

STRUCTURE AND LENGTH OF CHEMISTRY INDUCTION ZONE IN HYDROGEN-AIR DETONATIONS

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Abstract—The induction-zone structure of hydrogen-air detonation is analyzed by employing a reduced chemical kinetic mechanism for hydrogen oxidation chemistry in order to provide preliminary information for linear instability analysis of detonation. The reduced chemistry mechanism, derived by assuming O, OH, and HO₂ steady state, consists of the chain-initiation step, chain-branching step and radical-recombination step. In particular, near the onset condition of detonation instability, the temperature behind the leading shock is higher than the crossover temperature, so that the ignition process throughout the induction zone is found to be dominated by the exothermically neutral chain-branching step rather than the radical recombination step. Just behind the leading shock, the initial radical pool, in which radical concentration is comparable to the ratio of the chain-initiation rate to the chain-branching rate, is produced by the chain-initiation step. Following the initial build-up of a radical pool is the exponential growth of the radical concentration by the chain-branching step until a value of order unity at the end of the induction zone is reached. From the solution for the H-radical profile in the induction zone, the induction time is found to be proportional to the chain-branching time with a large constant multiplier of O(10) arising from the effect of the initial concentration of the radical pool formed by the chain-initiation step. The induction-zone length is calculated as a function of equivalence ratio and overdrive ratio. The results can be utilized in future analysis of linear instability of planar detonation.

Key words : Detonation, Induction Zone, von Neumann Spike, Chain-Branching Reaction

INTRODUCTION

Detonation is a combustion mode of fuel and oxidizer premixture, in which a chemical reaction zone accompanies a leading shock propagating into the fresh premixture with a speed much greater than the sound speed of the fresh premixture [Williams, 1985]. Detonation is of particular interest from the aspect of safety because overpressure behind a detonation wave is much higher than that of homogeneous explosion, thereby causing much more severe damage. However, predicting the physical properties of a detonation wave is still a daunting task because of the three dimensional nature of the detonation structure [Lee, 1984]. Detonation is not just a planar wave, but it involves the intersection of incident shock and reflection shock, called the triple point, from which the Mach stem and slip line bifurcate. The trajectory of the triple points usually leaves a pattern resembling fish-scale like cells with a well-defined characteristic cell size [Lee, 1984]. To date, the origin of the detonation cells is not fully understood although it is believed to arise from intrinsic instability of planar detonation.

Detonation is unstable under the acoustic interaction between the leading shock and exothermic reaction unless it is sufficiently overdriven [Erpenbeck, 1964]. There have been a few

theoretical attempts to analyze linear instability of an overdriven planar detonation wave by employing overall one-step exothermic chemical reaction with large activation energies [Buckmaster and Neves, 1988; Lee and Stewart, 1990; Bourlioux et al., 1991]. Such chemical kinetic mechanism has been successfully applied to a wide variety of problems in deflagration by using activation-energy asymptotics (AEA) [Linan, 1974], that is a special type of matched asymptotic expansion method developed for combustion problems with large activation energies. However, AEA for detonation instability analyses has not been equally successful in predicting the unstablest wavelength that should have been in a good agreement with detonation cell size. In fact, the predicted cell size was an-order-of-magnitude smaller than typical detonation cell size. Such an unrealistic result is most likely caused by the fact that an overall one-step chemistry with large activation energy is too nonlinear to describe detonation instability in a physically proper manner.

As a remedy to the failure of activation-energy asymptotics, multi-step chemistry, that is based on elementary reaction steps, would be considered [Clavin et al., 1997]. Central to multi-step chemistry are radicals, which form chain reaction steps. In general, chain reaction consists of three steps, namely, chain-initiation step, chain-branching step and radical-recombination step. The first two steps are responsible for producing radicals, while the last one is responsible for converting radicals into stable intermediates or products. The chain production step, i.e., the

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chain-initiation step plus chain-branching step, is in general exothermically neutral, but its reaction rate is temperature sensitive. On the other hand, the chain-termination step, i.e., radical-recombination step, produces a large amount of thermal energy by converting activated radicals into stable molecules, and its reaction rate is only weakly dependent on temperature variation. In view of the nature of the two-step chemical kinetic mechanism [Trevino and Mendez, 1991], the reaction zone structure behind the leading shock consists of two regions. An induction zone, in which radical concentration increases to a value of order unity, is followed by a heat-release zone, in which radical recombination produces thermal energy to sustain the overall detonation structure.

In comparison with overall one-step reaction with large activation energy, the main difference of two-step chemistry occurs in the heat-release zone in that temperature sensitivity of exothermic reaction for two-step chemistry is lower by an order of magnitude than that for single step chemistry. Consequently, acoustic interaction of heat release zone with leading shock can be tamed to predict a realistic detonation cell size by linear stability analysis. However, it must be kept in mind that the length of chemistry induction zone, determined mainly by radical-production steps, possesses a high sensitivity to temperature variation. Therefore, it is essential to precisely describe the location of the induction zone, which is the most nonlinear process in detonation structure, to obtain a realistic detonation cell size [Clavin et al., 1997].

The aforementioned two-step chemical kinetic mechanism is found to be applicable to most hydrocarbon oxidation chemistry. Particularly for hydrogen-air detonation systems, analytical description of the induction-zone length is possible because chemical reaction of hydrogen-air is well known and can be reduced to a simpler form. In the present paper, we attempt to derive an explicit formula for the induction-zone length of hydrogen-air detonation by employing a two-step reduced mechanism for hydrogen oxidation chemistry. The results can later be applied to linear stability analysis of hydrogen-air detonation to distinguish the physical origin of the detonation cellular structure

FORMULATION

1. Physical Setting

Schematic diagram of a planar hydrogen-air detonation is shown in Fig. 1. A fuel-oxidizer premixture is shock-compressed to attain high pressure and temperature to support exothermic reaction in supersonically propagating detonation wave. The condition behind the leading shock, corresponding to the von Neumann spike, can be simply obtained by the normal shock relationship. Since radical was initially absent prior to passing the leading shock, the radical concentration immediately behind the shock can be assumed to be zero because passage time for the leading shock is too short to produce any significant number of radicals.

Following the leading shock is the chemistry induction zone, in which radicals are produced under a constant temperature condition. Radicals are initially produced by chain-initiation

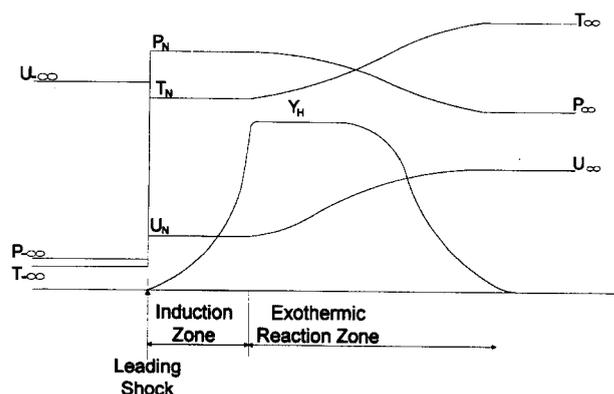


Fig. 1. Schematic diagram of planar hydrogen-air detonation, exhibiting the profiles of velocity, pressure and temperature variations. The subscripts " ∞ ", "N", " ∞ " denote the conditions at the upstream, immediately behind the leading shock (von Neumann spike), and at the downstream.

steps, in which hydrogen and oxygen molecules are collided to break up into radicals. Since chain-initiation reaction steps are much slower than chain-branching reaction steps, the chain production soon becomes dominated by a chain-branching reaction step once a small amount of radicals are produced by chain-initiation steps. Chain-branching steps stay dominant till the end of the induction zone, where the radical concentration reaches its saturation value of order unity. Once radical concentration is saturated, radical recombination steps begin to convert radicals into stable intermediates and products, leading to generation of thermal energy as a consequence of conversion of radicals into stable molecules. Consequently, the region following the induction zone is the exothermic reaction zone that is much thicker than the induction zone because radical recombination is slower than chain branching.

Chain branching steps are exothermically neutral and variations of hydrogen and oxygen molecule concentration are negligible unless flow is extremely close toward the end of the induction zone. It can therefore be assumed that the mean flow condition throughout the induction zone remains invariant. This simplification enables us to analytically describe the induction-zone length if the chain-branching reaction is sufficiently simplified.

2. Hydrogen Oxidation Chemistry

Since it is impossible to analytically treat the ignition process without sufficient simplification of the chemical kinetic mechanism, a reduced two-step ignition mechanism is introduced by assuming that O, OH, and HO_2 are in quasi-steady states and H_2O_2 is frozen during the ignition process. Then the corresponding two-step reduced chemical kinetic mechanism, describing the hydrogen-air ignition process, can be written as [Trevino and Mendez, 1991]



where the first reaction is responsible for radical production and the second is responsible for radical recombination. The

constant a in Eq. (2) is a ratio of the rates of the following two reactions, $\text{HO}_2 + \text{H} \rightarrow 2\text{OH}$ and $\text{HO}_2 + \text{H} \rightarrow \text{H}_2 + \text{O}_2$, and is considered to be independent of temperature variation. The rate of the first reaction is given by the sum of the following two elementary reaction steps,



where the reaction step in Eq. (3) is the dominant initiation step, while the reaction step in Eq. (4) is the dominant branching step. In addition, the rate of the second reaction is given by



For notational brevity, the rate constants of the reactions in Eqs. (3), (4) and (5) are respectively denoted by k_I , k_B and k_R , where the subscripts I, B and R denote initiation, branching and recombination step. Rate constants for each of these elementary reaction steps are listed in Table 1 [Trevino and Mendez, 1991].

The character of the above kinetic system can be classified by whether temperature is higher than a characteristic temperature, called crossover temperature T_c , at which the rates of chain branching and chain termination are equal. Under the condition of H, O and OH steady state, such radical balance is achieved if

$$2 k_B = k_R C_M \quad (6)$$

where k_j is rate constant of the elementary reaction step j and C_M is the concentration of the third body M. At temperatures higher than the crossover temperature, a chain-branching reaction is much faster than a radical-recombination reaction, that is in turn much faster than a chain-initiation reaction. Therefore, radical recombination reaction does not have to be considered during the chain-branching process. However, the chain-initiation step must be included although it is the slowest among the three reaction steps listed in Eqs. (3)-(5). Since the chain-branching reaction is first order to the H-radical concentration, it cannot proceed without the presence of the initial concentration of H radicals. Since H radical concentration is absent immediately behind the leading shock, the chain-initiation step is necessary to produce H radicals to bring the chain-branching step into the radical production process. Consequently, the chain-initiation and chain-branching steps suffice to describe the induction-zone structure.

3. Hydrogen Radical Profile in the Induction Zone

The conservation equation for the H-radical concentration is written in a coordinate system in which the coordinate origin is attached at the leading shock of the detonation wave. In addition, consumption of the major species is negligible until the end of the induction zone is reached, so that their concentrations are fixed at their initial values. The variation of the H radical can be then expressed as

$$dY_H/d\xi = Y_H + \epsilon Y_{H2} \quad (6)$$

Table 1. Rate constants for hydrogen oxidation chemistry

Elementary reaction step	A	n	E
$\text{H}_2 + \text{O}_2 \rightarrow \text{HO}_2 + \text{H}$	8.06×10^{13}	0.0	246.16
$\text{H} + \text{O}_2 \rightarrow \text{OH} + \text{H}$	2.00×10^{14}	0.0	70.30
$\text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{H}$	2.30×10^{18}	-0.8	0.00

Unit : A(cm, mole, s); E(KJ/mole); $k = A T^n \exp(-E/RT)$

where Y_i is the mass fraction of the species i . The dimensional coordinate x , the origin of which is attached at the leading shock, is nondimensionalized to form the nondimensional coordinate ξ as

$$\xi = x/u_N t_B \quad (7)$$

where u_N is the velocity at the von Neumann condition and t_B is the characteristic branching time. In terms of the rate constant for the chain-branching step, the characteristic branching time t_B is given as

$$t_B = W_{O_2} / 2\rho_N Y_{O_2}^0 k_B \quad (8)$$

where W_i is the molecular weight of the species i , ρ_N the density at the von Neumann condition and the superscript 0 denotes the condition of the fresh premixture. A small quantity ϵ is given to be $\epsilon = k_I / 2k_B$ and measures a ratio of the characteristic chain-initiation time to the characteristic chain-branching time. The small quantity ϵ is found to be of order 10^{-6} or less for the detonation conditions considered in the present study.

Eq. (6) is readily integrable to give the H-radical profile in the induction zone as

$$Y_H = \epsilon Y_{H2}^0 [\exp(\xi) - 1] \quad (9)$$

where Y_{H2}^0 is the initial mass fraction of H_2 . The above equation indicates that the chain-initiation step gives a linear growth of the H-radical concentration as $Y_H = \epsilon Y_{H2}^0 \xi$ only for $\xi \ll 1$. Once ξ becomes of order unity, growth of the H-radical concentration becomes exponential, indicating that H-radical is produced by the chain-branching step instead of the chain-initiation step. Then, the H-radical profile can be approximated as $Y_H = \epsilon Y_{H2}^0 \exp(\xi)$ for $\xi \geq 0(1)$.

The radical concentration grows throughout the chain-branching zone until being saturated with a value of order unity. Letting $Y_{H,s}$ be the saturation value, the induction zone ends approximately where

$$\xi = \ln(Y_{H,s} / \epsilon Y_{H2}^0) \quad (10)$$

Since $Y_{H,s}$ is divided by an asymptotically small quantity ϵ and the logarithm taken, putting $Y_{H,s} = Y_{H2}^0$ is sufficient to give a first approximation to the induction zone length. Therefore, the induction-zone length in a dimensional form, denoted by l , can be written as

$$l = u_N t_B \ln(\epsilon^{-1}) = u_N (W_{O_2} / 2\rho_N Y_{O_2}^0 k_B) \ln(2k_B/k_I) \quad (11)$$

The induction time, τ , being given as $\tau = l/u_N$, it is seen from Eq. (12) that the induction time can be written in a dimensional form as

$$\tau = t_b \ln(\epsilon^{-1}) = t_b \ln(2k_b/k_t) \quad (12)$$

The induction time is found to be much longer than the characteristic branching time by a large factor $\ln(\epsilon^{-1})$. Just behind the leading shock, the initial radical concentration is zero, so that the radical production is controlled by the chain-initiation step. Since the branching step is faster than the initiation step by an order of ϵ^{-1} , dominance of the initiation step lasts only until the H-radical concentration reaches of order ϵ , beyond which radical production is controlled by the chain-branching step leading to an exponential growth of the radical concentration, as indicated in the paragraphs below Eq. (9). The factor $\ln(\epsilon^{-1})$ in Eq. (12) represents the multiplier to the branching time that is required for the radical concentration to increase from $O(\epsilon)$ to $O(1)$ [Sanchez et al., 1997].

RESULTS AND DISCUSSION

The induction-zone length is calculated for various detonation conditions. The upstream temperature and pressure are set to be those of the standard condition. The condition at the von Neumann spike can be easily determined if the detonation propagation speed and the mixture condition are prescribed. First the equivalence ratio of the hydrogen-air mixture, denoted by Φ , is chosen. From the Rankine-Hugoniot relationship, the Chapman-Jouget (C-J) detonation speed is calculated by using the STANJAN code [Reynolds, 1987]. Once the C-J detonation speed is determined, the overdrive ratio is chosen to specify the detonation propagation speed, where the overdrive ratio f is defined as

$$f = D/D_{CJ} \quad (13)$$

and D_{CJ} is the C-J detonation speed while D is speed of the detonation under consideration. Since the detonation speed can be faster than the C-J detonation speed during the initial stage of the detonation initiation by adding ignition energy, the overdrive ratio is always greater than unity. Once mixture condition as well as detonation propagation speed is given, the von Neumann condition can be obtained from the normal shock relationship.

Properties of hydrogen-air detonation at the Chapman-Jouget propagation condition are shown in Fig. 2 as functions of the equivalence ratio with the fresh mixture at room temperature and pressure. First, detonation propagation speed D_{CJ} is seen to continuously increase with increasing equivalence ratio. This type of detonation speed variation is relevant only to hydrogen-air or hydrogen-oxygen detonation, while other hydrocarbon fuels exhibit maxima of their detonation speeds near stoichiometric mixing condition. Although the detonation Mach number for hydrogen-air detonation reaches its maximum value near the stoichiometric condition, the sound speed continuously increases with increasing hydrogen concentration because of a decrease in the average molecular weight. Since the increase of the sound speed is much greater than the decrease of the detonation Mach number, the detonation speed monotonically increases with increasing equivalence ratio. In addition, flow velocity just behind the leading shock, i.e. u_N , is

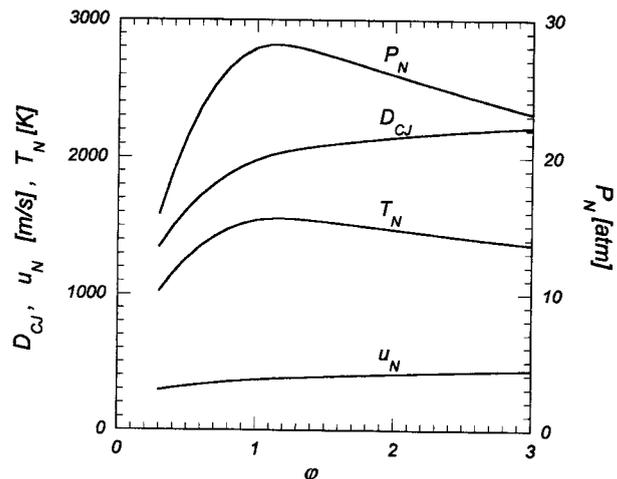


Fig. 2. Properties of the Chapman-Jouget detonation in terms of the detonation speed D_{CJ} [m/s], the von Neumann temperature T_N [K], the von Neumann pressure P_N [atm] and the von Neumann velocity u_N [m/s] as functions of the equivalence ratio Φ .

also found to increase with increasing equivalence ratio. On the other hand, other detonation properties, such as temperature and pressure at the von Neumann spike, exhibit their maximum values near the stoichiometric condition since they are not explicitly related to the sound speed.

For overdriven detonations with unity equivalence ratio, temperature and pressure at the von Neumann spike are presented in Fig. 3. As the overdrive ratio f increases, the temperature and pressure exhibit rapid increase. As pressure increases, the crossover temperature, above which chain branching is dominant over radical recombination, also increases because the rate of three-body recombination reaction is enhanced much faster than that of the two-body chain-branching reaction. Therefore, as the overdrive ratio increases, there is a competition between the increase of the von Neumann temperature and the increase of the crossover temperature caused by an

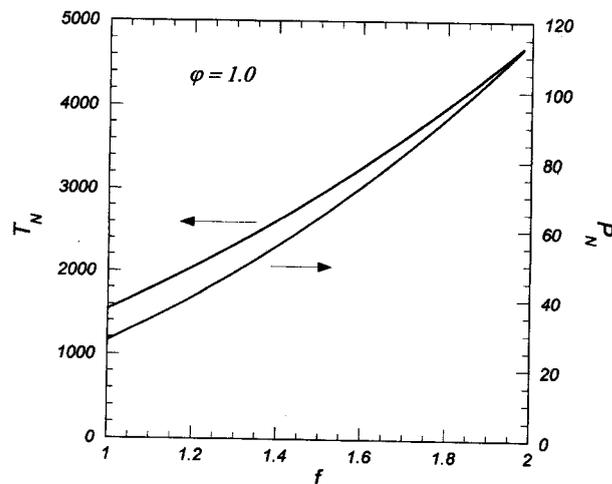


Fig. 3. Variations of the von Neumann temperature T_N [K], the von Neumann pressure P_N [atm] with the overdrive ratio f at the unity equivalence ratio.

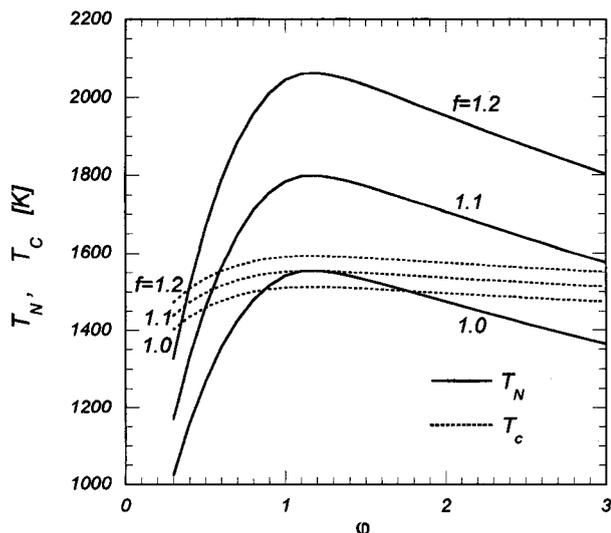


Fig. 4. Comparison of the von Neumann temperature T_N [K] with the crossover temperature T_c [K] for the equivalence ratio of $0.4 < \Phi < 3$ with the overdrive ratio $f=1.0, 1.1, 1.2$. The solid lines correspond to the von Neumann temperatures, while the dotted lines correspond to the crossover temperatures.

increase of the von Neumann pressure. Fig. 4 shows the variation of the crossover temperature T_c in comparison with the von Neumann temperature T_N for various values of equivalence ratio and overdrive ratio. For Chapman-Jouget detonations, i.e. $f=1$, the crossover temperature is seen to be lower than the von Neumann temperature only for a relatively narrow region near the stoichiometric condition. Ignition by chain-branching reaction can be applicable only in this region, while ignition, in the region of $T_c > T_N$, is known to be characterized by a thermal ignition process. However, as soon as the overdrive ratio f becomes slightly increased from unity, the increase of the von Neumann temperature is much greater than that of the crossover temperature. Consequently, the parametric range of the equivalence ratio, in which chain-branching ignition is applicable, becomes larger. For $\Phi > 1.2$, a slight overdriven condition, chain-branching ignition is found to be valid almost for an entire detonable equivalence ratio.

In particular, it is worthwhile to remember that the present analysis is performed as a preliminary study toward linear stability analysis of planar detonation waves. Strongly overdriven detonation, formed immediately after sudden injection of a sufficiently large energy to detonable mixture, is found to be strongly stable. As the detonation wave propagates, the influence of the initial ignition energy attenuates and detonation speed approaches the Chapman-Jouget detonation speed. Before reaching the Chapman-Jouget condition, instability of detonation ensues at a characteristic wavelength, that is likely corresponding to the detonation cell size, with an overdrive ratio still greater than unity. Therefore, near the onset condition of detonation instability, it would be assumed that the temperature in the induction zone is higher than the crossover temperature. It is also valid to describe the induction-zone structure by chain-branching ignition.

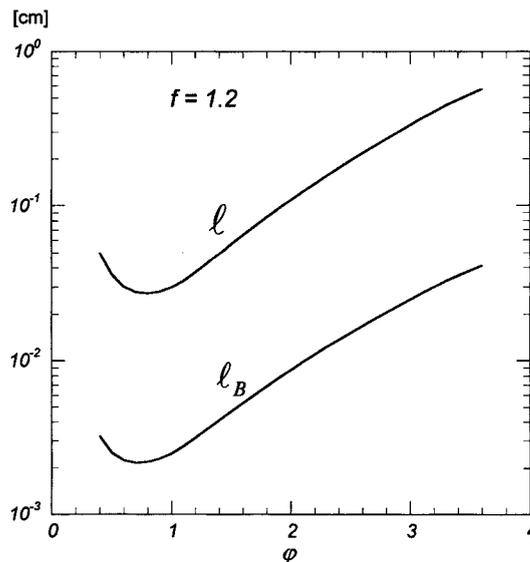


Fig. 5. Variations of the induction-zone length l [cm] and the characteristic branching length l_B [cm] with the equivalence ratio Φ at the overdrive ratio $f=1.2$.

For a prescribed overdrive ratio $f=1.2$, the induction-zone length l and the characteristic branching length l_B are shown in Fig. 5 as functions of the equivalence ratio Φ , where the characteristic branching length l_B is defined to be $l_B = u_N t_B$, measuring a distance that a flow particle can travel during the characteristic branching time t_B . Two points are apparent in Fig. 5. First, the minimum induction-zone length as well as the minimum branching length appears for a value of Φ less than unity although the characteristic branching time t_B exhibits its minimum near the stoichiometric condition. For a smaller value of the equivalence ratio, the sound speed for hydrogen-air mixture is lower, so that the velocity at the von Neumann spike is lower too. Consequently, the induction-zone length as well as the characteristic branching length shows it is minimum at an equivalence ratio somewhat smaller than unity. In addition, the induction-zone length is greater than the characteristic branching length by an order of magnitude. As discussed in the previous section, the difference in an order of magnitude is caused by the slowness of the chain-initiation step in comparison with the chain-branching step. From the results in Fig. 5, the value of ϵ is estimated to be of order 10^{-6} as previously estimated by Sanchez et al. [1997].

Variation of the induction-zone length with the overdrive ratio is presented for $0.4 < \Phi < 4$ in Fig. 6. The broken lines in the case of $f=1$, i.e., Chapman-Jouget detonation, indicates that the von Neumann temperature T_N is lower than the crossover temperature T_c in the corresponding parametric range. The induction-zone length monotonically decreases with increasing overdrive ratio. As detonation becomes overdriven, the temperature at the von Neumann spike becomes higher, thereby leading to a considerable decrease in the characteristic branching time. For the overdrive ratio $f=2$, the induction-zone length is seen to be decreased by a factor of 10^{-2} . In addition, the induction-zone length again exhibits its minimum for equivalence ratio smaller than unity. The estimated

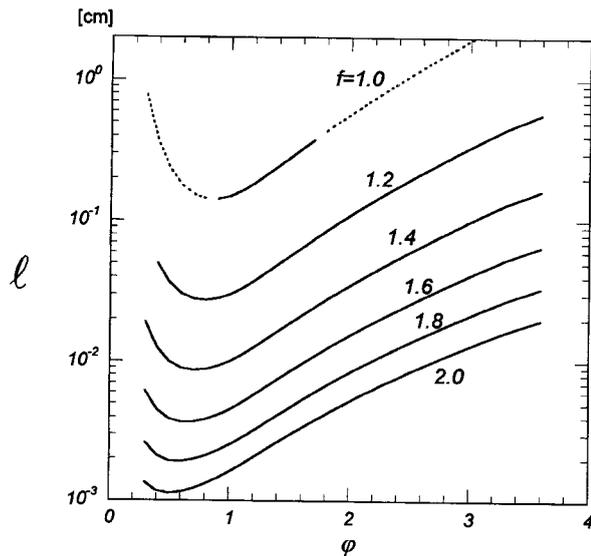


Fig. 6. Variations of the induction-zone length l [cm] with the overdrive ratio f for the equivalence ratio of $0.4 < \Phi < 3.6$. The dotted section in the case of $f=1.0$ indicates that the von Neumann temperature is lower than the crossover temperature and that the result might be in some error.

induction-zone length l is often found to be linearly correlated to the cell size λ for a wide range of the mixture condition, as $\lambda = A/l$ [Shchelkin and Troshin, 1965; Lee, 1984]. A simple estimate using the result for $f = 1$ in Fig. 6 gives a result that $\lambda \approx 10l$. This result is qualitatively in a good agreement that the proportionality constant A is of order 10. However, it is still premature to claim the above relationship without performing any dynamic analysis because the appearance of the detonation cell is arising from instability of planar detonation [Lee, 1984].

CONCLUDING REMARKS

The asymptotic structure for the induction zone of hydrogen-air detonation is analyzed by employing a reduced chemical kinetic mechanism of hydrogen oxidation in order to provide a simplified induction-zone structure suitable to be included in the future linear instability analysis of planar detonation. The analysis is an initial step to studying the cellular structure found in detonations. Although the cellular structure is a highly nonlinear phenomenon, its origin is believed to be a pulsating instability of weakly overdriven detonations. However, the results of linear analysis of the pulsating instability, with one-step Arrhenius-type chemical reaction, turned out to be pathological. As a remedy to this problem, the use of multi-step chemical reaction mechanisms is proposed. The present analysis is an effort to test a simplified two-step mechanism, which is intended to be used in the future linear stability analysis of hydrogen-air detonations.

As far as detonation becomes slightly overdriven, the temperature behind the leading shock is found to be higher than the crossover temperature, so that the ignition process is con-

trolled by the exothermically neutral chain-branching step rather than exothermic radical recombination step. Consequently, the ignition process can be characterized as a chain-branching ignition instead of thermal ignition process. By considering evolution of the hydrogen radical concentration, an analytical form for the induction-zone length, over which the H-radical concentration grows to a value of order unity, is presented.

The immediate extension of the present analysis could be made toward a simplified linear stability analysis of planar detonation. The square wave model, that was previously employed by Erpenbeck in his early analysis for detonation instability [Erpenbeck, 1964], can be employed in the analysis. In the square wave model, heat release is concentrated as a delta function at the end of the induction zone. However, the model that the present analysis suggests has a significant difference from that of Erpenbeck in that heat release viewed from the character of the present reduced chemistry is not temperature sensitive, while that of Erpenbeck is strongly temperature dependent because of high activation energy for heat-release reaction. Since it is conjectured that pathological results in the previous instability analysis arise from high temperature sensitivity of heat-release reaction, the proposed simplified model could yield qualitative reasonable instability results. In the later analysis, the instability model can be improved by considering distributed heat release by fully considering an exothermic radical recombination reaction step.

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APPENDIX RANKINE-HUGONIOT RELATIONSHIP

A first approximation to detonations can be obtained from the Rankine-Hugoniot relationship. The relationship is applicable to propagating waves with thin planar structures, so that the corresponding flows can be locally approximated to be one-dimensional. Then, the upstream and downstream conditions of detonation satisfy the mass, momentum and energy conservations as

$$\rho_0 u_0 = \rho_\infty u_\infty \quad (\text{A.1})$$

$$\rho_0 u_0^2 + p_0 = \rho_\infty u_\infty^2 + p_\infty \quad (\text{A.2})$$

$$h_0 + u_0^2/2 = h_\infty + u_\infty^2/2 \quad (\text{A.3})$$

where the subscripts "0" and " ∞ " denote the conditions at the downstream and upstream of the detonation and p and h are the pressure and specific enthalpy. In addition to the conservation equations, the equation of the state is applicable as

$$g(\rho_0, p_0, h_0) = g(\rho_\infty, p_\infty, h_\infty) \quad (\text{A.4})$$

where the function g is a generalized equation of the state.

In the above set of four equations, the thermodynamic conditions at the upstream are specified, so that there exist five unknowns, namely u_0 , ρ_∞ , u_∞ , p_∞ and h_∞ . In particular, the upstream speed u_0 is the quantity of primary interest because it is the propagation speed of the detonation. Since the above problem is under determined, an additional condition is required to calculate the propagation speed from Eqs. (A.1)-(A.4). A realistic choice of the additional constraint is found to be the Chapman-Jouget condition that the downstream speed u_∞ is the sonic speed. Consequently, the other four quantities, including the Chapman-Jouget detonation speed, are obtained by solving Eqs. (A.1)-(A.4). The equations are solved by the STANJAN code, which is capable of solving the equations with detailed thermodynamic properties and chemical equilibrium at the downstream.

While the Rankine-Hugoniot relationship is used to determine the detonation propagation speed and the detonation downstream conditions, the relationship can also be used to determine the state at the von Neumann spike, the condition corresponding to the immediate downstream of the leading shock of the detonation as illustrated in Fig. 1. When the conditions at the von Neumann spike are sought, the thermodynamic conditions as well as the propagation speed are already specified. Therefore the thermodynamic and flow conditions just behind the leading shock can be found by solving the Rankine-Hugoniot relationship with specified upstream conditions. Here, the detonation propagation speed can be either the Chapman-Jouget detonation speed, $u_0 = D_{CJ}$, or overdriven detonation speed, given as $u_0 = f D_{CJ}$, where f is the overdrive ratio. The Rankine-Hugoniot relationship with frozen chemistry is in fact the strong-shock relationship.

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