Prediction methods of detonation initiation using transient values and integral of reactivity gradient

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1 Introduction

Detonation initiation is a process that has been studied actively for next-generation aerospace propulsion systems due to its rapid energy conversion characteristic and efficiency (e.g., [1,2]). Zel'dovich proposed a theory relating reaction front propagation modes to spatial auto-ignition sequence, i.e., the reactivity gradient [3, 4]. In this theory, the speed of reaction front propagation relative to unburnt mixture is defined using the reactivity gradient as

$$u_r = \left(\frac{\partial \tau_i}{\partial r} \right)^{-1}, \tag{1}$$

where τ_i is the ignition delay time and r is the location in the spherical domain. For a hot spot induced deflagration to detonation transition (DDT), different reaction front propagation modes were identified by the normalized reactivity gradient, the ratio of the sound speed to the corresponding reaction front propagation speed [4, 5]:

$$\xi = \frac{a}{u_r} = \left(\frac{\partial \tau_i}{\partial r} \right) a, \tag{2}$$

where a is the sound speed. The occurrence of these different modes is strongly correlated to the reactive gradient of initial hot spot, ξ. If ξ approaches to unity, i.e., autoignition front propagation speed approximately approaches to acoustic wave speed, those two waves resonate and a detonation wave is likely to initiate.

2 Transient Reactivity Gradient

From the normalized reactivity gradient theory, it can be estimated that a detonation develops when $\xi \sim 1$. However, in the simulation results of [5], a detonation was not initiated even though $\xi = 1$. It was also found that although the initial ξ was higher than the order of unity, there was a developing detonation. The reason is that the value of ξ changes during the induction time due to conduction, diffusion, and chemical reaction.

Therefore, transient values of ξ in the unburnt mixture near ignition front are proposed instead of ξ based on the initial temperature gradient to analyze detonation initiation phenomena better. Moreover,

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the spatial distribution of ξ is employed rather than using one value of ξ. Equation 2 can be rewritten to calculate temporal evolution of ξ distribution:

$$\xi(r,t) = \frac{\partial \tau_i(r,t)}{\partial r} a(r,t), \tag{3}$$

where ξ, τ_i, and a are functions of location and time.

Temporal and spatial values of $(\partial \tau_i / \partial r)$ can be obtained from the local slope of the autoignition delay time versus temperature and the temperature profile from the numerical calculation. Transient values of local sound speed also can be deduced directly from the temperature profile.

A transient simulation of ignition and reaction front propagation was carried out using A-SURF [6], a solver for one-dimensional compressible multi-component reactive flows. A-SURF is suitable for the detonation study as in [7]. In the simulation, a one-dimensional spherical domain with a radius of 10 cm was used. Both the center and the outer boundaries had reflective boundary conditions. Initially, a hot spot of radius 3 mm was specified at the center, and the hot spot initiated an autoignition event generating a reaction front propagation outwardly. The initial temperature was 1077 K at the center and linearly decreased to 1066 K at r = 3 mm. pressure was 50 atm. The domain contained a stoichiometric 50%H_2-50%CO/air mixture at 50 atm. These initial conditions were chosen to be compared with previous studies [5, 7]. A 12-species skeletal chemical kinetic mechanism for the H_2/CO combustion was developed from GRI-Mech 3.0 [8] and used in the current study.

The normalized reactivity gradient of the initial hot spot (from 0 to 0.3 cm) in this simulation setup was around 25. As this value was larger than the order of unity, subsonic deflagration was estimated from the initial reactivity gradient. Figure 1 shows that development of pressure, temperature and ξ during a hot-spot induced reaction propagation. Based on the temperature profiles of each time sequence, $(\partial \tau_i / \partial r)$ and a were calculated, and ξ distributions were obtained using Equation 3. The subsonic deflagration was initiated and propagated until ~0.4 cm. At time sequence 4, ξ ahead of the reaction front reduced to the order of unity leading to a developing detonation until time sequence 7. The area ahead of detonation front at time sequences 8 and 9 had very small values of ξ, so the reaction front propagation became a supersonic deflagration without a sharp pressure peak followed by a near-instantaneous thermal explosion.

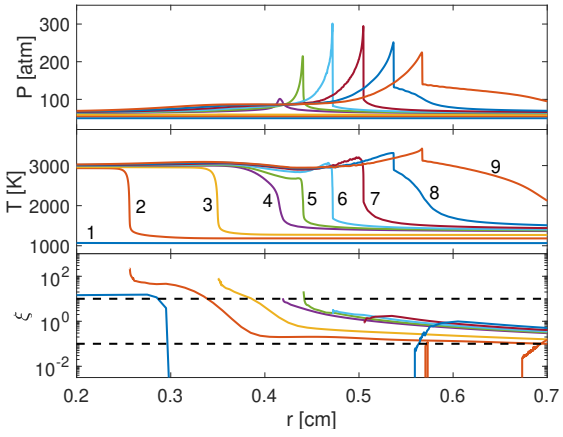


Figure 1: Development of pressure, temperature, and ξ for a hot spot with $\xi = 25$. Time sequence 1: 0.0, 2: 527.3, 3: 543.4, 4: 545.9, 5: 546.2, 6: 546.5, 7: 546.8, 8: 547.0, 9: 547.3 (μs). Dashed lines correspond to ξ = 10 and 0.1 respectively.

Using the transient ξ distribution, the effect of conduction, diffusion, and chemical reaction during the induction time on the reactivity gradient can be observed, and the transient reaction propagation modes

can be captured with a clear explanation. Even though the initial ξ is larger than the order of unity, the initial deflagration can transition to a detonation wave. Therefore, to predict detonation occurrences more precisely, a method including both direct detonation initiation and DDT is proposed in the next section.

3 Reactivity Gradient Integral

The normalized reactivity gradient calculated from the initial temperature profile is an indicator to estimate the mode of the reaction propagation from an inhomogeneous mixture. However, due to the conduction, diffusion, and chemical reaction during the induction time, it cannot successfully predict the occurrence of a detonation for the cases with a relatively long initiation time. If ξ is obtained after the induction time, it can predict the detonation occurrences more precisely. Therefore, the estimation of temperature profile after the induction time directly from the initial temperature gradient is useful to obtain an accurate ξ.

From the order-of-magnitude analysis of the energy conservation equation for a hot-spot condition during the induction time, the only dominant term to affect temperature is the chemical reaction. Therefore, during the induction time, the spatial temperature profile can be directly estimated by only the chemical reaction term of each location. The value of ξ based on the temperature distribution at the end of the induction time is a more accurate value than that from the initial temperature gradient, as it includes the effect of the chemical reaction during the induction time.

The normalized reactivity gradient can be simply expressed as the ratio of a to u_r. As the variation of sound speed is relatively small compared to that of reaction front propagation speed, the reaction propagation speed is a key factor to decide the detonation initiation. The spatial distribution of reaction propagation speed can be obtained from the temperature profile at the end of the induction time. Then, the effective reaction front propagation speed at $r = L$ is proposed as

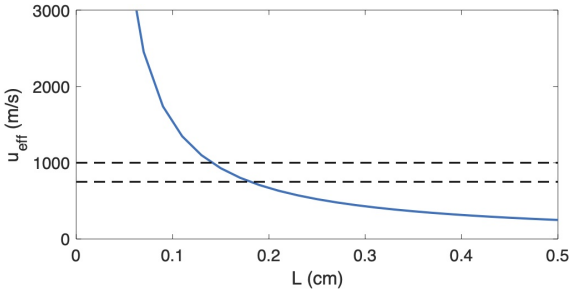
$$u_{eff}(L) = \frac{1}{L}\int_0^L u_r(r)dr, \tag{4}$$

where L is the location of the effective reaction front propagation speed. The effective reaction front propagation speed is an integral value, and represents the averaged reaction propagation speed from 0 to L. Then, the integral of normalized reactivity gradient, ξ_{eff}, at location L is defined as

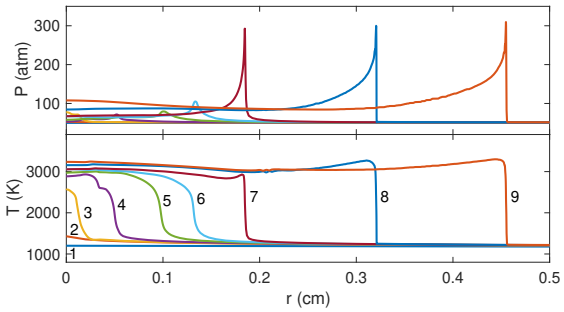
$$\xi_{eff}(L) = \frac{a}{u_{eff}(L)}. \tag{5}$$

Therefore, when u_{eff} approaches to the sound speed, the reactivity gradient integral is on the order of unity resulting in a detonation initiation. Figure 2a shows that the value of u_{eff} from $L = 0$ to $L = 0.5$ cm. The mixture was a stoichiometric 50%H_2-50%CO/air mixture at 1180 K and 50 atm with a 5 mm hot spot. The temperature in the center of hot spot was 1200 K. The same chemical kinetic mechanism was used with the previous section. The bounds of sound speed are approximately 750 and 1000 m/s for this condition, and shown in the figure with dashed lines. The values of u_{eff} are within the bounds of sound speed when $L \sim 0.15$ cm. Thus, the value of reactivity gradient integral at $L \sim 0.15$ cm is on the order of unity. Note that this result is directly from the initial values without any complex numerical simulations.

Figure 2b shows the A-SURF simulation results for this condition. In the simulation result, the reaction propagation is a supersonic deflagration initially, but transitions to the detonation between 0.1 and 0.2 cm. The estimated location of detonation initiation is $\sim$0.15 cm, which corresponds to the simulation



(a) Effective reaction front propagation speeds from $L = 0$ to $L = 0.5$ cm. Dashed lines correspond to bounds of sound speed, a = 750 and 1000 m/s.



(b) Development of pressure and temperature from A-SURF calculation. Time sequence 1: 0.00, 2: 51.56, 3: 51.95, 4: 52.73, 5: 53.5, 6: 53.90, 7: 54.29, 8: 55.07, 9: 55.86 (μs).

Figure 2: Detonation initiation from a stoichiometric 50%H_2-50%CO/air mixture at 1180 K and 50 atm with a 5 mm hot spot

results. Moreover, when $L < 0.15$, the effective reaction propagation speed is larger than the sound speed, and ξ_{eff} is smaller than the order of unity, which results in a supersonic deflagration. This supersonic deflagration also corresponds to the simulation result.

The method of reactivity gradient integral with the temperature profile after the induction time shows a good agreement with A-SURF simulation. The chemical reaction effect is considered in the method, and a detonation initiation by DDT with the initiation time also can be estimated directly from the initial conditions without any computationally expensive simulations.

4 Conclusions

The Zel'dovich gradient theory is a basic method to predict a detonation initiation. For better prediction, transient reactivity gradient and integral methods were proposed and evaluated. For the transient reactivity gradient method, temporal and spatial reactivity gradient distributions are directly employed, while the reactivity gradient integral estimates the location of detonation initiation based on the effective reaction front propagation speed from the spatial distribution. Both methods showed accurate predictions of detonation initiation with initiation time.

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