CALCULATING THE FUNDAMENTAL PARAMETERS TO ASSESS THE EXPLOSION RISK DUE TO CROSSOVER IN ELECTROLYSERS

Coudoro, K, Bernard, L. and. Jallais, S.
Centre de Recherche Paris-Saclay, AIR LIQUIDE Research & Development, 1, chemin de la Porte des Loges, Les Loges-en-Josas - BP 126, 78354, Jouy-en-Josas, France,
kodjo.coudoro@airliquide.com, laurence.bernard@airliquide.com,
simon.jallais@airliquide.com

ABSTRACT

With the predicted high demand of hydrogen projected to support the neutral carbon society transition in the coming years, the production of hydrogen is set to increase alongside the demand. As electrolysis is set to be amongst the main solutions for green hydrogen production, ensuring the safety of electrolysers during operation will become a central concern. This is mainly due to the crossover risk (hydrogen into oxygen or the other way around) in the separators as throughout the years several cases of incidents have been reported.

This study aims to evaluate the methodologies for calculating H_2/O_2 detonation cell size and laminar flame velocity using detailed kinetic mechanisms at the operating conditions of electrolysers (up to 35 bar and 360 K). Therefore, the modeling of H_2/O_2 and H_2/Air shock tube delay times and laminar flame speeds at initial different pressures and temperature based on the GRI mech 3.0 [1], Mevel et al.[2], Li et al.[3], Lutz et al. [4] and Burke et al. [5] kinetic mechanisms were performed and compared with the available experimental data in the literature. In each case, a best candidate mechanism was then chosen to build a database for the detonation cell size then for the laminar flame speeds up to the operating conditions of electrolysers (293-360K and 1-35 bar).

1. INTRODUCTION

Recent developments in the energy field indicate that the demand in hydrogen energy will increase rapidly over the coming years. As water electrolysis is set to play a major role in hydrogen production, some safety questions still remain about the process. For quite some time now, when dealing with alkaline eletrolyzers, several explosions have been reported in the US in 1969 and 1975; in Kosovo in 2014 and in Korea in 2019. As the explosions started from the separators, it became clear that the cause was hydrogen crossing over into the oxygen tank or the other way around. There are two main possibilities to generate overpressures that can lead to such explosions:

- A detonation when the mixture composition is in the detonable range and the initiation conditions are met. At electrolyser operating pressure and temperature (up to 30 bar and 363K) there is no experimental data on the detonability and flame propagation regimes for H_2/O_2 mixtures. In order to assess the occurrence risk and the consequences of an initiation of detonation in the separators in case of crossing over, it is important to calculate the detonation cell size for the mixtures at the operating conditions.
- A slow deflagration is first initiated which under the effect of instabilities will accelerate into a fast deflagration. Here again, the flame fundamental properties to allow the assessment of such phenomena are not available at the operation conditions of electrolysers. In this case evaluating the laminar flame speeds at operating conditions, is key to assessing the flame acceleration risk.

We propose in this work a calculation by extrapolation of the detonation cell sizes and laminar flame velocities for H_2/O_2 mixtures at high pressure and temperature based on the choice of a detailed kinetic model in each case.

2. METHODOLOGY

As it was mentioned during the introduction, there are very few experimental data available on H_2/O_2 mixtures in the literature. We propose a workaround using the detailed kinetic calculation software Cantera [6] and a detailed kinetic mechanism. The calculations will be split into two parts. The first one will focus on detonation cell sizes and the second one on laminar flame velocities.

At first, a set of kinetic mechanisms will be evaluated on H_2/O_2 experimental data, when available, otherwise on H_2/Air data of shock tube induction times (detonation cell sizes) and laminar flame velocities. For each fundamental parameter, the mechanism offering the best agreement with the experimental data will then be used to calculate either the detonation cell sizes or the laminar flame speeds. In the particular case of the detonation cell size, the Ng et al. [7] and the Westbrook et al. [8] correlations will be evaluated against experimental data. The correlation offering the best agreement will then be used to calculate the detonation cell sizes at high pressure and temperature up to the operating conditions of the electrolysers

3. DETONATION CELL SIZES

3.1 Model validation

H_2/O_2/Diluent mixtures in shock tube experiments

A set of experimental data available in the literature on shock tube experiments is selected to serve a comparison basis for the selected kinetic mechanisms. These experimental data are summarized in the following table.

Temperature (K)	Pressure (atm)	Equivalence ratio range	Reference
1000-1300	2.5	1	Bhaskaran et al.[9]
1000-1800	1-3	0.5-1	Cheng et al [10]
1000-1700	0.5-8.5	1-2	Cohen et al. [11]
1000-1350	1.2-2.7	1	Fujimoto et al. [12]
1100-1850	0.5-0.8	0.6-2	Jachimowski et al. [13]
1050-1250	1.41	1	Just et al. [14]
1190-1950	33-87	1	Petersen et al. [15]
1100-2600	0.5-9.5	0.12-3	Schott et al. [16]
1000-1100	5	2	Skinner et al. [17]
1010-1080	2-7	0.5-0.75	Snyder et al. [18]

Table 1: Summary of shock tube induction delay time database for H_2/O_2/Diluent mixtures

As shown in Table 1, the experimental database consists in a wide array of tested pressures and temperatures as well as equivalent ratios. The simulation results with all kinetic detailed mechanisms are reported in figure. 1. As this work is intended to determine the best fit to the experiments, all the experimental data has been aggregated and has been attributed the same statistical weight. Therefore the calculated induction times for all the mechanisms has been plotted against the experimentally measured

ones. Globally, the plot shows an acceptable agreement for all the mechanisms when compared with the experimental data.

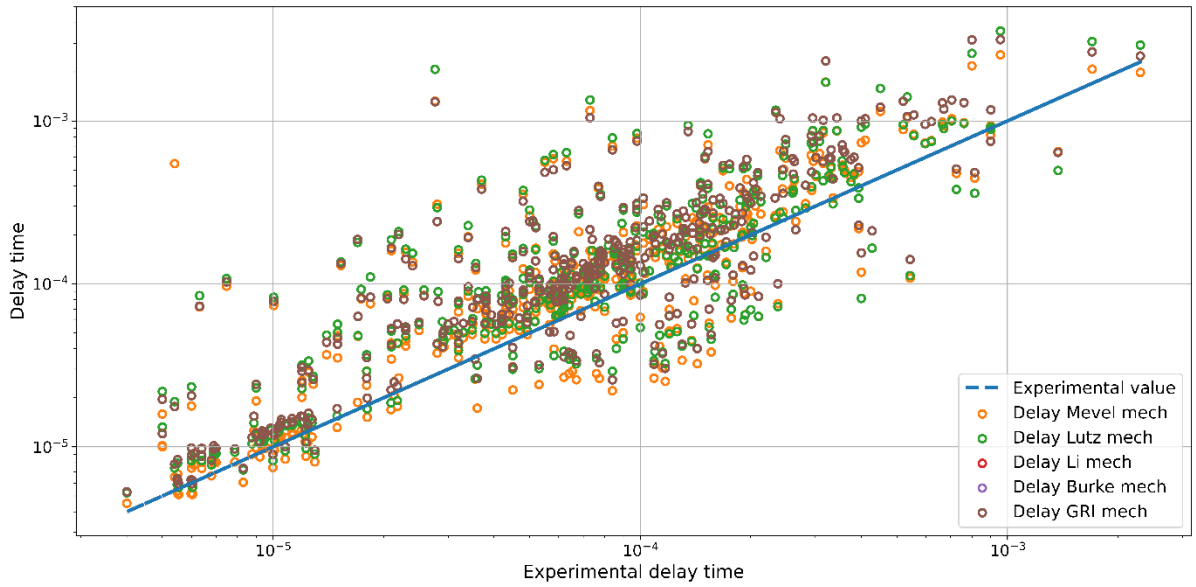

Figure 1: Simulated delay times against experimental delay times

Visually, no mechanism appears to provide the best fit. However, with such widely spread values, calculating the mean relative error provides an interesting basis of comparison. The values are reported in the following table.

Mech	Mevel	Lutz	Li	Burke	GRI
Mean relative error	6.0	6.7	7.4	11.2	16.4
% of data within +/-100% relative error	30.26%	29.31%	26.24%	21.99%	21.51%

Table 2: Mean relative error and percentage of data within +/- 100% relative error

From Table 2, it can be deduced that the Mevel et al. mechanism provides the lowest mean relative error amongst the tested mechanisms. It also presents the highest percentage of data within +/-100% relative error. On this basis, the calculation of the detonation cell sizes will be performed using the Mevel et al. mechanism.

It is however interesting to highlight that the models display a better agreement with part of the experimental data and a lower with others.

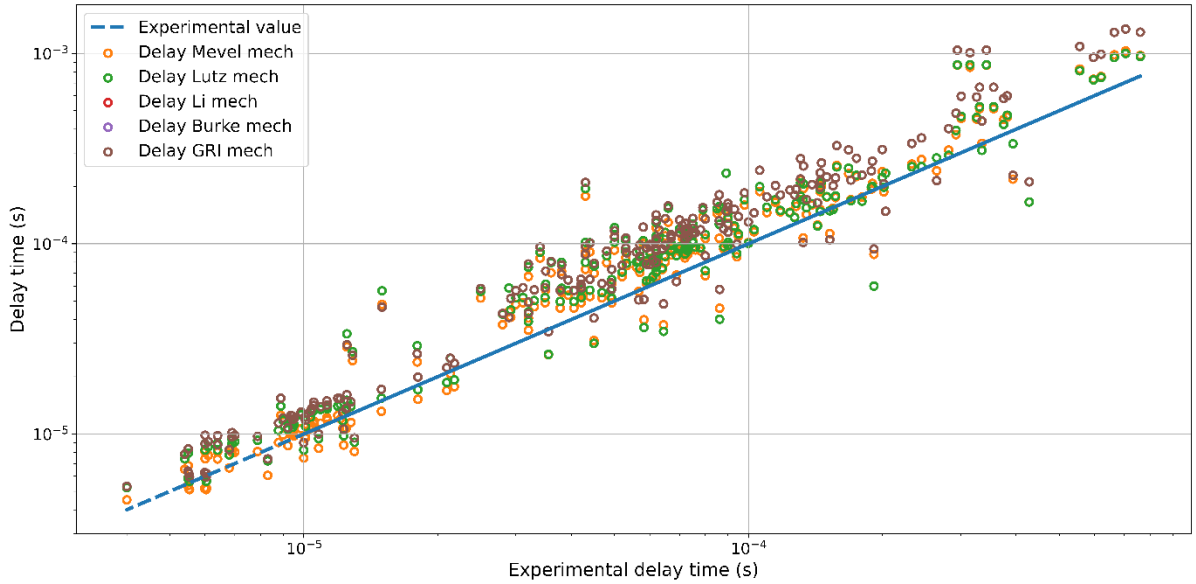

Figure 2: Experimental data comparison with model (reduced "best fit" database)

As shown on Figure 2, the comparison of the modeling results with the data from Bhaskaran, Cheng, Jachimwosky and Petersen, exhibits a better fit than with the entire database. With no particular specificity either on the equivalent ratio or the pressure or even on the diluent and its percentage, this hints towards a discrepancy in the experimental database. Although, this does not change the outcome on the best fitting mechanism as shown in the following table.

Mech	Mevel	Lutz	Li	Burke	GRI
Mean relative error	3.4	3.5	4.4	5.7	6.0
% of data within +/-100% relative error	38.46%	36.65%	33.48%	27.60%	26.24%

Table 3: Mean relative error and percentage of data within +/- 100% relative error using reduced database

3.2 Detonation cell size calculation

Cell size calculation at ambient temperature and pressure for H2/Air mixtures

Initial temperature (K)	Initial pressure (atm)	Equivalence ratio range	References
293	1	0.5-3.6	Guirao et al. (1982) [19]
298	1	0.3-5.5	Tieszen et al. (1986) [20]
298	1	0.5-4.5	Ciccarelli et al. (1994) [21]
293	0.83	0.3-5.6	Benedick et al. (1984) [22]

Table 4: List of detonation cell size at ambient pressure and temperature for comparison

On Figure 3, the comparison of both correlation with the set of experimental data is plotted. It appears that there is a good agreement between the Ng correlation and the experimental data on the lean side and around the stoichiometry (note the logarithmic plot). On the rich side, there is a slight underestimation of the cell size value but overall the agreement is fair. On the other hand, the Westbrook correlation give a fair agreement as well but lower than the performance of the Ng correlation. It can also be noted that there are some dispersions within the experimental data especially between the data from Ciccarelli et al. and the others. Globally the cell sizes measured by Ciccarelli et al. are lower than those from the other authors of the literature.

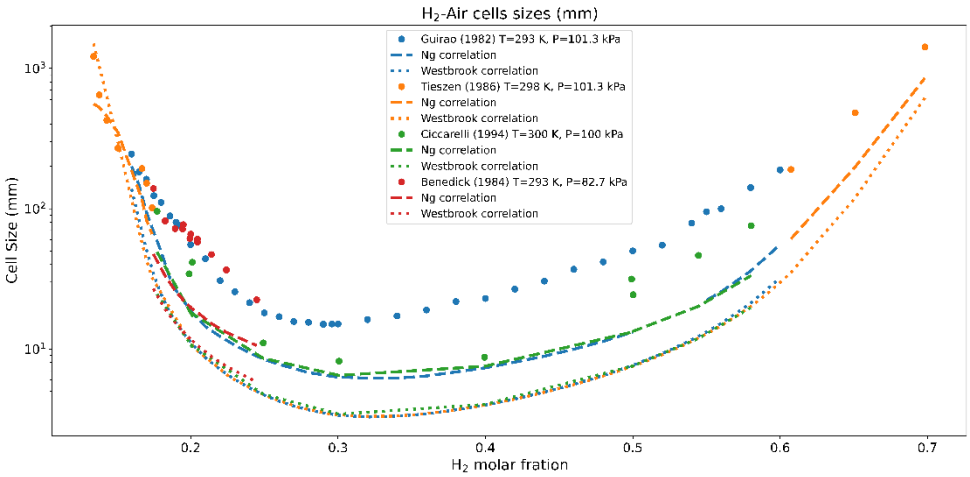

Figure 3: Comparison of cell size calculation using Westbrook and Ng correlation at ambient pressure and temperature

Cell size calculation at ambient pressure and elevated temperature for H2/air mixtures

The experimental set is based on the measurements performed by Ciccarelli et al [21] [23] in 1994 and 1997. With the increasing temperature, the detonation cell size decreases as shown in Figure 4. The figure also shows some important dispersions for experiments conducted in the same conditions. However, it can be noted that both models provide a fair agreement with the experimental data in these

conditions. The agreement is higher around stoichiometric values and then decreases as the hydrogen concentration decreases. In addition, the mechanism reproduces the experimental behavior: as the temperature increases, the cell size diminishes.

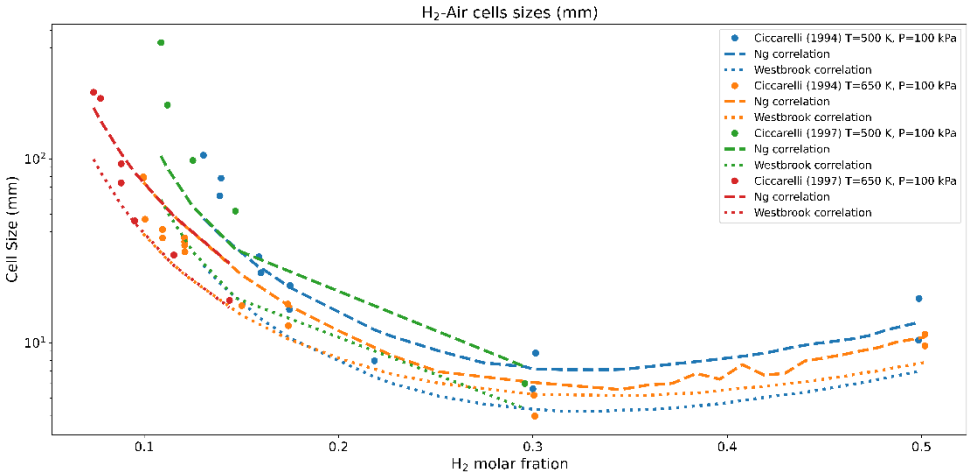

Figure 4: Comparison of cell size calculation using Westbrook and Ng correlation at ambient pressure and temperature

Cell size calculation at ambient pressure and elevated temperature for H2/O2 mixtures

The detonation cell size as a function of the pressure for stoichiometric H_2/O_2 mixtures is plotted on Figure 5. The comparison is based on a set of experiments available in the literature in stoichiometric conditions : [24]–[28].

As the pressure increases to reach the atmospheric pressure, the experimental detonation cell size decreases. Although the test conditions are the same, there is a strong discrepancy in the measurements. The same trend is observed on both Ng and Westbrook correlations. However, it appears that at low pressure the Westbrook correlation presents the best agreement with the experimental data. The trend seems to revert as the initial pressure increases but there is not enough experimental data to confirm it.

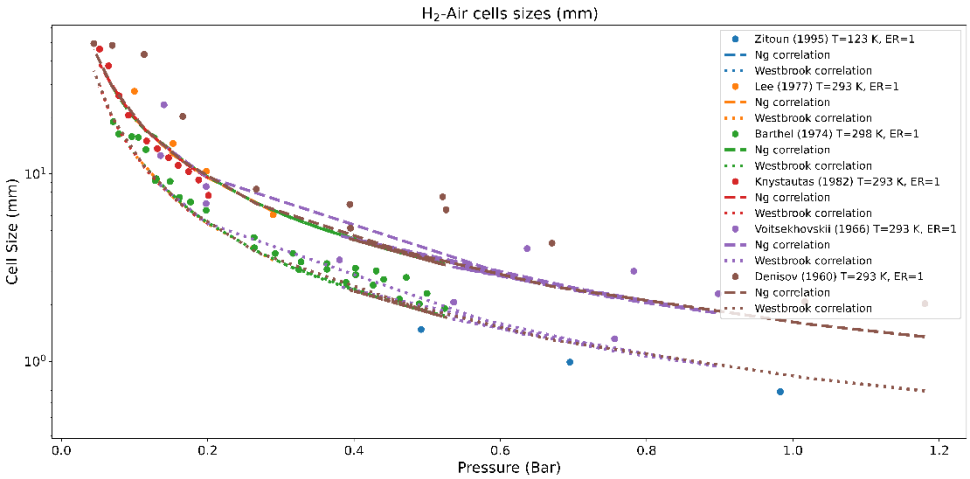

Figure 5: Effect of initial pressure on a stoichiometric H_2/O_2 mixture and comparison with Ng and Westbrook correlations

The comparison of the correlations based on the Mevel et al mechanism and the correlations by Ng and Westbrook highlights the difficulty in predicting the detonation cell size as only the ambient temperature

and pressure experiments present acceptable discrepancies. In that configuration, the Ng correlation presents the best agreement with the experimental data. Although the Westbrook correlation provides the best agreement for H_2/O_2 measurement at stoichiometric conditions and at low pressure, those conditions are marginal compared with the target of calculating the detonation cell size over the whole equivalence ratio range and at elevated temperature and pressure.

Figure 6 displays the simulation results at 363 K and for 1, 15 and 30 bar for hydrogen/oxygen mixtures. As the pressure increases, the detonation cell size decreases. A strong decrease is observed from 1 to 15 bar and a smaller decrease from 15 to 30 bar around the stoichiometric zone. Near the flammability limits, on the lean side, the plots are similar with a smooth slope while on the rich side the slope is steeper. This plot highlights the difficulty that may occur when predicting the detonability of such mixtures at high pressure and temperature especially on the rich side. With the addition of the calculation error and the error made in evaluating the composition of the mixture, the detonation risk assessment must be performed with important care.

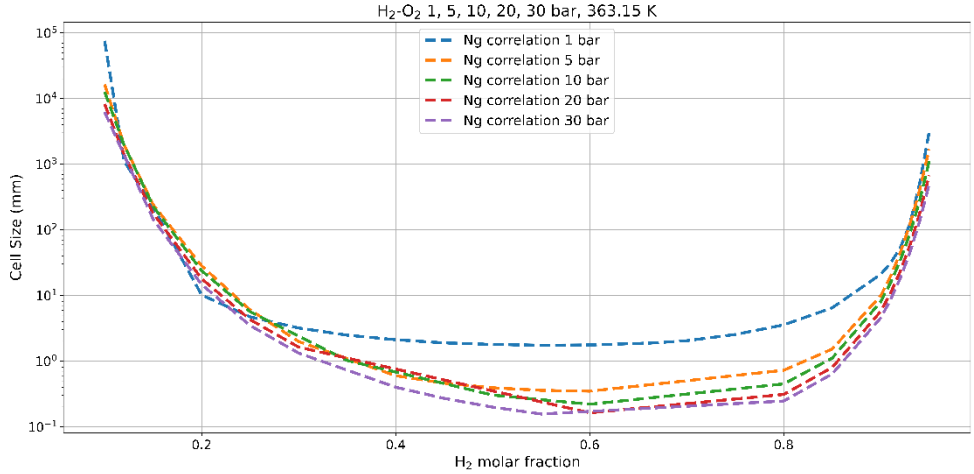

Figure 6: Detonation cell sizes for hydrogen/oxygen mixture using the Ng correlation

4. LAMINAR FLAME SPEEDS FOR FLAME ACCELERATION

4.1 Model validation

H2/Air mixtures at ambient temperature and pressure

In order to validate a detailed kinetic mechanism, a set of experimental data available in the literature is selected and will serve as the basis for model comparison. The following table summarizes the selected experimental data. All the selected experiments were conducted during the current century and include some of the most recent ones. The laminar flame speed plots were extracted from the figures shown in the papers.

On Figure 7, the laminar flame speeds for the selected experimental data were plotted against the H_2 percentage in the mixture. Although all the curves present the characteristic bell shape of the laminar flame velocity, a wide discrepancy can be observed. It goes from around a maximum value of 30 cm/s on the lean side to 50 cm/s on the rich side. This was observed by Han et al. [29] and they proposed some useful insights on the probable origins of the discrepancy. As the data available in the literature is not much detailed than the measured values of the laminar flame velocity, we cannot rule any of these data out based on the conclusions of Han et al.[29] Therefore, each of the experimental data will have the same statistical weight during our evaluation of the most suitable kinetic model.

Initial temperature (K)	Initial pressure (atm)	Equivalence ratio range	Reference
298	1	0.5-4	Tse et al., 2000
298	1	0.28-3.75	Lamoureux et al., 2003
298	1	0.5-4.5	Hu et al., 2009
293	1	0.3-5.6	Kuznetsov et al., 2012
303	1	0.5-4	Dayma et al., 2014
296	1	0.8-3.5	Grosseuvres et al., 2019

Table 5: Table of H2/Air experimental values considered in this work

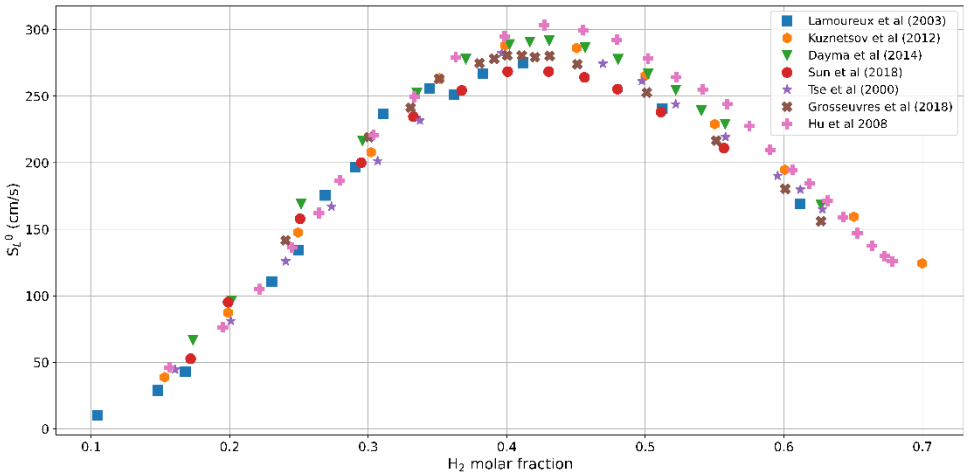

Figure 7: Experimental dataset for model validation

These data were modelled using the selected detailed kinetic mechanisms and are displayed on Figure 8

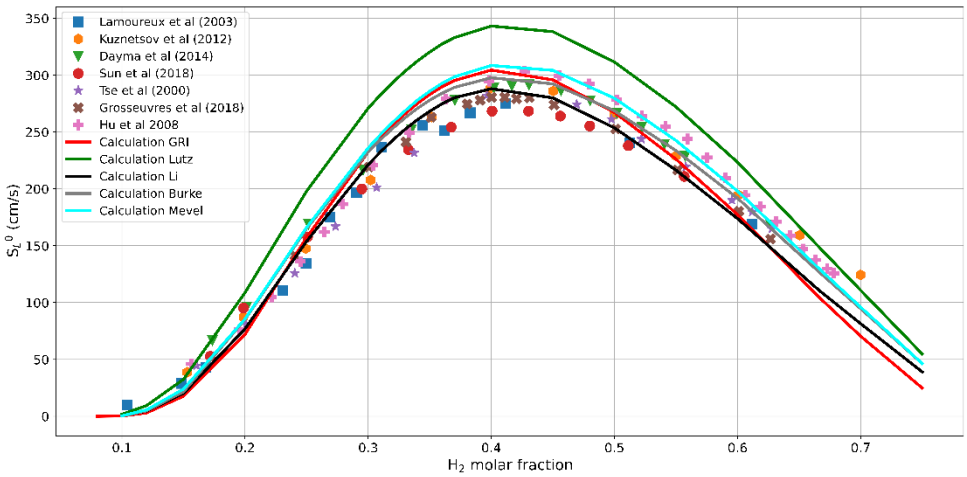

Figure 8: Comparison of experimental data with calculations

All of the most recent models present a good fit with the experimental data. The Lutz model, however, didn't provide a good agreement with the experience, as it was developed around 1990 and was validated against the data available at the time. In order to provide a rational comparison method for the models, a calculation of the deviation of the calculated S_L^0 from the S_L^0 measured from the literature are provided in Figure 9. The good agreement for the GRI, the Li, the Burke and the Mevel kinetic models are well illustrated by the plot as it appears that large part of the data are within +/- 10% of the experimental results regardless of the author. This figure also confirms the global overestimation of flame speed by the Lutz model with deviations higher 10% in a global view.

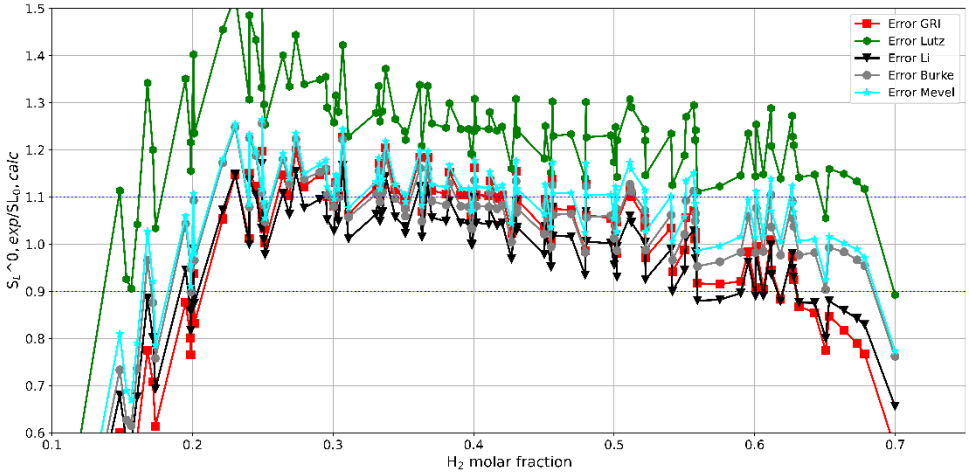

Figure 9: Deviation of the calculated S_L^0 from the experimental S_L^0

Moreover, calculating the standard error for each model (Table 6) based on all the experimental data selected for our work, it appears that the model from Li et al. gives the lowest standard error when compared to the experimental data. As it was previously mentioned, all experimental data are given the same weight. By doing so, it is the whole "cluster" of experimental data that is compared to each model. Thus, the comparison aims to find the model that fits better with the set of experimental data. It is also worth noting that the Li et al mechanism is the one that provides the most point within the +/- 10% deviation with the experiments (65%). The model from Burke et al. gives the second best agreement with the experiments.

Mech	Mevel	Lutz	Li	Burke	GRI
Standard error	26	55	16	20	23
% of data within +-/10% deviation	40%	5%	65%	63%	46%

Table 6: Standard error and 10% deviation percentage for each mechanism

H2/Air mixtures at 363K, 373K and ambient pressure

Very few data in the literature are available on the measurements of laminar flame velocity of hydrogen/air mixtures at high temperature and from the current century. Measurements have been done by Liu et al.[36] and Korrol et al [37] in the 80s and 90s using the burner method. As this method may be subject to errors, we ruled it out of our specification for experimental data. Therefore, only the Hu el al [32] experiments and the Grosseuvres et al [35] are taken into account in this part of the analysis. On Figure 10, the deviations from the experimental values a plotted and exhibit the same behavior as the ambient temperature calculations. Here again, the Lutz et al. mechanism is mostly outside the confidence interval of +/- 10% deviation. On the other hand, the Li et al. mechanism provides the best

agreement with the experimental data with a standard error of 20 cm/s and 81% of the points inside the confidence interval.

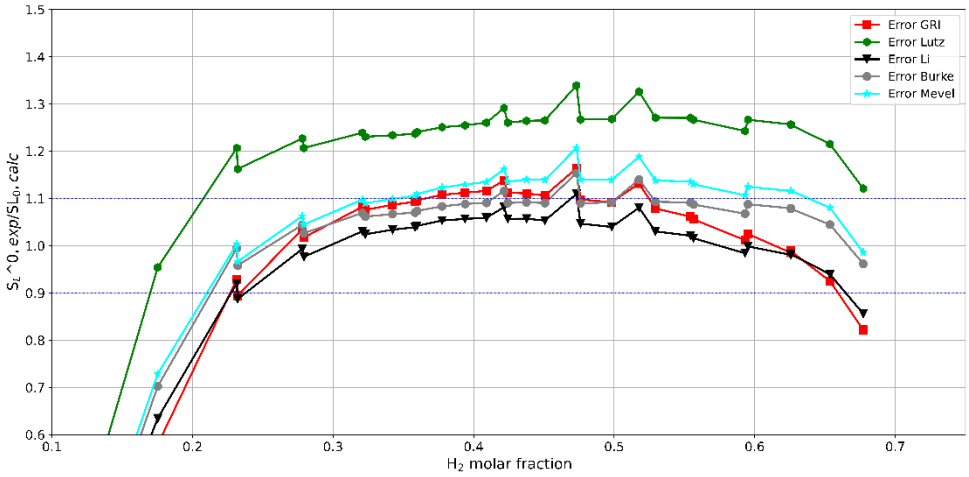

Figure 10: Deviation of the calculated S_L^0 from the experimental S_L^0 at 363K initial

The comparison of the standard error and the percentage of points in the +/-10% margin is reported in table

Mech	Mevel	Lutz	Li	Burke	GRI
Standard error	39	78	20	28	32
% of data within +-/10% deviation	28%	3%	81%	81%	56%

Table 7: Standard error and 10% deviation percentage for each mechanism at elevated temperature

H2/Air mixtures at elevated temperature and elevated pressure

As for the tests at elevated pressure, the data at elevated pressure and temperature are very scarce in the literature. The only data available for our study is the data from Hu et al. [32] which were performed at 373K at 0.25 MPa and at 0.5 MPa. Only rich side measurements were performed with few data for each condition. However, the trend is the same as for the previous calculations. The Li model is in good agreement with the experimental data and proves to be the best fit to the experimental dataset. Both Figure 11 and Table 8 show that the Li mechanism has the lowest standard error with the measurements and the highest percentage of data in the confidence interval.

Mech	Mevel	Lutz	Li	Burke	GRI
Standard error	53	93	17	35	30
% of data within +-/10% deviation	7%	0%	78%	30%	41%

Table 8: Standard error and 10% deviation percentage for each mechanism at elevated temperature and pressure

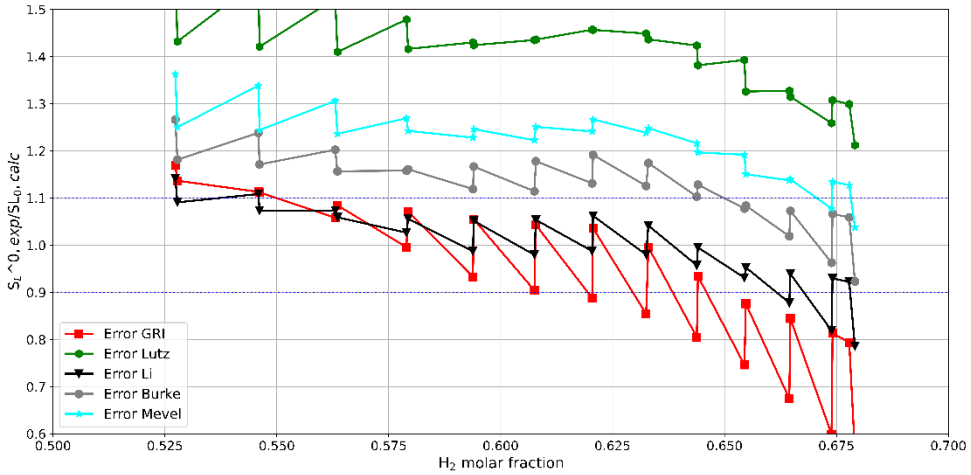

Figure 11: Deviation of the calculated S_L^0 from the experimental S_L^0 at elevated pressure and temperature

This analysis shows that the Li mechanism provides the best agreement overall in ambient and elevated pressure and temperature with the laminar flame speed experiments dataset that we considered for this work. Therefore, the extrapolation of the laminar flame speed at high temperature and pressure will be based on the Li mechanism. The results are displayed on the following figure.

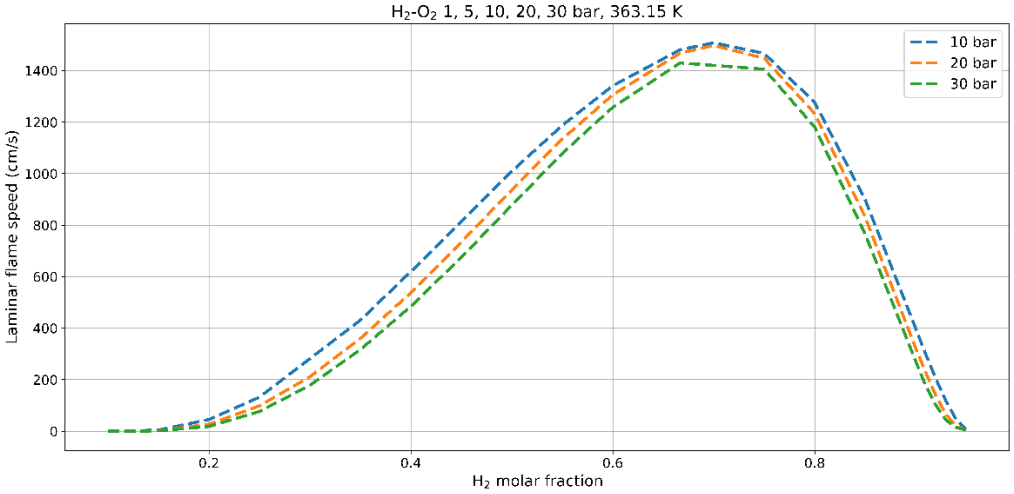

Figure 12: Laminar flame speeds for H_2/O_2 mixtures at high pressure and temperature based on the Li mechanism

CONCLUSION

Laminar flame speed and shock tube induction time simulations were performed using detailed kinetic models available in the literature.

On the shock tube side, the comparison of the experimental data against the simulated values shows a fair agreement. Analysing the relative errors showed that the best fit was obtained with the Mevel et al. mechanism. It was then used to compare the correlations from Ng et al. and Westbrook et al. using Cantera. By comparing with detonation cell size measurement from the literature, the Ng et al. mechanism displayed a better accuracy over the equivalence ratio range when the experiments presented little dispersion. Finally the mechanism was used to extrapolate the detonation cell sizes at electrolyser

operating temperature and varying pressure (1, 15, 30 bar) which can be used to predict the detonability of hydrogen/oxygen mixtures

On the laminar flame side, despite the differences in the experimental data, the Li et al. model has proven to reproduce better the measurements compared to the other mechanisms. Therefore it was a reasonable choice for extrapolating laminar flame speeds to the pressures and temperature of interest. This should in turn allow the evaluation of the fast deflagration potential and the run up distance for such phenomenon to occur.

Overall, this work has highlighted discrepancies in experimental data for laminar flame speeds and detonation cell sizes. In order to improve the quality of our extrapolation, a more thorough investigation of the sources of discrepancy on experimental measurement has to be performed. Additionally, a deeper experimental and modelling work on the ability of the chosen mechanisms to reproduce the effect of increasing both the pressure and temperature must be conducted to improve the confidence in the extrapolation.

REFERENCES

[1] 'GRI-Mech 3.0'. http://combustion.berkeley.edu/gri-mech/version30/text30.html (accessed Mar. 29, 2023).

[2] R. Mével, S. Javoy, F. Lafosse, N. Chaumeix, G. Dupré, and C.-E. Paillard, 'Hydrogen–nitrous oxide delay times: Shock tube experimental study and kinetic modelling', *Proceedings of the Combustion Institute*, vol. 32, no. 1, pp. 359–366, Jan. 2009, doi: 10.1016/j.proci.2008.06.171.

[3] X. Li, X. You, F. Wu, and C. K. Law, 'Uncertainty analysis of the kinetic model prediction for high-pressure H2/CO combustion', *Proceedings of the Combustion Institute*, vol. 35, no. 1, pp. 617–624, Jan. 2015, doi: 10.1016/j.proci.2014.07.047.

[4] A. E. Lutz, R. J. Kee, J. A. Miller, H. A. Dwyer, and A. K. Oppenheim, 'Dynamic effects of autoignition centers for hydrogen and C1,2-hydrocarbon fuels', *Symposium (International) on Combustion*, vol. 22, no. 1, pp. 1683–1693, Jan. 1989, doi: 10.1016/S0082-0784(89)80181-X.

[5] M. P. Burke, M. Chaos, Y. Ju, F. L. Dryer, and S. J. Klippenstein, 'Comprehensive H2/O2 kinetic model for high-pressure combustion', *International Journal of Chemical Kinetics*, vol. 44, no. 7, pp. 444–474, 2012, doi: 10.1002/kin.20603.

[6] D. G. Goodwin, H. K. Moffat, I. Schoegl, R. L. Speth, and B. W. Weber, 'Cantera: An Object-oriented Software Toolkit for Chemical Kinetics, Thermodynamics, and Transport Processes'. 2022.

[7] H. D. Ng, Y. Ju, and J. H. S. Lee, 'Assessment of detonation hazards in high-pressure hydrogen storage from chemical sensitivity analysis', *International Journal of Hydrogen Energy*, vol. 32, no. 1, pp. 93–99, Jan. 2007, doi: 10.1016/j.ijhydene.2006.03.012.

[8] C. K. Westbrook and P. A. Urtiew, 'Chemical kinetic prediction of critical parameters in gaseous detonations', *Symposium (International) on Combustion*, vol. 19, no. 1, pp. 615–623, Jan. 1982, doi: 10.1016/S0082-0784(82)80236-1.

[9] K. A. Bhaskaran, M. C. Gupta, and T. Just, 'Shock tube study of the effect of unsymmetric dimethyl hydrazine on the ignition characteristics of hydrogen-air mixtures', *Combustion and Flame*, vol. 21, no. 1, pp. 45–48, 1973.

[10] R. K.-C. Cheng, *Induction times and strong ignition limits for mixtures of methane with hydrogen*. University of California, Berkeley, 1977.

[11] A. Cohen and J. Larsen, 'Explosive mechanism of the H2-O2 reaction near the second ignition limit', *Report BRL*, vol. 1386, 1967.

[12] S. Fujimoto, 'Chemical reaction in a shock wave. I. The ignition delay of a hydrogen-oxygen mixture in a shock tube', *Bulletin of the Chemical Society of Japan*, vol. 36, no. 10, pp. 1233–1236, 1963.

[13] C. J. Jachimowski and W. M. Houghton, 'Shock-tube study of the initiation process in the hydrogen-oxygen reaction', *Combustion and Flame*, vol. 17, no. 1, pp. 25–30, 1971.

[14] F. JUST, 'Measurements of ignition delays of hydrogen air mixtures under simulated conditions of supersonic combustion chambers(Measurement of ignition delays of hydrogen-air under simulated conditions of supersonic combustion chambers)', 1968.

[15] E. L. Petersen, D. F. Davidson, M. Röhrig, and R. Hanson, 'High-pressure shock-tube measurements of ignition times in stoichiometric H2/O2/Ar mixtures', in *Proceedings of the 20th international symposium on shock waves*, 1996, pp. 941–946.

[16] G. L. Schott and J. L. Kinsey, 'Kinetic studies of hydroxyl radicals in shock waves. II. Induction times in the hydrogen-oxygen reaction', *The Journal of Chemical Physics*, vol. 29, no. 5, pp. 1177–1182, 1958.

[17] G. B. Skinner and G. H. Ringrose, 'Ignition delays of a Hydrogen—Oxygen—Argon mixture at relatively low temperatures', *The Journal of Chemical Physics*, vol. 42, no. 6, pp. 2190–2192, 1965.

[18] A. D. Snyder, J. Robertson, D. L. Zanders, and G. B. Skinner, 'Shock tube studies of fuel-air ignition characteristics', *Monsanto Research Corp., Technical Report AFAPL-TR-65-93*, 1965.

[19] C. M. Guirao, R. Knystautas, J. H. Lee, W. Benedick, and M. Berman, 'Hydrogen-air detonations', Sandia National Labs., Albuquerque, NM (USA); McGill Univ., Montreal, Quebec (Canada),

SAND-82-1494C; CONF-820801-11, Jan. 1982. Accessed: Mar. 31, 2023. [Online]. Available: https://www.osti.gov/biblio/5339784
[20] S. R. Tieszen, M. P. Sherman, W. B. Benedick, J. E. Shepherd, and R. Knystautas, 'Detonation cell size measurements in hydrogen-air-steam mixtures', *Dynamics of explosions*, pp. 205–219, 1986.
[21] G. Ciccarelli, T. Ginsberg, J. Boccio, C. Economos, K. Sato, and M. Kinoshita, 'Detonation cell size measurements and predictions in hydrogen-air-steam mixtures at elevated temperatures', *Combustion and Flame*, vol. 99, no. 2, pp. 212–220, Nov. 1994, doi: 10.1016/0010-2180(94)90124-4.
[22] W. B. Benedick, R. Knystautas, and J. H. Lee, 'Large-scale experiments on the transmission of fuel-air detonations from two-dimensional channels', Sandia National Labs., Albuquerque, NM (USA); McGill Univ., Montreal, Quebec …, 1983.
[23] G. Ciccarelli, T. Ginsberg, and J. L. Boccio, 'Detonation cell size measurements in high-temperature hydrogen-air-steam mixtures at the bnl high-temperature combustion facility', US Nuclear Regulatory Commission (NRC), Washington, DC (United States). Div …, 1997.
[24] H. O. Barthel, 'Predicted spacings in hydrogen-oxygen-argon detonations', *The Physics of Fluids*, vol. 17, no. 8, pp. 1547–1553, 1974.
[25] R. Knystautas, J. H. Lee, and C. M. Guirao, 'The critical tube diameter for detonation failure in hydrocarbon-air mixtures', *Combustion and Flame*, vol. 48, pp. 63–83, Jan. 1982, doi: 10.1016/0010-2180(82)90116-X.
[26] B. V. Voytsekhovskiy, V. V. Mitrofanov, and M. E. Topchiyan, 'The structure of a detonation front in gases', FOREIGN TECHNOLOGY DIV WRIGHT-PATTERSON AFB OH, 1966.
[27] Y. N. Denisov, 'Structure of gaseous detonation in tubes', *Z. Tekh. Fiz.*, vol. 450, 1960.
[28] J. H. Lee and H. Matsui, 'A comparison of the critical energies for direct initiation of spherical detonations in acetylene–oxygen mixtures', *Combustion and Flame*, vol. 28, pp. 61–66, Jan. 1977, doi: 10.1016/0010-2180(77)90008-6.
[29] W. Han, P. Dai, X. Gou, and Z. Chen, 'A review of laminar flame speeds of hydrogen and syngas measured from propagating spherical flames', *Applications in Energy and Combustion Science*, vol. 1–4, p. 100008, Dec. 2020, doi: 10.1016/j.jaecs.2020.100008.
[30] S. D. Tse, D. L. Zhu, and C. K. Law, 'Morphology and burning rates of expanding spherical flames in H2/O2/inert mixtures up to 60 atmospheres', *Proceedings of the Combustion Institute*, vol. 28, no. 2, pp. 1793–1800, Jan. 2000, doi: 10.1016/S0082-0784(00)80581-0.
[31] N. Lamoureux, N. Djebaïli-Chaumeix, and C.-E. Paillard, 'Laminar flame velocity determination for H2–air–He–CO2 mixtures using the spherical bomb method', *Experimental Thermal and Fluid Science*, vol. 27, no. 4, pp. 385–393, Apr. 2003, doi: 10.1016/S0894-1777(02)00243-1.
[32] E. Hu, Z. Huang, J. He, and H. Miao, 'Experimental and numerical study on laminar burning velocities and flame instabilities of hydrogen–air mixtures at elevated pressures and temperatures', *International Journal of Hydrogen Energy*, vol. 34, no. 20, pp. 8741–8755, Oct. 2009, doi: 10.1016/j.ijhydene.2009.08.044.
[33] M. Kuznetsov, S. Kobelt, J. Grune, and T. Jordan, 'Flammability limits and laminar flame speed of hydrogen–air mixtures at sub-atmospheric pressures', *International Journal of Hydrogen Energy*, vol. 37, no. 22, pp. 17580–17588, Nov. 2012, doi: 10.1016/j.ijhydene.2012.05.049.
[34] G. Dayma, F. Halter, and P. Dagaut, 'New insights into the peculiar behavior of laminar burning velocities of hydrogen–air flames according to pressure and equivalence ratio', *Combustion and Flame*, vol. 161, no. 9, pp. 2235–2241, Sep. 2014, doi: 10.1016/j.combustflame.2014.02.009.
[35] R. Grosseuvres, A. Comandini, A. Bentaib, and N. Chaumeix, 'Combustion properties of H2/N2/O2/steam mixtures', *Proceedings of the Combustion Institute*, vol. 37, no. 2, pp. 1537–1546, Jan. 2019, doi: 10.1016/j.proci.2018.06.082.
[36] D. D. S. Liu and R. MacFarlane, 'Laminar burning velocities of hydrogen-air and hydrogen-air–steam flames', *Combustion and Flame*, vol. 49, no. 1, pp. 59–71, Jan. 1983, doi: 10.1016/0010-2180(83)90151-7.
[37] G. W. Koroll, R. K. Kumar, and E. M. Bowles, 'Burning velocities of hydrogen-air mixtures', *Combustion and Flame*, vol. 94, no. 3, pp. 330–340, Aug. 1993, doi: 10.1016/0010-2180(93)90078-H.