



An analysis of the ignition limits of premixed hydrogen/oxygen by heated nitrogen in counterflow

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ABSTRACT

The non-monotonic ignition response of counterflowing premixed hydrogen/oxygen mixtures with nitrogen dilution versus heated nitrogen is studied numerically and theoretically. It is shown that the three ignition limits can be theoretically obtained by considering only the linear system involving at most only one radical in each reaction, while the influences of the nonlinear reactions, each involving two radicals, together with thermal feedback, introduce higher-order corrections, particularly for the third ignition limit. It is also demonstrated that the high diffusivity of H₂ promotes ignition at the third limit. On the other hand, the high diffusivity of the H atom suppresses ignition at the first limit, while the assumption of unity Lewis number for H yields remarkably good results for the other two limits. Furthermore, by solving the time evolution of the crucial H and HO₂ radicals, simplified formulations of the three individual limits and the two quadratic double limits are obtained analytically, in analogy with results for the homogeneous explosion problem.

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1. Introduction

The non-monotonic explosion limit of homogeneous mixtures of hydrogen and oxygen is among the most elegant demonstration of the inherently nonlinear and interacting nature of the participating chemical species in a reactive mixture. The nonlinear response of Z-curve shows that, over a range of the mixture's temperature, by gradually increasing its pressure the mixture is first non-explosive, then explosive, then non-explosive again, and finally explosive, as it traverses the first, second and third explosion limits. Such a complex response can be explained on the basis of chain branching versus termination reactions involving eight participating chemical species (H₂, O₂, H, O, OH, HO₂, H₂O₂, H₂O) in a detailed kinetic mechanism, together with the wall termination of the various participating radicals.

Analytical expressions have also been attempted for each of the single limits and the double (first-second and second-third) limits [1]. Comprehensive analysis that folds in the complete three limits, however, has only succeeded recently. Specifically, Wang and Law [2] analytically derived an explicit cubic equation describing the Z-shaped explosion curve, without considering the nonlinear

reactions involving two radicals, which could be important in the high-pressure regime relevant to the third limit. This restriction was subsequently removed by Liang and Law [3], yielding analytical expressions that accurately describe the entire three-limit explosion response.

Having successfully analyzed the Z-curve of the homogeneous H₂/O₂ explosion limits, we steer herein the ignition analysis to a substantially different system, namely the ignition limits in the inhomogeneous, counterflow configurations with the coupling between chemical kinetics and transport, as exemplified by the steady-state ignition limits of an initially cold premixed H₂/O₂ jet by a heated inert jet. Since in many practical situations, autoignition occurs within environments that often involve significant gradients in velocity, temperature, and species concentration [4], investigation of autoignition of premixed H₂/O₂ mixtures in counterflow is of great interest to the safe utilization of hydrogen and other fuels. Furthermore, understanding of the autoignition characteristics in turbulent reacting flows can stem from analysis of this simple, canonical, laminar configuration.

For such counterflow configurations, the limits are defined by the temperature and concentrations of the jets as well as the velocity gradient, namely the strain rate. Phenomenologically, this is a classical problem in combustion, notably represented by the seminal analysis of Liñán [5] for the general structure of laminar flames described by one-step chemistry, with the ignition limit

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Table 1
The adopted H₂/O₂ reaction mechanism, with $k(T) = BT^\alpha e^{-T_0/T}$. [3,11,12].

No.	Reaction	B (cm,mol,s,K)	α	T_0 (K)
Initial reaction				
(R6b)	H ₂ + O ₂ → HO ₂ + H	2.69E+12	0.36	27,888
Linear chain reactions				
(R1f)	H + O ₂ → O + OH	3.52E+16	-0.7	8590
(R2f)	H ₂ + O → OH + H	5.06E+04	2.67	3165
(R3f)	H ₂ + OH → H ₂ O + H	1.17E+09	1.3	1825
(R4f)	H + O ₂ + M → HO ₂ + M	k_0 5.75E+19	-1.4	0
		k_∞ 4.65E+12	0.44	0
(R10f)	H ₂ O ₂ + M → 2OH + M	k_0 7.60E+30	-4.2	25,703
		k_∞ 2.63E+19	-1.27	25,703
(R12f)	HO ₂ + H ₂ → H ₂ O ₂ + H	7.80E+10	0.61	12,045
Nonlinear chain reactions				
(R5f)	HO ₂ + H → 2OH	7.08E+13	0	148
(R6f)	HO ₂ + H → H ₂ + O ₂	1.66E+13	0	414
(R9f)	H + H + M → H ₂ + M	1.30E+18	-1	0
(R11f)	HO ₂ + HO ₂ → H ₂ O ₂ + O ₂	1.03E+14	0	5556
		1.94E+11	0	-709
(R13f)	HO ₂ + OH → H ₂ O + O ₂	2.89E+13	0	-252
(R14f)	H ₂ O ₂ + H → H ₂ O + OH	2.41E+13	0	1998
(R15f)	HO ₂ + O → O ₂ + OH	3.25E+13	0	0

defined by the lower turning point of the ignition-extinction S-shaped curve. Such a curve is obtained by plotting, say, a typical system response such as the perturbed temperature versus the Damköhler number, which represents the ratio of the characteristic flow time to that of the characteristic reaction time. Subsequently, Kreutz and Law [6] computationally simulated the weakly-reactive states leading to ignition for hydrogen versus heated air with a detailed kinetic mechanism. Results yield the characteristic homogeneous Z-shaped explosion curve for a given strain rate, with the second limits for the different strain rates aligned with each other. Zheng and Law [7] then studied the ignition of lean premixed hydrogen/air mixtures in a counterflow both experimentally and numerically. It is found that the larger diffusivity of H₂ compared with O₂ results in a hydrogen-enriched ignition kernel, while the diffusive loss of the H atom from the kernel typically reduces the amount of radical at the ignition location and hence makes ignition harder.

In terms of theory, Sánchez et al. [8,9] conducted a bifurcation analysis of nonpremixed hydrogen/oxygen autoignition in the high-temperature regime by employing a reduced chemical-kinetic scheme. It is demonstrated that with the oxidizer-stream temperature larger than the crossover temperature, the system has a different transcritical bifurcation behavior at the bifurcation point due to the competition between reactant consumption and chemical heat generation. It is noted that while the bifurcation analysis offers a simpler solution to describe the H₂/O₂ ignition criterion compared to a complete numerical simulation, it cannot fold in the entire three ignition limits and is also restricted to specific reduced chemical mechanism.

In view of the absence of general analytical solutions for the complete three-limit ignition response, we shall analytically study the counterflow ignition of H₂/O₂ mixtures versus heated N₂, governed by a comprehensive detailed kinetic mechanism developed recently, with additional computational simulation to support the analytical results. Considered at the broader scope, the analytical approach developed herein, using the premixed counterflow ignition for demonstration, is conceptually applicable to extensive problems involving ignition of both premixed and nonpremixed systems in various flow configurations.

In the next section we first define the problem of interest, to be followed by the numerical approach and the reaction mechanism adopted. With the insights provided by the simulation results, in Section 3 we study the subject problem by using eigenvalue analysis and asymptotic perturbation allowing, quite realistically, only

linear reactions in which either none or only one of the participating species is a radical. The more complete, and complex, problem involving nonlinear reactions, relevant for high-pressure situations, will be considered in further studies.

For simplicity, the analysis is first based on the assumption of unity Lewis number. Specifically, in Section 3.1–3.3 formulation of the problem is presented and the conservation equations are derived in a normalized coordinate. In Section 3.4 the dimension of the problem is reduced by using eigenvalue analysis and as such the asymptotic ignition limit is derived theoretically. The effects of the nonunity Lewis numbers of the hydrogen molecule and atom, and the role of the reactant composition are discussed respectively in Sections 3.5 and 3.6. In Section 3.7 the individual formulations of the three ignition limits are given with proper quasi-steady state assumptions. The analytical results are found to be in good agreement with the numerical results over a wide range of pressure and strain rate.

2. Numerical

Numerical simulation of the transient ignition of a hydrogen/oxygen mixture against heated nitrogen was performed based on the open source toolboxes, Cantera and Ember [10], in an axisymmetric counterflow configuration. The conservation equations of mass, momentum, species concentrations, and energy were solved along the stagnation streamline. Space-time adaptive mesh refinement is implemented to guarantee the accuracy of the results.

Recognizing [3] the realistic fact that, before the onset of ignition, consumption of the major reactants, H₂ and O₂, are nominally negligible, while the concentrations of the radicals, such as H and HO₂, are much lower than those of the major species, the various chain reactions in a reaction mechanism can be categorized as being either linear or nonlinear, which respectively involve reactant-radical and radical-radical reactions, as given in Table 1. Furthermore, the nonlinear reactions are expected to have primarily secondary effects because of the lower concentrations of both participating radicals.

The simulation uses an fourteen-step reduced hydrogen oxidation mechanism which consists of the initiation reaction, and six linear (reactant-radical) and seven nonlinear (radical-radical) reactions, shown in Table 1 [3,11,12]. The kinetic parameters are taken from Mueller et al. [11] and Sánchez et al. [12]. To simplify the analysis, the Lewis number of all the species, except for

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