



# Mechanisms of Ethylene Flame Propagation Enhancement by O ( $a^1\Delta g$ )

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# Mechanisms of Ethylene Flame Propagation Enhancement by $O_2(a^1\Delta_g)$

Recently estimated and updated quenching rates of  $O_2(a^1\Delta_g)$  by H and  $H_2$  have been added to a known and validated combustion mechanism to predict enhancement of  $C_2H_4$  flame propagation in the presence of  $O_2(a^1\Delta_g)$ . The results of experiments that targeted the isolated enhancement of  $O_2(a^1\Delta_g)$  on  $C_2H_4$  flame propagation were used as a means to compare the effects of different chain-initiation, chain-branching, and quenching rates. The ratio of chain-branching to quenching rates of 0.25 to 0.33 for  $H+O_2(a^1\Delta_g)$  was found to accurately predict the enhancement trends found in the  $C_2H_4$  flame propagation experiments. The results suggest that flame propagation enhancement of hydrocarbon fuels may not be strongly dependent on the reactions of intermediate hydrocarbon fragments with  $O_2(a^1\Delta_g)$  since the dominant pathways may solely lie with primary radicals such as H.

## Introduction

Understanding in the field of plasma-assisted combustion has advanced considerably over the past decade, showing significant enhancement and making mainstream practical applications increasingly more realistic [1-3]. Many of the applications are motivated by the need for higher performance and more efficient combustion systems ranging from small internal combustion engines to high-speed air-breathing propulsion devices. These systems can require ignition at low temperatures, within restricted residence times, burning outside normal flammability limits, and flame stabilization in high-speed flows. Therefore, there has been significant effort focused on attempting to gain a fundamental understanding of the mechanisms of plasma-assisted combustion. This has naturally motivated investigations that identify and target specific plasma-produced species and enhancement pathways by decoupling the potential thermal, kinetic, transport, and hydrodynamic effects.

One of the areas of research that has emerged with regard to decoupling the plasma-flame interaction in order to understand combustion enhancement is to produce specific species via a plasma discharge and examine their effects on flame propagation. Since the propagation of a flame is driven by how the reactants are conditioned and brought to sufficiently high temperatures allowing for rapid oxidation, thermal conduction and radical diffusion upstream are vital. Therefore there is the potential to affect flame propagation rates by either providing a source of heat or by modifying the kinetics to increase chemical heat release in the lower temperature preheat portions of a flame. The application of plasma touches upon both of these enhancement mechanisms by producing species in the reactants somewhere

upstream that will allow for modification of kinetics in the early stages of the flame. For example, the low temperature preheat zone will significantly benefit from the activation of new kinetic pathways through the introduction of specific species that affect chain-initiation and chain-branching reactions. This in turn couples with the enhanced early reactivity and heat release that ultimately results in a more rapid propagating or stable flame. For this to be accomplished, the species causing the enhancement need to survive until the flame front, and therefore results in either in situ production for short lifetime species, or potential remote production for longer lifetime species. This creates a challenge as to discerning where and how the species are produced, and therefore properly defining the boundary conditions for modelling. An attractive plasma-produced species that can be produced and introduced to a flame for enhancement is  $O_2(a^1\Delta_g)$ , the first electronically excited state of  $O_2$ . While  $O_2(a^1\Delta_g)$  is typically produced among many other plasma species that have the potential to enhance a flame, one of the key points is that  $O_2(a^1\Delta_g)$  requires very low excitation levels with only 0.98 eV/molecule. Therefore, it has the potential to be generated across a wide range of systems. More importantly,  $O_2(a^1\Delta_g)$  has very high reactivity. For example, take one of the most important chain-branching reactions in combustion systems,



If the  $O_2$  in the system is excited to the first electronic level,  $O_2(a^1\Delta_g)$ , it is shown in figure 1 that the reaction rate becomes significantly faster (up to 6 orders of magnitude), especially at temperatures below 1000 K. Furthermore, if only 1% of the  $O_2$  is converted to  $O_2(a^1\Delta_g)$ , there remains an order of magnitude increase in the reaction rate at temperatures as high as 1000 K. Therefore, if plasma can activate the

oxidizer of a combustion system to produce  $O_2(a^1\Delta_g)$ , there is great potential to enhance the overall combustion process with small energy input through chain-branching because of the high chemical selectivity and radical production. Furthermore,  $O_2(a^1\Delta_g)$  has a significantly long radiative lifetime ( $> 4000$  s) because of a spin forbidden transition to the ground state [4]. Therefore, it can be produced remotely, quantitatively measured, and transported to a flame, allowing for a clear definition of the boundary conditions for any experiment, and therefore subsequent modelling efforts.

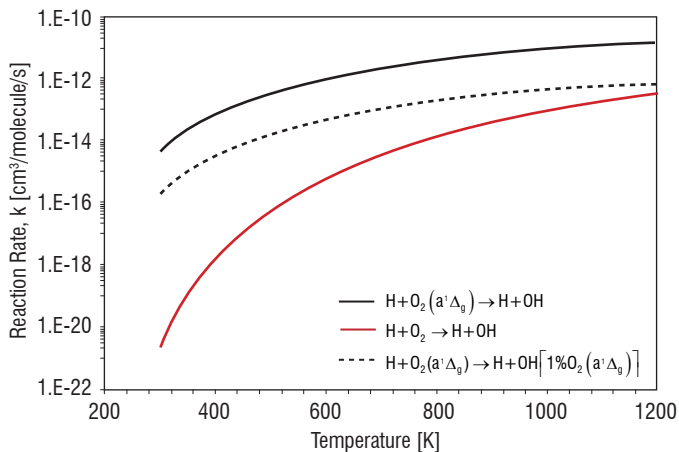


Figure 1 – Calculated reaction rate as a function of temperature for H with  $O_2$  and  $O_2(a^1\Delta_g)$  [5, 6]

Because of the potential benefits of  $O_2(a^1\Delta_g)$ , there have been many works targeting an understanding of the enhancement mechanism using a variety of fuels [7-15]. The experiments and kinetic models have shown that the induction and ignition delay times can be reduced significantly and the laminar flame speeds can be enhanced. Initially Basevich *et al.*, apparently for the first time, used the reactions involving  $O_2(a^1\Delta_g)$  to explain flame speed enhancement in  $H_2/O_2$  mixtures after the excitation of  $O_2$  by a discharge [7]. The oxygen flow was excited by a DC discharge ( $I=5-85$  mA), and then  $H_2$  was added to the flow. The obtained mixture was ignited by a pulsed spark discharge with subsequent measurements of normal flame velocity and the axial profile of translational gas temperature. For discharge currents exceeding 17 mA, the flame velocity almost doubled, while the increase in the translational gas temperature did not exceed 5-10 K. The results of the simulations in reference [5] confirmed the assumption that the impact of a glow discharge in  $O_2$  on the flame velocity was likely associated with the effect of  $O_2(a^1\Delta_g)$  molecules.

Kozlov *et al.* [11] also investigated flame propagation enhancement by performing numerical simulations of  $H_2/O_2$  flames with the addition of  $O_2(a^1\Delta_g)$  under the conditions of the experiments in reference [7]. The results showed that a 10% conversion of  $O_2$  to  $O_2(a^1\Delta_g)$  gave more than a 50% increase in the laminar flame velocity. Lean mixtures were enhanced more than stoichiometric and rich mixtures because of the chain-initiation and chain-branching reactions involved. It should be noted though that gas heating may not be neglected with such a significant concentration of  $O_2(a^1\Delta_g)$ . With having 10% of the  $O_2$  excited to  $O_2(a^1\Delta_g)$ , its thermalization exceeds a temperature change of 100 K for a stoichiometric  $H_2/O_2$  mixture and greater than 300 K for a lean ( $\phi = 0.1$ )  $H_2/O_2$  mixture.

Bourig *et al.* extended the numerical modeling by investigating flame propagation, as well as flame stabilization by  $O_2(a^1\Delta_g)$  [15]. More recently, Starik *et al.* numerically examined the effects of  $O_2(a^1\Delta_g)$  on  $CH_4$ -air flame propagation with a detailed kinetic mechanism

developed [13]. Similar to previous investigations, the flame propagation enhancement was up to 40% for fuel rich mixtures and up to 70% for fuel lean mixtures with 10% conversion of  $O_2$  to  $O_2(a^1\Delta_g)$ . Nevertheless, there was a lack of clean experiments for detailed comparisons of the enhancement, and therefore left question as to how valid the enhancement predictions were.

Recent advancements in experiments have provided some data on the individual effects of  $O_2(a^1\Delta_g)$  on flame propagation. In the previous work of Ombrello *et al.* [16], experiments were designed and conducted to isolate  $O_2(a^1\Delta_g)$  from other excited species for transport to sub-atmospheric pressure lifted tribrachial flames. The details of the experiments can be found in reference [16], and therefore only a brief description is given here for clarity of the motivation. The experimental set-up, shown in figure 2, consisted of a high velocity (20-40 m/s) 1.04 mm diameter  $C_2H_4$  fuel jet within a low velocity (0.15-0.2 m/s) 90 mm diameter  $O_2/Ar$  co-flow to make the burner, which was placed in a variable pressure chamber. This burner configuration created a mixing layer with a stoichiometric contour where the premixed flame head was always anchored, followed with a diffusion flame tail (shown in the right inset in figure 2). Because of the slow laminar boundary layer development and the velocity and concentration gradients created, the lifted flame height was very sensitive to the changes in flame speed, and therefore provides favorable flame geometry for the direct observation of flame speed enhancement. Therefore, for a fixed flow field, the flame was located in a stationary position where the lifted flame speed at the premixed flame head was balanced with the local flow velocity. If the flame speed was increased because of the presence of plasma species, the liftoff height decreased to re-establish a local dynamic balance between the flame speed and flow velocity. Importantly, since the fuel and oxidizer were not mixed far upstream of the flame, there was very short residence time for the fuel and oxidizer to react in the cold flow, isolating the enhancement effects to be directly from reactions in the flame zone and not far upstream in the cold un-reacted flow.

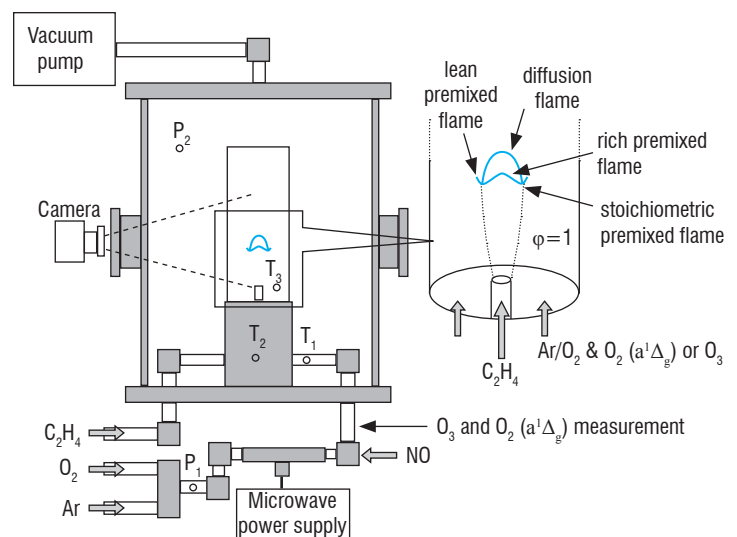
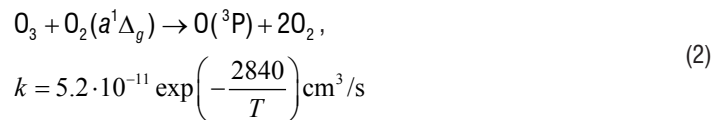


Figure 2 – Set-up for experiments in reference [16]

Upstream of the burner, the  $O_2/Ar$  mixture was excited with a self-sustained microwave discharge which produced excited Ar, as well as multiple oxygen containing species such as  $O$ ,  $O_3$ ,  $O_2(v)$ ,  $O(^1D)$ ,  $O(^1S)$ ,  $O_2(a^1\Delta_g)$ , and  $O_2(b^1\Sigma_g^-)$ . Pressures and reactant flow rates were chosen to provide long residence times (0.91-1.68 s) between the discharge and burner to allow for quenching and recombination of most species except  $O_3$  and  $O_2(a^1\Delta_g)$ . These two species could be

selectively quenched with the addition of NO in the plasma afterglow. Without NO injection, the  $O_2(a^1\Delta_g)$  was quenched via reaction with O and  $O_3$ . With NO injection, the O and  $O_3$  were catalytically removed and the  $O_2(a^1\Delta_g)$  concentration was preserved. Additionally, the NO did not have any effect on the flame speed with the concentrations that were injected.

The isolation of  $O_2(a^1\Delta_g)$  from all other plasma species was vital to develop an understanding of the kinetic pathways involved because of the strong combustion enhancement from other species, such as O and  $O_3$ , as well as their ability to rapidly quench  $O_2(a^1\Delta_g)$ . For example, the reaction of [17]:



rapidly quenches  $O_2(a^1\Delta_g)$  and produces atomic oxygen, potentially in the high temperature region in a flame front. The atomic oxygen can then take part in critical chain chemical reactions which significantly increase flame propagation speeds.

Therefore, with the plasma turned on and off, with and without NO injection, the isolated effects of  $O_3$  and  $O_2(a^1\Delta_g)$  on flame speed were observed by changes in flame liftoff height. Significantly, the results were the first isolated enhancement effects of  $O_2(a^1\Delta_g)$  on  $C_2H_4$  flame speed, with clear correlations between increased change in flame liftoff height (and hence increase in flame speed) with increased  $O_2(a^1\Delta_g)$  concentration. Interestingly, the results (shown in figure 3) revealed that approximately 500 parts per million (ppm) of  $O_3$  produced the same amount of flame speed enhancement as approximately 5500 ppm of  $O_2(a^1\Delta_g)$ . Since the flame speed enhancement kinetics with  $O_3$  is fairly well known, it can be used as a metric for comparison to flame speed enhancement kinetics with  $O_2(a^1\Delta_g)$ . This is a key point that is vital to the discussion to follow in this paper.

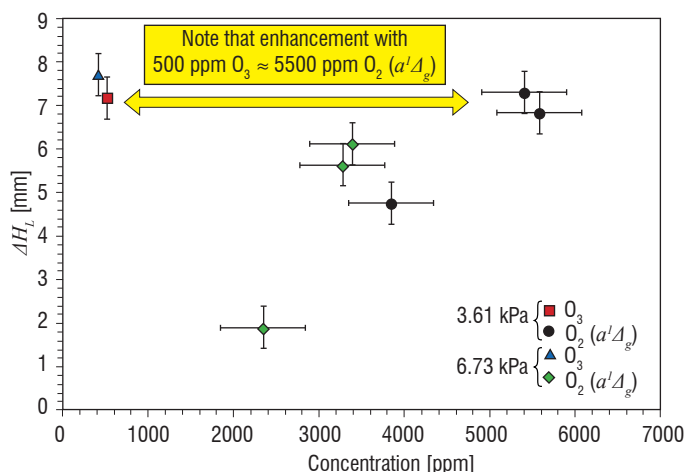


Figure 3 – Experimental results of flame liftoff change with  $O_2(a^1\Delta_g)$  and  $O_3$  concentration. The error bars denote the experimental uncertainties in the concentrations and change in flame liftoff height [16]

The goal of the present work was to use the experimental data shown in figure 3 from reference [16] as a target to assess the sensitivity of chain-initiation, chain-branching, and quenching rates of  $O_2(a^1\Delta_g)$  on  $C_2H_4$  flame speed enhancement. The roles of specific reactions are sought in order to better understand and validate the flame speed enhancement kinetics with the presence of  $O_2(a^1\Delta_g)$ .

## Initial Simulations and Kinetics

Originally in reference [16], simulations were performed in an attempt to explain the flame speed enhancement and understand the mechanisms involved with the presence of  $O_2(a^1\Delta_g)$ . To accomplish this, a kinetic sub-mechanism was added to a validated combustion mechanism [18] and simple one-dimensional flame simulations [19] were performed. The tribrachial flames that were used in the experiments of reference [16] are established in the mixing layer between the fuel and the oxidizer. Even though there is a non-premixed boundary condition for the reactants, the leading edge and stabilization point of the flame is premixed and at a stoichiometric equivalence ratio [20-25]. Therefore simple one-dimensional premixed stoichiometric freely propagating flame simulations can be performed and used for valid comparison. The one-dimensional laminar flame speed can be converted to the tribrachial flame speed by the square root of the unburned to the burned density ratio [20]. Through the original calculations in reference [16], it was found that there was a significant mismatch in enhancement between  $O_2(a^1\Delta_g)$  and  $O_3$  compared to the experiments. In the experiments, approximately 500 ppm of  $O_3$  was yielding the same change in flame liftoff height (and hence increase in flame speed) as approximately 5500 ppm of  $O_2(a^1\Delta_g)$  (see figure 3), whereas the simulations were showing significantly elevated levels of enhancement with  $O_2(a^1\Delta_g)$  (~5%) as compared to  $O_3$  (~1%) (figure 4). Since the kinetics are simple and fairly well known for  $O_3$ , there was concern that the  $O_2(a^1\Delta_g)$  mechanism was in error. Specifically, the thought was that  $O_2(a^1\Delta_g)$  quenching reactions were missing, leading to higher concentrations surviving throughout the early stages of the flame and hence elevated levels of flame propagation enhancement.

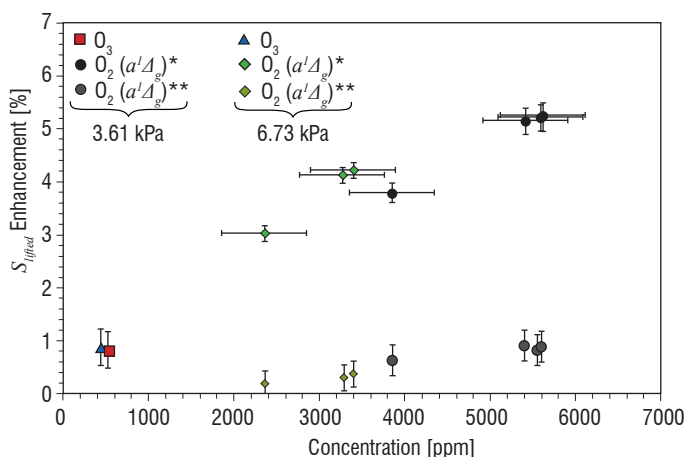


Figure 4 – Computational results of lifted flame speed enhancement with  $O_2(a^1\Delta_g)$  and  $O_3$  using the original kinetics (\*) and the inclusion of the estimated fictitious collisional quenching rate of  $C_2H_4$  with  $O_2(a^1\Delta_g)$  to fit trend of experimental results (\*\*) [16]

To rectify, there was emphasis placed on the quenching of  $O_2(a^1\Delta_g)$  via the fuel,  $C_2H_4$ . Unfortunately, there was a lack of temperature dependent quenching rate data of  $O_2(a^1\Delta_g)$  by hydrocarbon species that was suspected to be the main cause for the discrepancy. The only rates that could be found were at 298 K [26]. Therefore, a temperature dependent quenching reaction rate was estimated for



in order to explain the mismatch in enhancement as compared to the experiment. Since the temperature dependence of  $O_2(a^1\Delta_g)$  quenching

by other parent fuels, such as  $H_2$ , are approximately Arrhenius,[27] it was assumed that  $C_2H_4$  might also follow. Therefore, originating with the quenching rate of  $O_2(a^1\Delta_g)$  at 298 K given in reference [27], a temperature dependent rate was found that would explain the discrepancy between the experimental results in reference [16] and the original kinetics. The estimated rate is shown in figure 5, and the results of the calculated flame speed enhancement are shown in figure 4. While the enhancement by  $O_2(a^1\Delta_g)$  could be decreased to the levels of  $O_3$  as shown in the experiments with the estimated rate for (3), it was unrealistic and therefore motivated more detailed studies into the kinetics.

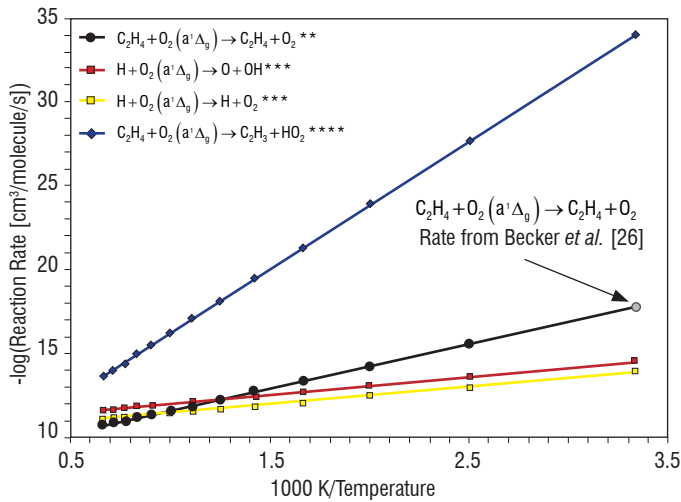


Figure 5 – Arrhenius temperature dependent collisional and reactive quenching rates of  $O_2(a^1\Delta_g)$  by H and  $C_2H_4$ . Estimated quenching rate of  $C_2H_4$  with  $O_2(a^1\Delta_g)$  to fit trend of experimental results (\*\*), rate from reference [28] (\*\*\*), and rate from reference [13] (\*\*\*\*)

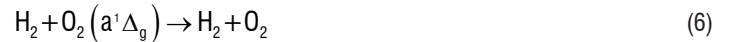
## Simulations with Updated Kinetics

Recently there have been advancements in the kinetic understanding of  $O_2(a^1\Delta_g)$  based upon the collective interpretation of many experimental and computational studies. One temperature dependent reaction rate of importance to a  $C_2H_4$  fueled system that was shown in reference [13] is



While this reaction has the potential to affect  $O_2(a^1\Delta_g)$  concentration and the overall reaction mechanism (see figure 5), simulations showed that it had no effect on the flame speed enhancement.

The focus of another recent work dealing with the enhancement kinetics via  $O_2(a^1\Delta_g)$  was on  $H_2/O_2$  reactants for simplicity and greatest comparison to experimental results [28]. It was found that in order to explain a wide range of experimental observations, there was an error in  $O_2(a^1\Delta_g)$  quenching. In short, this meant that the original kinetics used in the simulations shown in figure 4 were overestimating the enhancement compared to the experiments. The focus of the discrepancy was on the balance between the chain-initiation and quenching pathways of  $H_2$  with  $O_2(a^1\Delta_g)$  and the chain-branching and quenching pathways of H with  $O_2(a^1\Delta_g)$  via the reactions:



The concern was that the weighting of the chain-initiation and chain-branching pathways were higher than they should be, and therefore would lead to significantly elevated levels of flame enhancement. Specifically, the balance between (7) and (8) was suspect because of how critical  $H + O_2$  is to all combustion systems. The result of the study [28] showed that the ratio of chain-branching to quenching (7/8) should not be greater than 0.25. In order to provide some level of experimental validation, a comprehensive numerical study of the ignition of  $H_2/O_2$  mixtures for the experimental conditions of [29] was carried out by Chukalovsky *et al.* [30]. Similarly, it was shown that the probability of the chain-branching to the collisional quenching pathway (7/8) decreased to approximately 0.11 at high temperature. This weighting of the quenching reaction versus the branching reaction was a departure from previous thoughts on the kinetics, and since these two reactions are so dominant in all combustion systems, it was prudent to assume that they might have implications beyond just  $H_2/O_2$  systems, specifically for hydrocarbon fuels.

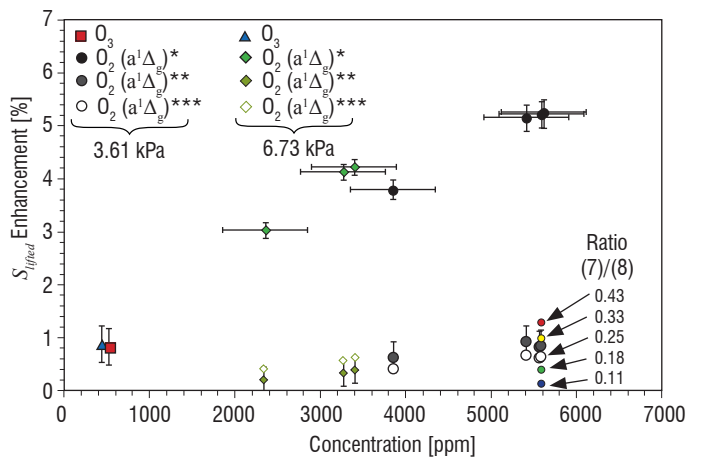


Figure 6 – Computational results of lifted flame speed enhancement with  $O_2(a^1\Delta_g)$  and  $O_3$  using the original kinetics (\*), the inclusion of the fictitious rate for reaction (3) [16] (\*\*), and the updated kinetics with H and  $H_2$  from reference [28] (\*\*\*)

The experimental and simulation results from reference [16] were then revisited with the knowledge garnered in the  $H_2/O_2$  reactant study. Since it was clear that the fictitious reaction of  $O_2(a^1\Delta_g)$  quenching via  $C_2H_4$  (3) was able to explain the discrepancy, it was compared to the updated reactions of (7) and (8) across the temperature range experienced in a flame. The results are shown in figure 5. The collisional quenching rate (8) is very comparable to the fictitious rate of (3) at temperatures above 700 K, which is in the regime that would most affect the early stages of the flame.

The flame propagation enhancement was then computed using the updated kinetics and removing (3) to see if it also explained the discrepancy compared to the experiments. Figure 6 shows the results of using the updated rates for  $O_2(a^1\Delta_g)$  involved in chain-branching



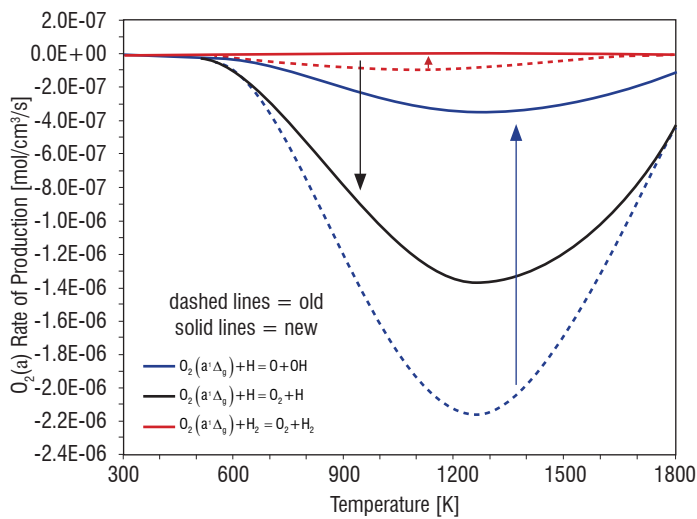


Figure 7 – Computed rate of production of  $O_2(a^1\Delta_g)$  versus temperature showing the major consumption pathways of  $O_2(a^1\Delta_g)$  with the original and updated H and  $H_2$  kinetics

and collisional quenching with the suggested (7/8) ratio of 0.25 from reference [28]. The new ratio gives computed flame speed enhancement that nearly matches the experimental trends, as well as when using the fictitious reaction (3). This clearly shows that the collisional quenching reaction of (8) plays a critical role in explaining the enhancement for the  $C_2H_4$  fueled system. Additional simulations were performed with varying the ratio of (7/8) from 0.11 to 0.43. The results showed that a ratio of 0.25 to 0.33 provided a comparable level of enhancement via  $O_2(a^1\Delta_g)$  to match  $O_3$ .

A more detailed investigation of the kinetic processes involved was achieved by examining the rate of production of  $O_2(a^1\Delta_g)$ . This allowed for an understanding of what the differences were in terms of the reactions with  $O_2(a^1\Delta_g)$  with the original and updated kinetics. The major pathways with H and  $H_2$  are shown in figure 7. The differences can be seen in the decreased importance of (6) and (7), but increased reactivity via (8). The shifting of importance of the reaction makes sense since H is present in the early stages of the flame because of back diffusion from the high-temperature reaction front.

When compared to the past kinetics with the fictitious rate for (3) in figure 8, it became more apparent why the updated kinetics correctly captured the effect on the flame enhancement. In the past work of reference [16] the fictitious rate for (3) had a peaked consumption

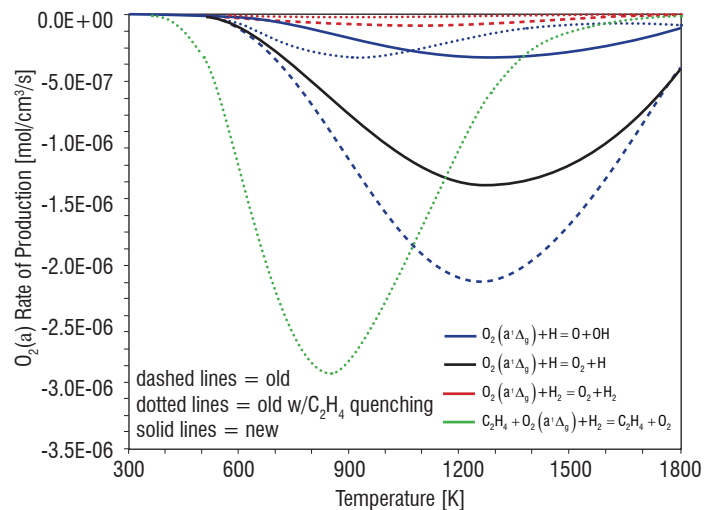


Figure 8 – Computed rate of production plot of  $O_2(a^1\Delta_g)$  versus temperature showing the major consumption pathways of  $O_2(a^1\Delta_g)$  with the past and updated kinetics

rate at much lower temperatures than reasonable because of having to compensate for the elevated branching rates via (7). The updated kinetics suppressed the chain-branching reaction (7) and increased the quenching reaction (8), resulting in a more accurate and realistic explanation of the enhancement.

## Summary and Conclusions

It has become evident through the inclusion of recently updated kinetics that careful attention needs to be paid to the balance between chain-initiation, chain-branching, and quenching rates when interrogating  $O_2(a^1\Delta_g)$ . Specifically, since the H atom is one of the most dominant and important intermediate radicals in all combustion systems, its contribution to collisional quenching needs to be heavily weighted and considered for an accurate description of any combustion enhancement mechanisms. The results of new H and  $H_2$  kinetics with  $O_2(a^1\Delta_g)$  has provided a more accurate explanation of the flame propagation enhancement of  $C_2H_4$  by  $O_2(a^1\Delta_g)$ . The implications are far ranging, indicating that the development of the kinetics involved in the enhancement of hydrocarbon fuels may not have to include intermediate hydrocarbon fragment reactions with  $O_2(a^1\Delta_g)$  to accurately predict flame propagation enhancement. The dominant pathways may solely lie with primary radicals such as H ■

## References

- [1] A. STARIKOVSKIY and N. ALEKSANDROV – *Plasma-Assisted Ignition and Combustion*. Progress in Energy and Combustion Science, Vol. 39, pp. 61-110, 2013.
- [2] S. M. STARIKOVSKAIA – *Plasma Assisted Ignition and Combustion: Nanosecond Discharges and Development of Kinetic Mechanisms*. Journal of Physics D: Applied Physics, Vol. 47, pp. 353001, 2014.
- [3] I. V. ADAMOVICH and W. R. LEMPET – *Challenges in Understanding and Development of Predictive Models of Plasma Assisted Combustion*. Plasma Physics Controlled Fusion, Vol. 57, pp. 014001, 2015.
- [4] A. A. IONIN, I. V. KOCHETOV, A. P. NAPARTOVICH and N.N. Yuryshv – *Physics and Engineering of Singlet Delta Oxygen Production in Low-Temperature Plasma*. Journal of Physics D: Applied Physics, Vol. 40, R25-R61, 2007.
- [5] V. Ya. BASEVICH and A. A. BELYAEV – *Evaluation of Hydrogen-Oxygen Flame Velocity Increase at Singlet Oxygen Addition*. Chemical Physics Reports, Vol. 8, pp. 1124, 1989.
- [6] L. IBRAGIMOVA, G. SMEKHOV and O. SHATALOV – *Recommended Rate Constants of Chemical Reactions in an  $H_2$ - $O_2$  Gas Mixture with Electronically Excited Species  $O_2(^1\Delta)$ ,  $O(^1\Delta)$ ,  $OH(^2\Sigma)$  Involved*. Institute of Mechanics of Lomonosov, Moscow State University, 2003.
- [7] V. Y. BASEVICH and S. M. KOGARKO – *To Mechanism of the Influence of Glow Discharge Products on the Hydrogen-Oxygen Flame Velocity in Conditions of Inflammation Peninsula*. Kinetics and Catalysis, Vol. 7, pp. 393, 1966.

- [8] G. D. SMEKHOV, L. B. IBRAGIMOVA, S. P. KARKACH, O.V. SKREBKOV and O. P. Shatalov – *Numerical Simulation of Ignition of Hydrogen-Oxygen Mixture in View of Electronically Excited Components*. High Temperature, Vol. 45, n° 3, pp. 395-407, 2007.
- [9] O. V. SKREBKOV and S. P. KARKACH – *Vibrational Nonequilibrium and Electronic Excitation in the Reaction of Hydrogen with Oxygen Behind a Shock Wave*. Kinetics and Catalysis, Vol. 48, n° 3, pp. 367-375, 2007.
- [10] A. M. STARIK and N.S. TITOVA – *Kinetics of Detonation Initiation in the Supersonic Flow of the  $H_2 + O_2$  (air) Mixture in  $O_2$  Molecule Excitation by Resonance Laser Radiation*. Kinetics and Catalysis, Vol. 44, n° 1, pp. 28-39, 2003.
- [11] V.E. KOZLOV, A. M. STARIK and N. S. Titova – *Enhancement of Combustion of a Hydrogen-Air Mixture by Excitation of  $O_2$  Molecules to the Singlet State*. Combustion, Explosion, and Shock Waves, Vol. 44, n° 4, pp. 371-379, 2008.
- [12] A. M. STARIK, V. E. KOZLOV and N. S. TITOVA – *On Mechanisms of Flame Velocity Increase Upon Activation of  $O_2$  Molecules in Electrical Discharge*. Journal of Physics D: Applied Physics, Vol. 41, 125206, 2008.
- [13] A. M. STARIK, V. E. KOZLOV and N. S. TITOVA – *On the Influence of Singlet Oxygen Molecules on the Speed of Flame Propagation in Methane-Air Mixture*. Combustion and Flame, Vol. 157, n° 2, pp. 313-327, 2010.
- [14] A. S. SHARIPOV and A. M. STARIK – *Kinetic Mechanism of  $CO-H_2$  System Oxidation Promoted by Excited Singlet Oxygen Molecules*. Combustion and Flame, Vol. 159, n° 1, pp. 16-29, 2012.
- [15] A. BOURIG, D. THÉVENIN, J. P. MARTIN, G. JANIGA and K. ZÄHRINGER – *Numerical Modeling of  $H_2-O_2$  Flames Involving Electronically-Excited Species  $O_2(a^1\Delta_g)$ ,  $O(^1D)$  and  $OH(^2\Sigma^+)$* . Proceedings of the Combustion Institute, Vol. 32, pp. 3171-3179, 2009.
- [16] T. OMBRELLO, S. H. WON, Y. JU and S. WILLIAMS – *Flame Propagation Enhancement by Plasma Excitation of Oxygen. Part II: Effects of  $O_2(a^1\Delta_g)$* . Combustion and Flame, Vol. 157, pp. 1916-1928, 2010.
- [17] J. I. STEINFELD, S. M. ADLER-GOLDEN and J. W. GALLAGHER – *Critical Survey of Data on the Spectroscopy and Kinetics of Ozone in the Mesosphere and Thermosphere*. Journal Physical Chemistry Reference Data, Vol. 16, n° 4, pp. 911-951, 1987.
- [18] H. WANG, X. YOU, A. V. JOSHI, S. G. DAVIS, A. LASKIN, F. EGOLFOPOULOS and C. K. LAW – *USC Mech Version II. High-Temperature Combustion Reaction Model of  $H_2/CO/C_1-C_4$  Compounds*. [http://ignis.usc.edu/USC\\_Mech\\_II.htm](http://ignis.usc.edu/USC_Mech_II.htm), May 2007.
- [19] PREMIX from the CHEMKIN package, Reaction Design, 6440 Lusk Boulevard, Suite D-205, San Diego, CA 92121. <http://www.reactiondesign.com>.
- [20] S. H. CHUNG – *Stabilization, Propagation and Instability of Tribrachial Triple Flames*. Proceedings of the Combustion Institute, Vol. 31, n° 1, pp. 877-892, 2007.
- [21] J. LEE, S. WON, S. JIN and S. CHUNG – *Lifted Flames in Laminar Jets of Propane in Coflow Air*. Combustion and Flame, Vol. 135, n° 4, pp. 449-462, 2003.
- [22] J. JU and Y. XUE – *Extinction and Flame Bifurcations of Stretched Dimethyl Ether Premixed Flames*. Proceedings of the Combustion Institute, Vol. 30, pp. 295-301, 2005.
- [23] Y. XUE and Y. JU – *Combustion Science and Technology*. Vol. 178, pp. 2219-2247, 2006.
- [24] M. KIM, S. WON and S. CHUNG – *Effect of Velocity Gradient on Propagation Speed of Tribrachial Flames in Laminar Coflow Jets*. Proceedings of the Combustion Institute, Vol. 31, pp. 901-908, 2007.
- [25] G. RUETSCH, L. VERVISCH and A. LINAN – *Effects of Heat Release on Triple Flames*. Physics of Fluids, Vol. 7, pp. 1447-1454, 1995.
- [26] K. H. BECKER, W. GROTH and U. SCHURATH – *The Quenching of Metastable  $O_2(a^1\Delta_g)$  and  $O_2(b^1\Sigma_g^-)$  Molecules*. Chemical Physics Letters, Vol. 8, pp. 259-262, 1971.
- [27] P. BORRELL and D.S. RICHARDS – *Quenching of Singlet Molecular Oxygen,  $O_2(a^1\Delta_g)$  and  $O_2(b^1\Sigma_g^-)$ , by  $H_2$ ,  $D_2$ ,  $HCl$  and  $HBr$* . Journal of the Chemical Society: Faraday Transactions 2, Vol. 85, n° 9, pp. 1401-1411, 1989.
- [28] N. A. POPOV – *Effect of Singlet Oxygen  $O_2(a^1\Delta_g)$  Molecules Produced in a Gas Discharge Plasma on the Ignition of Hydrogen-Oxygen Mixtures*. Plasma Sources Science and Technology, Vol. 20, n° 4, 2011.
- [29] V. V. SMIRNOV, O. M. STELMAKH, V. I. FABELINSKY, D. N. KOZLOV, A. M. STARIK and N. S. TITOVA – *On the Influence of Electronically Excited Oxygen Molecules on Combustion of Hydrogen-Oxygen Mixture*. Journal of Physics D: Applied Physics, Vol. 41, pp. 192001, 2008.
- [30] A. A. CHUKALOVSKY, K. S. KLOPOVSKY, M. A. LIBERMAN, Y. A. MANKELEVICH, N. A. POPOV, O. V. PROSHINA and T. V. RAKHIMOVA – *Study of Singlet Delta Oxygen  $O_2(a^1\Delta_g)$  Impact on  $H_2-O_2$  Mixture Ignition in Flow Reactor: 2D Modeling*. Combustion Science and Technology, Vol. 184, n° 10-11, pp. 1768-1786, 2012.

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