

Investigation of different chemical kinetics reaction rates and its relevant modelling for H₂-O₂ combustion

Sayed Ebrahim Hashemi, Pratap Jung Rai, Sudeep Parajuli, Arash Abbasi

Department of Process, Energy and Environmental Technology, University College of Southeast Norway, Porsgrunn, Norway

ABSTRACT

The chemical reaction rate is considered as an essential requirement for modelling of different combustion phenomena. Several parameters such as temperature, pressure and reaction steps of combustible fuel influence the accuracy of modelling. Investigation of different reaction steps of modelling hydrogen mixture is reckoned in the present work. Accomplished modelling for H₂-O₂ in the scientific literature has been studied and tried to find the correct value of constants in the Arrhenius form of reaction rate. One and two-step reaction rates have been modelled and found an oxidizer concentration in the one-step reaction will decrease much more than in two-step reaction whereas concentration will be zero at the end, while hydrogen consumed faster in a two-step reaction. Both temperature and pressure had a great impact on reaction rates for one-step modelling whereas the rate of reaction increased exponentially.

Keyword: Chemical Reaction Steps, Hydrogen mixture, Reaction Rate, Arrhenius Constants

1. INTRODUCTION

The chemical reaction rate is the rate of change in concentrations or amounts of either reactants or products. The chemical reaction mechanism is stepwise descriptions of what comes on molecular level while chemical reaction takes place. An elementary chemical reaction is introduced to obtain the detailed information about the chemical reaction during the process which helps to understand the flame and reaction shock wave behaviours [1].

To understand and predict the behaviour of a chemical system one must consider chemical kinetics. The application of the numerical method in combustion processes for modern technologies needs some modification and information to achieve precise results. Nevertheless, detailed information sometimes creates more complexity which explores arduous result of concepts [2].

Among all combustible fuel, hydrogen is considered as one of the most ideal fuels that can reduce the greenhouse gas and air pollutant emissions in the world. However, the safety issues of hydrogen should be resolved carefully before it being widely used, particularly in cities. In addition, hydrogen is one of the most promising fuel for the supersonic air flow system and it fascinates researchers' attention these days.

In this work, a brief explanation of different reaction steps, especially for H₂ combustion under a scientific investigation is considered. Furthermore, a study of different models of chemical kinetics reaction steps is investigated and eventually, created a model for H₂-O₂ combustion by using numerical methods to determine rates of chemical reaction.

2. LITERATURE REVIEW OF DIFFERENT CHEMICAL REACTION STEPS

2.1. Single step kinetic reaction

The reactants are converted into the products in a single step and the reaction is called a one-step reaction. Figure 1 shows the schematic diagram for a hypothetical one step reaction when two or more atoms or molecules collide with each other. An elementary step is a reaction which takes place by such a collision process [3]. An elementary step is characterised by its molecularity, the number of reactant particle in the step.

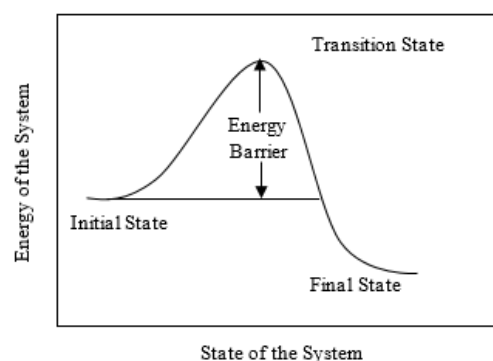


Figure 1: Schematic diagram for a hypothetical one-step reaction [4].

The position of maximum energy is called the transition state of the reaction, and the differences in energy between the transition state and the initial state are the energy barrier to the reaction. A one-step reaction has a single transition state; such a process is called an elementary reaction. The transition state is more unstable than either reactants or products. Thus, it either continues to form the products or returns to the reactants [4, 5].

Many researchers have worked on the study of the application of one-step mechanism. In most of the applied systems, the combustion shows highly turbulent to the fluid velocity. A one-step global kinetic model has been used in current numerical fluid calculations by many scholars [3].

Fernández et al. [6] studied the use of one step reduced kinetics to calculate the flammability limits and burning velocities of planar deflagration. Moreover, an explicit one-step reaction rate expression has been derived for the hydrogen oxidation reaction, which is then used for the calculation of lean flammability limit and laminar burning velocities of hydrogen-air systems. The study is limited to fuel lean mixture, and the system is depending upon the pressure and initial temperature.

Similarly, the study modelled in [6] shows that the accuracy of the steady-state expression is limited to lean conditions, and when the mixtures become richer, it degrades, that leads to the failure of the one step reduced kinetics, which must be replaced by the two-step or three-step mechanisms. In the study it is assumed that O, OH, and HO_2 maintain steady states throughout the flame, for the hydrogen-air combustion, and thus H doesn't follow the steady-state approximation [7]. To make this mechanism a one-step mechanism, H also should behave as steady state.

Bane et al. [8] worked to develop a one-step model for use in flame, ignition and large-scale combustion simulation, which is based on constant pressure and constant volume. The research intended to develop the model that extracts the physical parameters which will use in the one-step model for flame and ignition simulation. A method was developed to calculate the effective reaction order and activation energy for a range of hydrogen-air mixtures for one step reaction.

Yinhe Liu et al. [9] studied the premixed hydrogen flame propagation experimentally and by using the numerical simulation, where they used the one step global reaction mechanism. They mainly focused on the impact of initial temperature, hydrogen concentration and steam concentration on hydrogen/air flame propagation.

2.2. Two step kinetic reaction

Many chemical reaction models such as the C-J model, the two-step reaction model, and the detailed chemical reaction model has been applied to numerical simulations of detonation waves. The two-step chemical reaction model can describe the chemical reaction process. Thus, the two-step chemical reaction model is also studied by many scholars [10].

The main superiority of two-step reaction to single step is the ability of modelling delayed zone in combustion processes. Specifically, attention is directed towards developing two-step models, the first step pertaining to the nearly isothermal induction and subsequent abrupt temperature increase, and the second to the later slow temperature rise. Two-step reactions are categorized below with respect to complexity:

A. Two-step models (delayed parameter) [11, 12].

Principally, the delayed parameter model is preferred to single step reaction due to considering delayed zone of reaction. Moreover, accounting a few empirical parameters in

this model caused to have a more close approximation to experimental data by numerical simulation. However, those empirical parameters were different for each mixture.

B. Reduced mechanisms [13].

Due to the computational cost of using detailed models, reduced mechanisms are more popular. In fact, reduced mechanisms are derived from detailed mechanisms to smaller models with less number of species which has been using since very longer time for flame studies.

Two-step chemical kinetic descriptions for H_2 - O_2 and other hydrocarbon fuels was considered by Varatharajan et al. [14]. They tried to simplify different elementary steps of combustion with regards to detonation application in two steps. Those reaction mechanisms were developed via reduction processes from the detailed mechanism which comprises 193 reactions, among them 41 species have been examined comprehensively against shock tube ignition times and counter flow flame structure measurements.

Liu et al. [15] studied detonation propagation characteristic of the H_2 - O_2 - N_2 mixture in a tube with considering two-step chemical kinetic reactions of hydrogen. Their research showed that various initial condition had a huge influence on detonation.

Huang et al. [16] studied the effect of H_2O mass fraction by using two different chemical kinetics mechanism of the turbulent diffusion combustion of H_2 - O_2 in supersonic flow. They employed namely the two-step mechanism of Rogers and Chinitz [17] and the seven-step mechanism of Jachimowski [18]. The obtained results showed that the predicted mole fraction profiles for different components have good connection with the investigated data under the supersonic mixing and combustion condition, and there was no significant impact of chemical reaction on the overall performance of turbulent diffusion combustion.

2.3. Three step kinetic reaction

Three Step Reactions are step-by-step of elementary reaction process till the third step that occurs on a molecular level in chemical reactions. There are different factors which has to be kept in mind while determining the three-step rate of reaction such as concentration, surface area, temperature, and catalysts [19]. The three-step chemical reaction comprises two intermediate species (I_{1-2}) and three activated complexes number (X_{1-3}), which is shown in Figure 2.

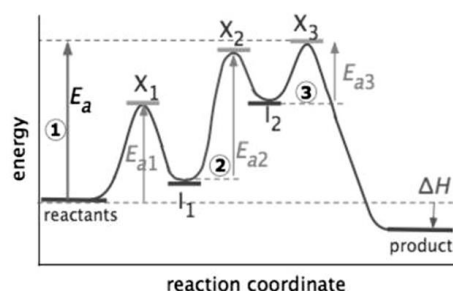


Figure 2: Schematic diagram for a hypothetical three-step reaction [20].

Pierre et al. [21] studied about universal reduced chemistry for H₂-O₂ combustion focused on H₂ oxidation including premixed and non-premixed on the basis of flammability and autoignition. According to research, four step chemistry has been used to determine autoignition time which found above the second explosion limit. And also, two separated three step reduced chemistry has been used for flames and autoignition, considered best mechanism, but does not applicable for universal reduced chemistry. From many discussions shown in [21-23], three step chemical kinetic is suitable for autoignition and planar detonation, including premixed and non-premixed combustion, in the both condition; above and below second explosion limit.

Jiménez et al. [24] used San Diego mechanism for three step reaction mechanism to test explicitly reduced mechanism for H₂-O₂ combustion and found three step reaction is an excellent mechanism for laminar flame burning velocities induction time, oxidizer stream temperature at autoignition [25]. To compute steady planar deflagration and non-premixed counter-flow flames. The most interesting observation is higher the pressure at steady state assumption associated in reduced chemistry has higher accurate ingrate predictions. In fact, these simplified mechanism [24] would be suitable and sufficiently accurate for deflagration, detonation, and ignition, at both speed; low-speed and supersonic combustion.

Many scholars suggested that HO₂ at steady state assumption is a reasonable approximation for three step reaction mechanism than four step chemistry when the homogeneous ignition of the hydrogen-oxygen mixture under the crossover temperature and pressure at initial condition [22, 23].

From the discussion given in [26], Figure 3 along with different pressure and ignition time shows the resulted equivalence ratios within flammability condition range changes from very lean to very rich mixtures and also found temperature and error at very lean mixtures have proportional relation if the temperature increases error also increases proportionally.

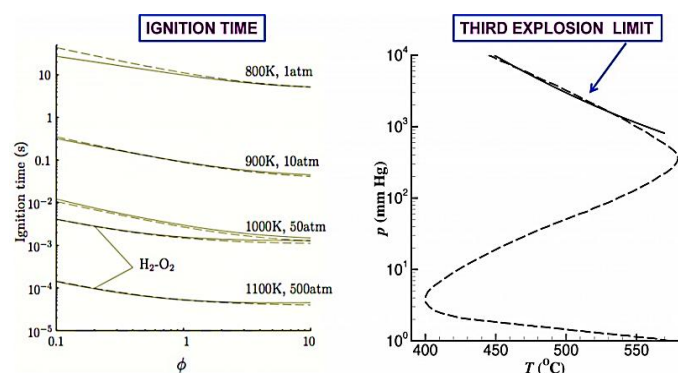


Figure 3: Below crossover temperature of hydrogen-oxygen ignition. Left-hand-side indicates the variation of ignition time with equivalence ratio and right-hand-side indicates by dashed line experimentally determined explosion limits of the hydrogen-oxygen and solid line representing analytic prediction developed by third explosion [27].

2.4. Four and more kinetic reaction steps

The four and more steps reaction mechanism present reasonable results at different condition. However, it takes more computational time than reduced reaction steps such as one, two and three steps.

Boivin et al. [21] studied the four-step mechanism with O and OH at steady-state condition reduce to 3-step mechanism in order to reduce the computational time. The principle of their method is based on reduced mechanism and nominated a single species, introducing HO₂ for high temperature and H₂-O₂ for low-temperature ignition.

Zacharias et al. [2] studied five steps chemical kinetic mechanism for using in gas turbine combustion. Skeletal and reduced mechanism were applied for laminar flame speed, the delay time of ignition and structure of flame, as they compared their results with some experimental data. Their results showed mechanisms can be applied in a wide range of pressures and temperatures; furthermore, with using the reduced mechanism reduced the computational time to the GRI mesh 3.0 and increase the accuracy.

Location of second explosion limit and progress time of hydrogen-air mixing layer that a branched-chain explosion determines the process of ignition is studied by [28]. Moreover, they compared some articles about the problem of Hydrogen-air auto-ignition time with experimental data [29].

Cao et al. [30] investigated the influence of the reaction mechanism in finite-rate chemistry large-eddy simulation of self-ignition, and three different hydrogen-air reaction mechanisms were employed. They found that the one-step mechanism results in a too early ignition and a more stable flame, and the seven-step mechanism is the only model that can match the wall pressure amplitudes and the OH distributions.

Strohle et al. [31] evaluated a reaction mechanism for hydrogen combustion in a gas turbine combustor, and six different chemical reaction mechanisms were selected for comparisons.

3. NUMERICAL DESCRIPTION

The way of calculating differential equations has been a challenge in all research [18, 28]. Although, considering the only reaction rate as a differential equation is very easy to handle. Increasing in detailed reaction steps needs to develop equations and couple them to each other. There are several methods to compute ordinary differential equation such as simple Forward or Backward Euler method. Moreover, it is possible to employ several advanced methods like Rung Kutta and Huen's method to calculate the concentration changes in combustor numerically. A Forward Euler method was used in modelling of hydrogen combustion to compute single and two-step reactions numerically, where two-step reaction rates were needed to couple reactions to each other.

4. MODELLING FOR ONE AND TWO STEP REACTION

The main issue we encountered while modelling was to find relevant and accurate pre-exponential factors on the Arrhenius reaction rate. The detailed reaction and its relevant

Arrhenius constants are tabulated in Appendix I (Table 1) for several reaction steps. During the combustion process, a constant temperature was assumed to calculate concentrations and rate constants. Moreover, using a differential form of energy balance would give more accurate results even in single step reaction. However, the effect of varying temperature and pressure was considered in the rate of reaction.

5. RESULT AND DISCUSSION

The numerical results of reaction rates in a combustible mixture of H_2-O_2 under a specific condition of temperature and pressure for one-step and two-step reactions are shown in Figure 4 and 5 respectively. In a single step reaction, the primary concentration of oxygen is half of hydrogen according to stoichiometry reaction. Initially, the H_2O production rate is high and goes on decreasing gradually while the fuel (H_2) is being consumed.

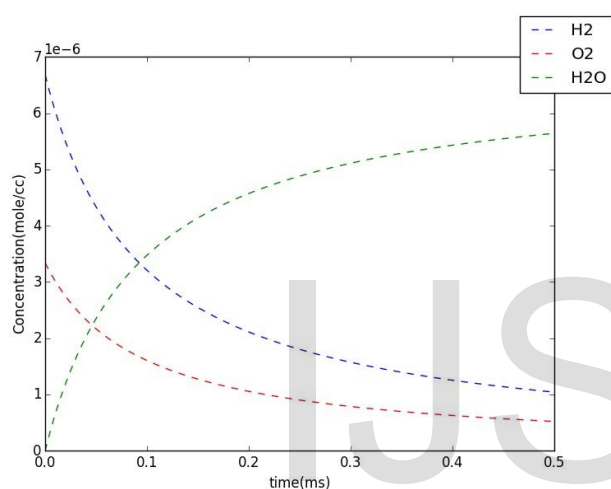


Figure 4: Concentration as a function of time for H_2 combustion in one step reaction at $T= 1200$ K and $P =1$ bar

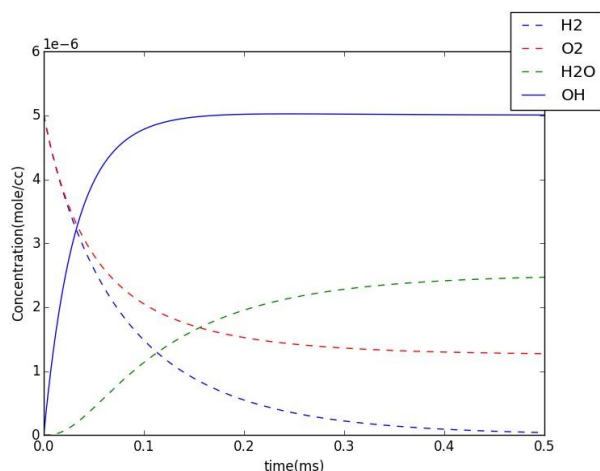


Figure 5: Concentration as a function of time for H_2 combustion in two-step reactions at $T= 1200$ K and $P =1$ bar

In Figure 5, both concentrations of hydrogen and oxidizer had the same amount with regards to stoichiometric reactions. In two-step reactions, the rate of consuming H_2 is higher than a single step. However, Figure 5 shows that the final concentration of water as a product is lower than it contained

in a one-step reaction. Moreover, OH as an intermediate product is counted as the major product in two-step reactions. Figure 4 and 5 illustrate that the initial fuel consumption in two step reaction is much faster than one step, however producing intermediate radicals is considered as its drawbacks. After a certain time, the concentration of oxygen becomes zero in one-step reaction while it reaches to a particular concentration in the two-step reaction.

The effect of temperature on reaction rate for a single step reaction is demonstrated in Figure 6 which shows that the reaction rate of H_2O increases exponentially with the increase in temperature. However, the reaction rate of H_2 and O_2 goes on decreasing as the temperature increases. After certain temperature (approx. 1300 K), the rate of reaction changes dramatically. Therefore, the suitable range of temperature should be considered for single-step reaction of H_2 mixture combustion to achieve an accurate computational model for the simulation in different applications,

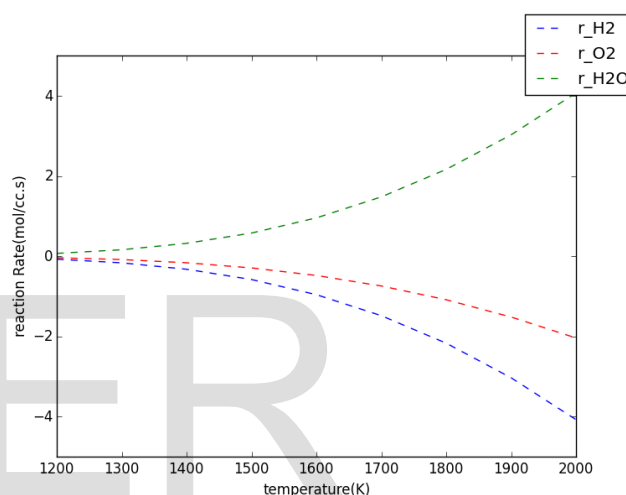


Figure 6: Reaction rate comparison for different range of temperature at $P =1$ bar

The impact of pressure on the reaction rate of H_2 mixture combustion is illustrated in Figure 7 which shows the same trend as that of temperature. The rate of reaction of H_2O increases as the pressure rises.

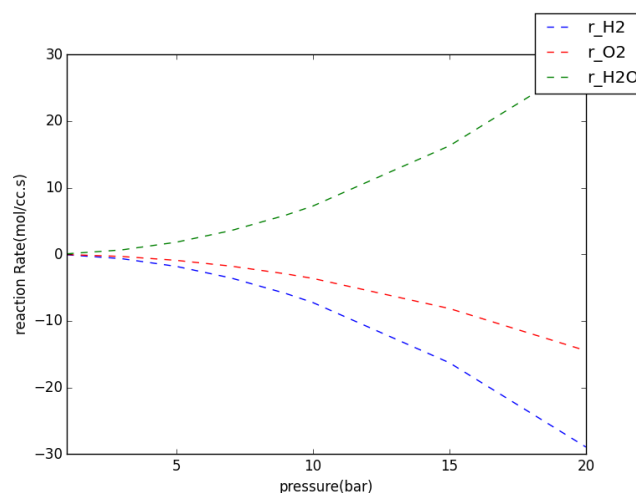


Figure 7: Reaction rate comparison for different range of pressure at $T=1200$ K

Results show that the reaction rate is sensitive to temperature and pressure. The effect of temperature and pressure is not linear on reaction rate. Consumption of fuel increases while reaction rate increases, to produce a product (in single step reaction the only product is water).

6. CONCLUSION

According to discussed models above, the following conclusions are possible to formulate:

- Different reaction steps are used for specific applications.
- Increasing reaction rate may give more accurate results. However, the computational costs outweigh.
- Solving differential equation of reaction rates is the challenging task to decide between numerical errors and computing run time.
- Oxidizer concentration decreased much more in one-step reaction whereas it reached to zero concentration at the end.
- The main production in two-step reaction was OH radical while in one-step, water was the only product.
- The concentration of product in the single-step reaction of the hydrogen-oxygen mixture was higher than two-step reactions.
- Hydrogen consumed faster in a two-step reaction.
- Both temperature and pressure had a great impact on reaction rates for one-step modelling where the rate of reaction increased exponentially.

ACKNOWLEDGEMENT

We would like to express our special thanks of gratitude to our supervisor Ass. Professor Andre Vagner Gaathaug who gave us the golden opportunity to do this wonderful project, as well as we would also like to thank our friends and entire college personnel who helped us a lot in finalizing this project report within the time frame.

REFERENCES

- [1] S. McAllister, J.-Y. Chen, and A. C. Fernandez-Pello, *Fundamentals of combustion processes*: Springer, 2011.
- [2] Z. M. Nikolaou, J.-Y. Chen, and N. Swaminathan, "A 5-step reduced mechanism for combustion of CO/H₂/H₂O/CH₄/CO₂ mixtures with low hydrogen/methane and high H₂O content," *Combustion and Flame*, vol. 160, pp. 56-75, 1// 2013.
- [3] G. L. Borman and K. W. Ragland, *Combustion Engineering*: McGraw-Hill Science/Engineering/Math, 1998.
- [4] K. A. Connors, *Chemical Kinetics: The Study of Reaction Rates in Solution*. New York: VCH Publishers, Inc., 1990.
- [5] Richard F. Daley and S. J. Daley, *Organic Chemistry*: Daley Press, 2013.
- [6] D. Fernández-Galisteo, A. Sánchez, A. Liñán, and F. Williams, "One-step reduced kinetics for lean hydrogen-air deflagration," *Combustion and flame*, vol. 156, pp. 985-996, 2009.
- [7] N. Peters and B. Rogg, *Reduced kinetic mechanisms for applications in combustion systems* vol. 15: Springer Science & Business Media, 2008.
- [8] S. Bane, J. Ziegler, and J. Shepherd, "Development of one-step chemistry models for flame and ignition simulation," *GALCIT Report GALCITFM*, vol. 2010, 2010.
- [9] Y. Liu, Y. Zhang, X. Liu, Z. Liu, and D. Che, "Experimental and numerical investigation on premixed H₂/air combustion," *International Journal of Hydrogen Energy*, 2016.
- [10] J. Ning, X. Yuan, T. Ma, and C. Wang, "Positivity-preserving moving mesh scheme for two-step reaction model in two dimensions," *Computers & Fluids*, vol. 123, pp. 72-86, 12/21/ 2015.
- [11] S. Taki and T. Fujiwara, "Numerical Analysis of Two-Dimensional Nonsteady Detonations," *AIAA Journal*, vol. 16, pp. 73-77, 1978/01/01 1978.
- [12] E. S. Oran, T. R. Young, J. P. Boris, J. M. Picone, and D. H. Edwards, "A study of detonation structure: The formation of unreacted gas pockets," *Symposium (International) on Combustion*, vol. 19, pp. 573-582, // 1982.
- [13] A. S. Tomlin, T. Turányi, and M. J. Pilling, "Chapter 4 Mathematical tools for the construction, investigation and reduction of combustion mechanisms," in *Comprehensive Chemical Kinetics*. vol. Volume 35, M. J. Pilling, Ed., ed: Elsevier, 1997, pp. 293-437.
- [14] B. Varatharajan, M. Petrova, F. A. Williams, and V. Tangirala, "Two-step chemical-kinetic descriptions for hydrocarbon-oxygen-diluent ignition and detonation applications," *Proceedings of the Combustion Institute*, vol. 30, pp. 1869-1877, 1// 2005.
- [15] Y. Liu and X. Liu, "Detonation propagation characteristic of H₂-O₂-N₂ mixture in tube and effect of various initial conditions on it," *International Journal of Hydrogen Energy*, vol. 38, pp. 13471-13483, 10/8/ 2013.
- [16] W. Huang, Z.-g. Wang, S.-b. Li, and W.-d. Liu, "Influences of H₂O mass fraction and chemical kinetics mechanism on the turbulent diffusion combustion of H₂-O₂ in supersonic flows," *Acta Astronautica*, vol. 76, pp. 51-59, 7// 2012.
- [17] R. R and C. W, "On the use of a global hydrogen-air combustion model in the calculation of turbulent reacting flows," in *20th Aerospace Sciences Meeting*, ed: American Institute of Aeronautics and Astronautics, 1982.
- [18] C. J. Jachimowski, "An analytical study of the hydrogen-air reaction mechanism with application to scramjet combustion," 1988.

- [19] T. A. M. U. Department of Chemistry. (2015). *Kinetics : Factors Affecting Reaction Rates*. Available: <https://www.chem.tamu.edu/class/majors/tutorialnote/files/factors.htm>
- [20] S. Lower. (2014). *Chem1 virtual textbook*. Available: <http://www.chem1.com/acad/webtext/dynamics/mech.html>
- [21] P. Boivin, A. L. Sánchez, and F. A. Williams, "Four-step and three-step systematically reduced chemistry for wide-range H₂-air combustion problems," *Combustion and Flame*, vol. 160, pp. 76-82, 1// 2013.
- [22] E. Fernández-Tarrazo, A. L. Sánchez, and F. A. Williams, "Hydrogen-air mixing-layer ignition at temperatures below crossover," *Combustion and Flame*, vol. 160, pp. 1981-1989, 10// 2013.
- [23] P. Boivin, "Reduced-kinetic mechanisms for hydrogen and syngas combustion including autoignition," 2011.
- [24] P. Saxena and F. A. Williams, "Testing a small detailed chemical-kinetic mechanism for the combustion of hydrogen and carbon monoxide," *Combustion and Flame*, vol. 145, pp. 316-323, 2006.
- [25] P. Boivin, C. Jiménez, A. L. Sánchez, and F. A. Williams, "An explicit reduced mechanism for H₂-air combustion," *Proceedings of the Combustion Institute*, vol. 33, pp. 517-523, 2011.
- [26] P. Boivin, A. L. Sánchez, and F. A. Williams, "Explicit analytic prediction for hydrogen-oxygen ignition times at temperatures below crossover," *Combustion and Flame*, vol. 159, pp. 748-752, 2012.
- [27] Antonio L. Sánchez, César Huete, a. Daniel Martínez-Ruiz, and D. M. Boza. *Reactive Flows*. Available: <http://asanchez.ucsd.edu/research-2/chemical-kinetic-studies/>
- [28] P. Boivin, A. Dauplain, C. Jiménez, and B. Cuenot, "Simulation of a supersonic hydrogen-air autoignition-stabilized flame using reduced chemistry," *Combustion and Flame*, vol. 159, pp. 1779-1790, 4// 2012.
- [29] P. Boivin, "Reduced-kinetic mechanisms for hydrogen and syngas combustion including autoignition," PHD, Universidad Carlos III de Madrid, 2011.
- [30] C. Cao, T. Ye, and M. Zhao, "Large eddy simulation of hydrogen/air scramjet combustion using tabulated thermo-chemistry approach," 2015.
- [31] J. Ströhle and T. Myhrvold, "An evaluation of detailed reaction mechanisms for hydrogen combustion under gas turbine conditions," *International Journal of Hydrogen Energy*, vol. 32, pp. 125-135, 1// 2007.
- [32] G. Balakrishnan, M. D. Smooke, and F. A. Williams, "A numerical investigation of extinction and ignition limits in laminar nonpremixed counterflowing hydrogen-air streams for both elementary and reduced chemistry," *Combustion and Flame*, vol. 102, pp. 329-340, 8// 1995.
- [33] A. L. Sánchez, E. Fernández-Tarrazo, P. Boivin, A. Liñán, and F. A. Williams, "Ignition time of hydrogen-air diffusion flames," *Comptes Rendus Mécanique*, vol. 340, pp. 882-893, 11// 2012.

Appendix I

Table 1: Rate parameters for Arrhenius form ($k = A_0 T^n \exp(-\frac{E_a}{RT})$) for different H₂-O₂ mechanisms

Reaction	A ₀ [m ³ mol ⁻¹ s ⁻¹]	T [K]	n	Reference
Single-step reaction				
$2H_2 + O_2 \xrightarrow{I} 2H_2O$	$9.9 \cdot 10^{14}$	15,155	0.0	[15]
Two-step reaction				
$H_2 + O_2 \xrightarrow{I} 2OH$	$2.30 \cdot 10^{16}$	5,134	0.0	[16]
$2OH + H_2 \xrightarrow{II} 2H_2O$	$1.83 \cdot 10^{18}$	11,067	0.0	
Three-step reaction				
$H + O_2 \xrightarrow{I} OH + O$	$3.52 \cdot 10^{16}$	94	-0.7	[24]
$H_2 + O \xrightarrow{II} HO + H$	$5.06 \cdot 10^4$	1,756	2.7	
$H_2 + OH \xrightarrow{III} H_2O + H$	$1.17 \cdot 10^9$	5,182	1.3	
Four-step reaction				
$H + O_2 \xrightarrow{I} OH + O$	$3.52 \cdot 10^{16}$	8,589	-0.7	[32]
$O + H_2 \xrightarrow{II} HO + H$	$5.06 \cdot 10^4$	3,165	2.67	
$H_2 + OH \xrightarrow{III} H_2O + H$	$1.17 \cdot 10^9$	1,825	1.3	
$H + H + M \xrightarrow{IV} H_2 + M$	$1.80 \cdot 10^{18}$	0	-1	
Five-step reaction				
$H + O_2 \xrightarrow{I} OH + O$	$3.52 \cdot 10^{16}$	8,589	-0.7	[33]
$H_2 + O \xrightarrow{II} OH + H$	$5.06 \cdot 10^4$	3,165	2.67	
$H_2 + OH \xrightarrow{III} H_2O + H$	$1.17 \cdot 10^9$	1,829	1.3	
$H + O_2 + M \xrightarrow{IV} HO_2 + M^b$	$5.75 \cdot 10^{19}$	0	-1.4	
$H_2 + O_2 \xrightarrow{V} HO_2 + H$	$2.69 \cdot 10^{12}$	2,789	0.36	
Seven-step reaction				
$H + OH + M^a \xrightarrow{I} H_2O$	$2.21 \cdot 10^{22}$	0.0	-2.0	[16]
$H + H + M^a \xrightarrow{II} H_2 + M^a$	$7.30 \cdot 10^{17}$	0.0	-1.0	
$H_2 + O_2 \xrightarrow{III} 2OH$	$1.70 \cdot 10^{13}$	48,000	0.0	
$H + O_2 \xrightarrow{IV} OH + O$	$1.20 \cdot 10^{17}$	16,800	-0.9	
$OH + H_2 \xrightarrow{V} H_2O + H$	$2.20 \cdot 10^{13}$	5,150	0.0	
$O + H_2 \xrightarrow{VI} OH + H$	$5.06 \cdot 10^{14}$	6,268	2.7	
$2OH \xrightarrow{VII} H_2O + O$	$6.30 \cdot 10^{12}$	1,090	0.0	

^a [M] = 2.5[H₂] + 16.0[H₂O] + 1.0[OTHER]