an idea for further experimental investigations. This study offers valuable insights into the advantages and challenges of oxyfuel combustion of hydrogen-methane mixtures, supporting the development of sustainable and environmentally friendly combustion technologies.

Keywords: Oxyfuel combustion; CO_2-reduction; Methane combustion; Hydrogen combustion; Mechanism development

---

*Corresponding author.

1. Introduction

The demand for the reduction of CO_2 emissions in industrial activities is increasing at a large rate nowadays, and several technologies are being developed to reach a transition to net-zero carbon emissions soon. One of these technologies, oxyfuel combustion, is a thermal process in which a fuel is burnt using near-pure oxygen as an oxidant as opposed to conventional combustion, which uses air. By switching from air to oxygen, the behaviour of the whole process can be changed, including the flame characteristics and heat transfer, the composition of the flue gas, the pollutant formation, and the degree of corrosion [1]. Since the nitrogen component of air is not heated, fuel consumption is reduced, and higher flame temperatures are possible. Oxyfuel combustion has also received much attention in recent decades as a potential carbon capture and storage technology, which can be a great step towards net carbon emissions. Hydrogen is a promising alternative to traditional fuels due to its CO_2-free combustion and possible renewable production of the fuel, while methane (natural gas) is still widely used in the co-combustion of alternative fuels. The oxyfuel combustion of these fuels is of high practical significance, and to facilitate their application, detailed combustion mechanisms are necessary.

Turányi et al. [2] developed a method to test reaction mechanisms, and this method was applied for hydrogen combustion by Olm et al. [3] and methane combustion by Zhang et al. [4-5]. In these papers, several detailed mechanisms were tested against a large amount of experimental data, which did not include oxyfuel conditions. Some detailed mechanisms and large experimental data series are irrelevant to oxyfuel combustion. However, only a limited number of oxyfuel combustion studies are available in the literature. The experiments that have been conducted so far include laminar burning velocity, ignition delay time and species concentration measurements but do not cover all important temperature, pressure and equivalence ratio intervals that might be important for mechanism optimization. This statement is especially true for hydrogen and hydrogen/methane mixtures.

In this study, the literature on burning velocity, ignition delay, and species concentration measurements is extensively reviewed, focusing on reaction mixtures that may contain water, carbon dioxide and small amounts of noble gases but no nitrogen. The available detailed combustion mechanisms suitable for methane and hydrogen combustion are also presented along with highlighting their strengths and weaknesses.

2. Literature oxyfuel combustion experiments

Our aim was to collect a significant amount of oxyfuel combustion experiments available in the literature. We collected 1292 data points in 243 data series and encoded them in ReSpecTh Kinetic Data (RKD) v2.5 format [6] XML files. The collected publications with the experimental conditions are shown in Table 1. To visualize the data series and the condition ranges they cover, the experimental data are plotted in Fig. 1. In the next section, the most important laminar burning velocity and other experiments focusing on oxyfuel combustion are reviewed in detail.

2.1 Laminar burning velocity experiments

The laminar burning velocity (LBV) is a key property of combustible mixtures, defined as the speed at which an unstretched planar adiabatic laminar flame front propagates relative to the unburned gas. LBV is essential for optimizing combustion engine performance, modelling turbulent flames, validating chemical kinetic mechanisms, and ensuring safety in applications such as explosion protection and fuel tank venting. Additionally, it provides insight into the reactivity, diffusivity, and heat release of fuel–air mixtures and is critical for predicting flashback, determining ignition energy, and analyzing flame stability. Laminar burning velocity depends on factors such as fuel composition, equivalence ratio, pressure, and temperature. Accurate measurements are vital for advancing combustion research, improving efficiency, and enhancing safety in fuel systems [1].

Extensive databases for commonly used fuels - such as hydrogen, carbon monoxide, C1–C4 hydrocarbons, small alcohols, and esters - are available in the literature, with notable contributions by Konnov et al. [7] covering a wide range of fuels, and Wan et al. [8] focusing on H_2 and H_2/CO, among other comprehensive reviews. However, data availability becomes limited when exploring temperatures beyond 500 K and pressures above 10 bar (see Figure 1. This limitation is primarily due to the significantly higher setup costs and inherent constraints of certain measurement techniques, which have been evaluated and discussed in reviews by Egolfopoulos et al. [9], Konnov et al. [7], and others. Common methods reported in the literature include the cone flame, spherical vessel, and heat flux burner, along with frequent use of the counterflow burner and diverging channel. Less common approaches, such as shock tube LBV measurements and stepwise tube methods, have also been documented.

Table 1 List of the collected experimental publications on hydrogen and methane oxyfuel combustion with the conditions and the number of collected data. Notations and abbreviations: LBV: laminar burning velocity measurement; ST: shock tube; FR: flow reactor; *T*: (cold side) temperature; *p*: pressure *φ*: fuel-to-oxygen equivalence ratio.

Experiment type	Author	Year	Ref.	Data series/points	*T* / K	*p* / atm	*φ*
LBV-H_2	Kuznetsov et al.	(2011)	[10]	5/44	390 – 573	0.99-29.61	1.0
	Koroll et al.	(1988)	[11]	3/16	298 – 373	0.99	1.0
	Qiao et al.	(2005)	[12]	3/7	300	0.70	1.0
	Tse et al.	(2000)	[13]	2/10	298	1.00-20.00	1.5
	Burke et al.	(2010)	[14]	4/24	295	1.0 – 25.0	2.5
LBV-CH_4	Li et al.	(2015)	[15]	1/4	353	5.0 – 25.0	2.5
	Hu et al.	(2014)	[16]	1/9	300	1.0	0.6 – 1.4
	Zhu et al.	(1989)	[17]	2/11	298	1.0	0.39 – 1.14
	Xie et al.	(2013)	[18]	11/67	1169– 1285	0.99 – 2.96	0.40 – 1.61
	Mazas et al.	(2011)	[19]	3/31	373	1.0	0.5 – 1.5
	Oh et al.	(2012)	[20]	1/16	300	1.0	0.5 – 2.0
	Sentko et al.	(2015)	[21]	5/45	300 – 455	1.0	2.38 – 3.33
	Chen et al.	(2007)	[22]	3/17	298	1.0 - 5.0	0.5 – 0.8
	Almansour et al.	(2016)	[23]	4/22	295	1.0	0.8 – 1.3
	Khan et al.	(2017)	[24]	3/15	300	0.99	0.6 – 1.4
	Wang et al.	(2020)	[25]	16/14	298	0.99 – 3.45	0.6 – 1.6
ST-CH_4	Asaba et al.	(1963)	[26]	6/74	905 – 1794	7.0	0.22 – 3.00
	Petersen et al.	(1999)	[27][28]	9/27	1128 – 1607	12.0 – 91.3	5.99 – 6.00
	Skinner et al.	(1959)	[29]	1/13	1152 – 1328	6.0	3.0
	Pryor et al.	(2017)	[30]	9/37	1724 – 2038	0.61 – 1.09	1.0
	Liu. et al.	(2018)	[31]	2/21	1503 – 1785	0.74 – 1.98	0.50
FR-CH_4	Rasmussen et al.	(2008)	[32]	14/126	598 – 763	98.69	40.90 – 113.64
	Chellappa et al.	(1997)	[33]	76/137	623 – 703	33.56 – 49.35	16.00 – 32.00
	Cho et al.	(2008)	[34]	15/75	973 – 1073	1.0	10.0
	Rytz et al.	(1991)	[35]	35/195	723 – 748	29.61 – 49.46	38.0
	Giménez-L. et al.	(2015)	[36]	8/96	771 – 1674	1.0	0.50 – 5.00

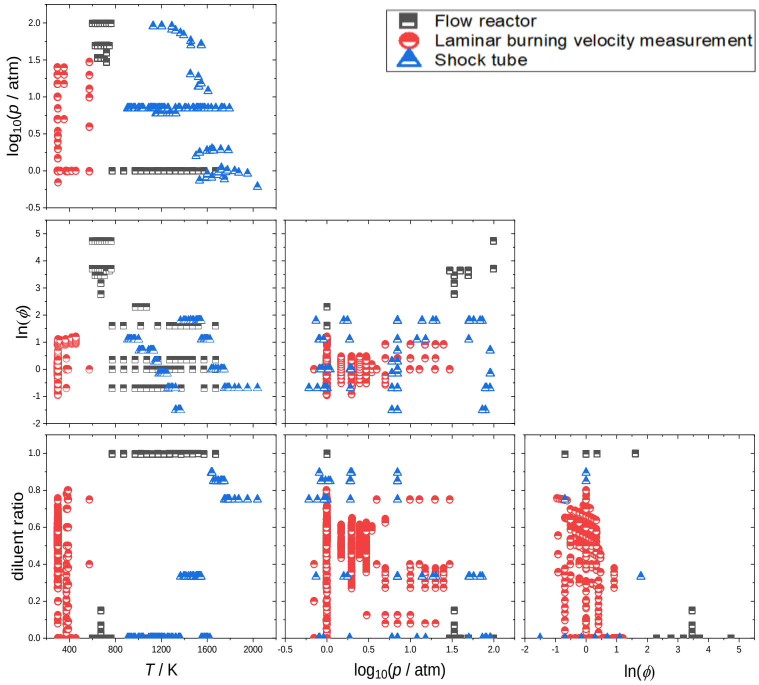

Figure 1 Measured hydrogen and methane oxyfuel data as a function of temperature, equivalence ratio, pressure and diluent ratio.

For methane–hydrogen mixtures, most studies use dry, particle-free compressed air as the oxidizer, reflecting industrial practice and ease of use. However, some studies investigate variations, including oxygen dilution by argon, nitrogen and helium, water vapor addition, exhaust gas recirculation, and oxygen-enriched combustion. The use of pure oxygen as an oxidizer, known as oxyfuel combustion, is rarely addressed in the literature. Since LBV is measured in premixed flames, oxygen enrichment intensifies reactions, increasing burning velocities and raising flashback risks. As a result, identifying suitable setups for mixtures from CH_4–O_2 to H_2–O_2 becomes a key challenge.

Setups like heat flux burners and counterflow burners are not perfectly suitable for oxyfuel combustion due to their velocity limits and structural constraints. Diverging channels also struggle with heat loss from high temperatures. As a result, only spherical and cone flame setups are commonly used for very high burning velocities (>1 m/s). Spherical flames involve igniting a premixed mixture in a closed vessel, with flame dynamics captured via pressure sensors and high-speed cameras. However, for fast oxyfuel flames, only a few usable frames are typically obtained due to ignition and wall effects.

Data on CH_4-O_2 measurements is limited. Oh and Noh [20] measured the laminar burning velocity (LBV) of CH_4-O_2 flames using a Bunsen burner and the cone method, employing CH chemiluminescence and Schlieren techniques. They found an LBV of 291 cm/s at φ=1.1. Mazas et al. [19] measured LBVs of methane-oxyfuel flames using a premixed cone flame and Schlieren method, finding 430 cm/s for stoichiometric methane-oxygen mixtures at 373 K.

Hu et al. [16] measured LBVs of preheated hydrogen-air flames at 443 K, reaching 500 cm/s using a cylindrical setup and an HG-100K camera at 10,000 fps. Krejci et al. [37] replicated these experiments with a FastCam SA 1.1 camera, facing limitations in resolution and frame rate. Kuznetsov et al. [10] performed LBV measurements for hydrogen-oxygen flames with water vapor addition, finding discrepancies of up to 35% between pressure and optical methods, with LBVs ranging from 1200-1300 cm/s for mixtures with 4% H_2O.

Koroll and Mulpuru [11] measured LBVs for H_2-O_2 flames using the nozzle-burner method, finding 1100 cm/s at 298 K and 1400 cm/s at 393 K, with nonlinear trends for water vapor, Ar, and He dilution. Mével et al. [38] used a constant-volume chamber and a PHOTRON APX camera, obtaining hydrogen-oxygen LBV values between 1039-1079 cm/s, with discrepancies in simulations ranging from 20% to 45%.

Qiao et al. [12] examined the effects of flame stretch and diluents on the laminar burning velocities of hydrogen premixed flames through both experimental and computational methods. Oxygen ratio was maximum at 30 %. It was found that flame stretch significantly affected the laminar burning velocities. Chemically passive suppression agents, such as helium, argon, nitrogen, and carbon dioxide, were found to reduce the unstretched laminar burning velocity in the order of their increasing specific heats and decreasing transport properties.

Tse et al. [13] examined the morphology of constant-pressure expanding spherical flames at elevated pressures up to 60 atm, revealing that flame instabilities, particularly hydrodynamic cell development, dominated the flame dynamics. These instabilities were observed for all fuels and equivalence ratios, highlighting their importance in internal combustion engine processes. Helium dilution was shown to be an effective technique for suppressing instabilities in laminar flames, with new stretch-free flame speed data obtained for $H_2/O_2/He$ mixtures at pressures up to 20 atm. The results also emphasize the need to address uncertainties in third-body efficiency factors and transport coefficients, especially at high pressures and varying equivalence ratios, while the apparatus used offers potential for further studying transient, high-pressure flame phenomena.

Burke et al. [14] investigated the pressure and flame temperature dependence of mass burning rates for $H_2/CO/O_2$/diluent mixtures across various conditions. Results showed that at low pressures, mass burning rates increased with pressure, but at higher pressures, they decreased, with CO addition and CO_2 dilution strengthening these dependencies.

Li et al. [15] conducted a quantitative uncertainty analysis of an H_2/CO kinetic model using the Data Collaboration method. They identified dataset inconsistencies when including literature data on laminar flame speeds for $H_2/O_2/CO_2$ mixtures at 15–25 atm, but the new experimental data, obtained under similar conditions, aligned well with the existing dataset.

Hu et al. [16] investigated the effects of equivalence ratio, O_2 concentration (max 35 %), and CO_2 dilution on the laminar flame speeds of premixed oxy-methane flames through experimental measurements (cone flame) and kinetic simulations.

Two key contributions are made in the study by Zhu et al. [17]. Stretch-free laminar flame speeds for methane/(Ar, N_2, CO_2)-air mixtures were accurately determined over a wide range of stoichiometries, pressures, and flame temperatures.

2.2 Other experiments available in literature

As the number of available laminar burning velocity experiments under oxyfuel conditions is limited, other experiments were also included in our study. These experiments were ignition delay time measurements in shock tube [26-31] and outlet concentration measurements in flow reactors [32-36].

Although there are several experiments dealing with oxyfuel combustion, the low number of collected data points indicates that more experiments should be conducted, as is also obvious from Fig. 1.

3. Performance of existing reaction mechanisms and possible mechanistic improvements

Our final aim is to develop a more accurate reaction mechanism describing oxyfuel processes. For this reason, 16 existing models were collected. These were developed primarily for methane combustion but contain detailed hydrogen chemistry as well.

The collected experimental data were reproduced using the 16 detailed mechanisms. Simulation framework Optima++ [39] was used to perform the simulations, while Cantera [40] was applied as a kinetic solver package. However, not all models were suitable for simulating all points, as 4 mechanisms do not contain helium but in some of the experiments it was used as a diluent gas. For this reason, the helium-containing experiments were treated separately and simulated with only 12 models.

Agreement of the simulation results with the experimental data was investigated comprehensively using the following error function:

$$E = \frac{1}{N}\sum_{f=1}^{N_f}\sum_{s=1}^{N_{fs}}\frac{1}{N_{fsd}}\sum_{d=1}^{N_{fsd}}\left(\frac{Y_{fsd}^{\mathrm{sim}} - Y_{fsd}^{\mathrm{exp}}}{\sigma(Y_{fsd}^{exp})}\right)^2 \quad (1)$$

In equation (1), *N* is the number of experimental data series in the data collection, N_f is the number of datasets (i.e. the number of RKD files), N_{fs} is the number of data series in dataset *f*, and N_{fsd} is the number of data points in data set *f* and data series *s*. y_{fsd}^{sim} and y_{fsd}^{exp} are the simulated and experimental values, respectively, of the *d*-th experimental data point of the *s*-th data series in the *f*-th dataset. $\sigma(Y_{fsd}^{\mathrm{exp}})$ is the estimated standard deviation of the data point y_{fsd}^{exp}. The corresponding simulated value y_{fsd}^{sim} is obtained from a simulation using a detailed mechanism and an appropriate simulation method. If a measured value is characterized by absolute errors (the scatter is independent of the magnitude of y_{fsd}), then $Y_{fsd} = y_{fsd}$. If the experimental results are described by relative errors (the scatter is proportional to the value of y_{fsd}), then option $Y_{fsd} = \ln(y_{fsd})$ is used.

When estimating the standard deviation of the data points, both uncertainty $\sigma_{\mathrm{exp},ij}$ provided by the authors of the publications or estimated in this study, and the $\sigma_{\mathrm{stat},i}$ statistical scatter of the data points were considered:

$$\sigma_{fsd} = \sqrt{\sigma_{\mathrm{exp},fsd}^2 + \sigma_{\mathrm{stat},fs}^2} \qquad (2)$$

Table 2 Comparison of the investigated reaction mechanisms based on the error function values calculated for all experimental data and various subsets of them. The final order in this table is based on the overall error function values for the helium-free experiments. Mechanisms not containing helium-chemistry are indicated with a *. Colours from green to red indicate growing error function values.

		LBV-H_2	LBV-CH_4	ST-CH_4	FR-CH_4	Overall	Failed	Overall (He)	Failed (He)
Number of data series		12	48	15	91	166		13	
Number of data points		68	338	86	394	886		40	
FFCM-1-2016	[41]	9.2	14.1	12.7	68.3	28.0	3	38.6	0
USC-II-2007	[42]	9.8	21.6	17.8	83.1	36.4	3	58.4	0
GRI3.0-1999*	[43]	17.4	30.5	15.1	71.5	37.9	3	-	-
SanDiego-2014	[44]	12.5	44.6	7.6	88.3	47.3	3	16.0	0
SanDiego-2016	[45]	12.5	46.9	8.4	84.7	47.6	4	18.4	0
Shrestha-2019	[46]	10.7	4.7	9.2	243.1	70.9	4	26.7	0
CaltechMech-2016*	[47]	9.0	4.7	27.3	264.4	79.1	5	-	-
Konnov-2017	[48]	5.1	13.9	11.3	284.4	86.1	3	11.6	0
Aramco2.0-2016	[49]	3.0	7.8	10.6	320.0	92.5	3	7.8	0
Le Cong-Dagaut-2009*	[50]	11.3	22.3	12.4	292.7	93.1	7	-	-
NUIGMech-2021	[51]	10.3	10.6	9.7	316.1	93.5	3	8.2	0
Hashemi-2016	[52]	5.5	18.5	23.4	309.7	96.8	5	8.8	0
Glarborg-2018	[53]	5.7	29.6	9.2	315.2	101.5	3	7.6	0
Konnov-2009*	[54]	34.3	32.9	26.1	313.0	108.2	3	-	-
CRECK-2014	[55]	21.4	62.4	17.2	352.6	130.0	3	22.8	0
GDFKin-2012	[56]	32.2	39.5	21.9	465.7	151.9	13	19.8	10

The calculated error function values by experiment type and overall can be seen in Table 2 for the non-helium experiments. The overall results for the helium-containing experiments are also shown. However, not all data points were included in the comparison. Those data points were excluded from the comparison for which the error function values were greater than 9 for all mechanisms. As a few data points with extremely high error function value (over 10,000) remained, these were excluded as well. The data points with failed simulations were also not considered, but their number is indicated for each mechanism in Table 2.

A mechanism can be considered good if it can reproduce experimental data in their 3σ uncertainty range, which corresponds to an error function value not greater than 9. The results show that the FFCM-1-2016 performs the best for the flow reactor measurements and overall, considering only the helium-free experiments. However, its error function values are greater than 9 for each experiment type., There are mechanisms for which the error function values are smaller than 9 for certain experiment types, for example Aramco2.0-2016, which is the best-performing mechanism with an excellent result for hydrogen-LBV measurements and is also good for the methane-LBV experiments, for which Shrestha-2019 and CaltechMech-2016 are the best-performing models. SanDiego-2016 can simulate shock tube measurements the best, also under 3σ on average.

However, none of the mechanisms can reproduce the flow reactor experimental data within 3σ, and the overall values are much greater than 9 as well. This indicates that further development of the models is necessary. It also needs to be noted that more data points are needed to get a reliable picture of the performance of the mechanisms.

4. Conclusions

Experimental data from several publications on methane and hydrogen oxyfuel combustion was collected and the data was reviewed extensively to show the shortcomings of the available literature data. Based on this it can be said that more reliable experiments are necessary over temperatures above 500 K and pressures over 10 bar.

Kinetic simulations were performed with existing detailed mechanisms to reproduce the data. FFCM-1-2016 was the best-performing model but no mechanism could simulate experimental data within their 3σ uncertainty range on average, meaning that further development of the models is necessary focusing on oxyfuel conditions.

While the collected 1292 data points in 243 data series were enough to get a basic picture of the performance of the mechanisms, more experiments should be conducted to get more reliable conclusions.

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.

Acknowledgements

The authors acknowledge the support of the NKFIH grant OTKA K147024 of the Hungarian National Research, Development and Innovation Office. ÁVR was also supported by the DKOP-23 Doctoral Excellence Program of the Ministry for Culture and Innovation of Hungary from the source of the National Research, Development, and Innovation Fund.

References

[1] P. Mathieu, Developments and innovation in carbon dioxide (CO_2) capture and storage technology, Woodhead Publishing (2010).

[2] T. Turányi, T. Nagy, I.Gy. Zsély, M. Cserháti, T. Varga, B. T. Szabó, Determination of rate parameters based on both direct and indirect measurements. Int. J. Chem. Kinet. 44 (2012) 284–302.

[3] C. Olm, I.Gy. Zsély, R. Pálvölgyi, T. Varga, T. Nagy, H. J. Curran, Comparison of the performance of several recent hydrogen combustion mechanisms. Combust. Flame 161 (2014) 2219–34.

[4] P. Zhang, I. Gy. Zsély, V.Samu, T. Nagy, T. Turányi, Comparison of methane combustion mechanisms using shock tube and rapid compression machine ignition delay time measurements. Energy & Fuels 35 (2021) 12329–51.

[5] P. Zhang, I. Gy. Zsély, M. Papp, T. Nagy, T. Turányi, Comparison of methane combustion mechanisms using laminar burning velocity measurements. Combust. Flame 238 (2022) 11867.

[6] T. Varga, C. Olm, M. Papp, Á. Busai, A. Gy. Szanthoffer, I. Gy. Zsély, T. Nagy, T. Turányi. ReSpecTh Kinetics Data Format Specification v2.5. Chemical Kinetics Laboratory, ELTE Institute of Chemistry (2024). https://respecth.elte.hu/rkdformat (accessed March 2025).

[7] A.A. Konnov, A. Mohammad, V.R. Kishore, N.I. Kim, C. Prathap, S. Kumar, A comprehensive review of measurements and data analysis of laminar burning velocities for various fuel+air mixtures, Prog. Ener. Combust. Sci. 68 (2018) 197-267.

[8] W. Han, P. Dai, X. Gou, Z. Chen, A review of laminar flame speeds of hydrogen and syngas measured from propagating spherical flames, App. Ener. Combust. Sci. 100008 (2020).

[9] F.N. Egolfopoulos, N. Hansen, Y. Ju, K. Kohse-Höinghaus, C.K. Law, F. Qi, Advances and challenges in laminar flame experiments and implications for combustion chemistry, Prog. Ener. Combust. Sci. 43 (2014) 36-67.

[10] M. Kuznetsov, R. Redlinger, W. Breitung, J. Grune, A. Friedrich, N. Ichikawa, Laminar burning velocities of hydrogen-oxygen-steam mixtures at elevated temperatures and pressures, Proc. Combust. Inst. 33 (2011) 895-903.

[11] G.W. Koroll, S.R. Mulpuru, The effect of dilution with steam on the burning velocity and structure of premixed hydrogen flames. Symp. (Int.) Combust. 21 (1988) 1811–1819.

[13] J. Oh, D. Noh, Laminar burning velocity of oxy-methane flames in atmospheric condition, Energy 45 (2012) 669-675.

[12] L. Qiao, C.H. Kim, G.M. Faeth, Suppression effects of diluents on laminar premixed hydrogen/oxygen/nitrogen flames, Combust. Flame 143 (2005), 79-96.

[13] S.D. Tse, D.L. Zhu, C.K. Law, Morphology and burning rates of expanding spherical flames in H_2/O_2/inert mixtures up to 60 atmospheres, Proceedings of the Combustion Institute 28 (2000), 1793–1800.

[14] M. P. Burke, M. Chaos, F. L. Dryer, Y. Ju, Negative pressure dependence of mass burning rates of $H_2/CO/O_2$/diluent flames at low flame temperatures, Combust. Flame, 157, (2010), 618-631.

[15] X. Li, X. You, F. Wu, C. K. Law, Uncertainty analysis of the kinetic model prediction for high-pressure H2/CO combustion, Proceedings of the Combustion Institute, 35, (2015), 617-624.

[16] E. Hu, Z. Huang, J. He, H. Miao, Experimental and numerical study on laminar burning velocity and flame instabilities of hydrogen-air mixtures at elevated pressures and temperatures. Int. J. Hydro. Ener. 34 (2009) 8741-8755.

[17] D.L. Zhu, F.N. Egolfopoulos, C.K. Law, Experimental and numerical determination of laminar flame speeds of methane/(Ar, N_2, CO_2)-air mixtures as function of stoichiometry, pressure, and flame temperature, Symp. (Int.) Combust. 22 (1989), 1537-1545.

[18] Y. Xie, J. Wang, M. Zhang, J. Gong, W. Jin, Z. Huang, Experimental and numerical study on laminar flame characteristics of methane oxy-fuel mixtures highly diluted with CO_2, Energy & Fuels 27, (2013), 6231-6237.

[19] A.N. Mazas, B. Fiorina, D.A. Lacoste, T. Schuller, Effects of water vapor addition on the laminar burning velocity of oxygen-enriched methane flames. Combust. Flame 158 (2011) 2428-2440.

[20] J. Oh, D. Noh, Laminar burning velocity of oxy-methane flames in atmospheric condition, Energy 45 (2012) 669-675.

[20] J. Oh, D. Noh, Laminar burning velocity of oxy-methane flames in atmospheric condition, Energy 45 (2012) 669-675.

[21] M.M. Sentko, C. Weis, S.R. Harth, P. Habisreuther, N. Zarzalis, D. Trimis, Proceedings of the European Combustion Meeting (2015), 1-6.

[22] Z. Chen, On the extraction of laminar flame speed and Markstein length from outwardly propagating spherical flames, Combust. Flame 158 (2011) 291-300.

[23] B. Almansour, L. Thompson, J. Lopez, G. Barari, S. S. Vasu, Laser ignition and flame speed measurements in oxy-methane mixtures diluted with CO_2, J. Energy Resour. Technol. 138 (2015) 032201.

[24] A.R. Khan, S. Anbusaravanan, Lokesh Kalathi, Ratnakishore Velamati, C. Prathap, Investigation of dilution effect with N_2/CO_2 on laminar burning velocity of premixed methane/oxygen mixtures using freely expanding spherical flames, Fuel 196 (2017), 225-232.

[25] S. Wang, Z. Wang, Y. He, X. Han, Z. Sun, Y. Zhu, M. Costa, Laminar burning velocities of CH4/O2/N2 and oxygen-enriched $CH_4/O_2/CO_2$ flames at elevated pressures measured using the heat flux method, Fuel 259 (2020) 116152.

[26] K. Y. Asaba, N. Kakihara, T. Hikita, A shock-tube study of ignition of methane-oxygen mixtures, Proc. Combust. Inst. 9 (1963) 193-200.

[27] E.L. Petersen, D.F. Davidson, R.K. Hanson, Kinetics modeling of shock-induced ignition in low-dilution CH4/O2 mixtures at high pressures and intermediate temperatures, Combust. Flame 117 (1999), 272-290.

[28] E. L. Petersen, D. F. Davidson, R. K. Hanson, Ignition delay times of ram accelerator CH/O/Diluent Mixtures, J. Prop. Pow. 15 (1999), 82-91.

[29] G. B. Skinner, R. A. Ruehrwein, Shock tube studies on the pyrolysis and oxidation of methane, J. Phys. Chem. 63 (1959), 1736-1742.

[30] O. Pryor, S. Barak, B. Koroglu, E. Ninnemann, S. S. Vasu, Measurements and interpretation of shock tube ignition delay times in highly CO_2 diluted mixtures using multiple diagnostics, Combust. Flame 180 (2017), 63-76.

[31] Y. Liu, C. Zou, J. Cheng, H. Jia, and C. Zheng, Experimental and numerical study of the effect of CO_2 on the ignition delay times of methane under different pressures and temperatures, Energy & Fuels 32 (2018), 10999-11009.

[32] C. L. Rasmussen, P. Glarborg, Direct partial oxidation of natural gas to liquid chemicals: chemical kinetic modeling and global optimization, Ind. Eng. Chem. Res. 47 (2008), 6579-6588.

[33] A. S. Chellappa, S. Fuangfoo, and D. S. Viswanath, Homogeneous oxidation of methane to methanol: effect of CO_2, N_2, and H_2 at high oxygen conversions, Ind. Eng. Chem. Res. 36 (1997), 1401-1409.

[34] Y. C. Cho, K-H. Choi, Y. R. Kim, S. H. Lee, Kinetic investigation of oxidative methane pyrolysis at high CH_4/O_2 ratio in a quartz flow microreactor below 1073 K, Bulletin of The Korean Chemical Society 29 (2008), 1609-1612.

[35] D. W. Rytz, A. Baiker, Partial oxidation of methane to methanol in a flow reactor at elevated pressure, Ind. Eng. Chem. Res. 30 (1991), 2287-2292.

[36] J. Giménez-López, A. Millera, R. Bilbao, M. U. Alzueta, Experimental and kinetic modeling study of the oxy-fuel oxidation of natural gas, CH_4 and C_2H_6, Fuel 160 (2015), 404-412.

[37] M.C. Krejci, O. Mathieu, A.J. Vissotski, S. Ravi, T.G. Sikes, E.L. Petersen, A. Kérmonès, W. Metcalfe, H.J. Curran, Laminar flame speed and ignition delay time data for the kinetic modeling of hydrogen and syngas fuel blends, J. Eng. Gas Turb. Pow. 135 (2013) 021503.

[38] R. Mével, J. Sabard, J. Lei, N. Chaumeix, Fundamental combustion properties of oxygen enriched hydrogen/air mixtures relevant to safety analysis: Experimental and simulation study. Int. J. Hydr. Ener. 41 (2016) 6905–6916.

[39] M. Papp, T. Varga, Á. Busai, I. Gy. Zsély, T. Nagy, T. Turányi: Optima++ v2.5: A general C++ framework for performing combustion simulations and mechanism optimization (2024); available at http://respecth.hu/ (accessed March 2025)

[40] D. G. Goodwin, H. K. Moffat, I. Schoegl, R. L. Speth, B. W. Weber. Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes (2023). https://www.cantera.org (accessed March 2025)

[41] G.P. Smith, Y. Tao, H. Wang, Foundational fuel chemistry model Version 1.0, (2016), https://web.stanford.edu/group/haiwanglab/FFCM1/pages/FFCM1.html (accessed March 2025)

[42] H. Wang, X. You, A.V. Joshi, S.G. Davis, A. Laskin, F. Egolfopoulos, C.K. Law, USC Mech version II. High-temperature combustion reaction model of H_2/CO/C1-C4 compounds (2007), http://ignis.usc.edu/USC_Mech_II.htm (accessed March 2025)

[43] G.P. Smith, D.M. Golden, M. Frenklach, N.W. Moriarty, B. Eiteneer, M. Goldenberg, C.T. Bowman, R.K. Hanson, S. Song, W.C. Gardiner Jr, V.V. Lissianski, Z. Qin, GRI-Mech 3.0 (1999), http://www.me.berkeley.edu/gri_mech/ (accessed March 2025)

[44] Mechanical and Aerospace Engineering (Combustion Research) University of California at San Diego, Chemical-kinetic mechanisms for combustion applications San Diego Mechanism (2014) https://web.eng.ucsd.edu/mae/groups/combustion/mechanim.html (accessed March 2025)

[45] Mechanical and Aerospace Engineering (combustion research) University of California at San Diego, chemical-kinetic mechanisms for combustion applications San Diego Mechanism (2016) https://web.eng.ucsd.edu/mae/groups/combustion/mechanism.html (accessed March 2025)

[46] K. P. Shrestha, L. Seidel, T, Zeuch, F. Mauss, Kinetic Modeling of NO_x formation and consumption during methanol and ethanol cxidation. Comb. Sci. Tech. 191 (2009), 1627–1659.

[47] The FORCE - California Institute of Technology, CaltechMech detailed kinetic model (version 2.3), (2015), https://www.theforce.caltech.edu/CaltechMech/ (accessed March 2025)

[48] M. Christensen, A. A. Konnov, Laminar burning velocity of diacetyl + air flames. Further assessment of combustion chemistry of ketene, Combust. Flame 178 (2017) 97-110.

[49] NUI Galway Combustion Chemistry Centre, AramcoMech 2.0, 2017, http://www.nuigalway.ie/combustionchemistrycentre/mechanismdownloads/aramcomech20/ (accessed March 2025)

[50] T. Le Cong, Philippe Dagaut, G. Dayma. Oxidation of Natural Gas, Natural Gas/Syngas Mixtures, and Effect of Burnt Gas Recirculation: Experimental and Detailed Kinetic Modeling. J. Eng. Gas Turb. Pow. 130 (2008), 041502.

[51] Y. Wu, S. Panigrahy, A. B. Sahu, C. Bariki, J. Beeckmann, J. Liang, A. A.E. Mohamed, S. Dong, C. Tang, H. Pitsch, Z. Huang, H. J. Curran, Understanding the antagonistic effect of methanol as a component in surrogate fuel models: A case study of methanol/n-heptane mixtures, Combust. Flame 226 (2021), 229-242.

[52] H. Hashemi, J. M. Christensen, S. Gersen, H. Levinsky, S. J. Klippenstein, P. Glarborg, High-pressure oxidation of methane, Combust. Flame 172 (2016) 349-364.

[53] P. Glarborg, J. A. Miller, B. Ruscic, S. J. Klippenstein, Modeling nitrogen chemistry in combustion, Prog. Energ. Comb. Science, 67, 2018, 31-68.

[54] A.A. Konnov, Implementation of the NCN pathway of prompt-NO formation in the detailed reaction mechanism, Combust. Flame 156 (2009) 2093-2105.

[55] CRECK modeling Group C1-C3 kinetic mechanism Version 1412, (2014), http://creckmodeling.chem.polimi.it/index.php (accessed March 2025)

[56] Y.Yu. Cinétique d'auto-inflammation de carburants gazeux a haute pression: etude experimentale et de modelisation, L'Universite des Sciences et Technologies de Lille (2012).