Autoignition and detonation development from a hot spot in hydrogen/air mixture

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1 Introduction

Engine knock is one of the main constrains for the development of high-efficiency spark ignition engines (SIEs). It is generally accepted that knock in SIEs is caused by end-gas autoignition. Heat release during end-gas autoignition can generate pressure pulse/wave propagating across the system and it corresponds to the normal knock with the pressure oscillation around 2 MPa. A new engine knock mode with extremely high pressure oscillation (above 20 MPa) has been recently found in highly boosted SIEs and it has been called as super-knock [1-3]. The super-knock was attributed to developing detonations induced by the coherent coupling between pressure wave and local reaction/autoignition [1]. Such kind of detonation development can be explained by the SWACER mechanism [4] and reactivity gradient theory [5].

To quantify the critical conditions for detonation development, Bradley and coworkers [6-8] proposed an operational peninsula within which detonation can develop from temperature inhomogeneity (e.g., a hot spot). The detonation limits were described by two non-dimensional parameters: one is the normalized temperature gradient (ξ); and the other is the ratio of acoustic time to excitation time (ε). The detonation peninsula was used by Bradley and Kalghatgi [2, 9] to study engine knock. It was demonstrated that the detonation peninsula helps to determine the critical conditions for detonation development in engines. Therefore, detonation peninsula is a very useful tool in the study of engine knock [2, 10]. However, the detonation peninsula was original determined for syngas [6, 7]. Though Bates et al. [8] showed that this detonation peninsula also works for iso-octane, recent study [11] indicated that the detonation development regime in terms ξ and ε might depend on fuel. Moreover, it is not clear whether the detonation peninsula is affected by the initial pressure, initial temperature and equivalence ratio.

Therefore, further study is needed to understand how fuel, initial pressure, initial temperature and equivalence ratio affect detonation development regime and autoignitive reaction front propagation from a hot spot. This motivates the present study. The objectives are to obtain the detonation development regimes for fuels other than syngas and to examine the effects of initial pressure, initial temperature and equivalence ratio on detonation development. Furthermore, the mechanism for detonation development is interpreted with the help of SWACER mechanism. Since hydrogen is the simplest fuel with well-established chemical mechanism, it is considered in the present work.

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2 Numerical model and specifications

One-dimensional numerical simulation is conducted to investigate the propagation modes of autoignitive reaction front evolving from a hot spot in hydrogen/air mixture. Spherical symmetry is assumed and thereby it is one-dimensional. The initial temperature distribution for a hot spot located at the center is

$$T(t=0,r)=\begin{cases} T_0+(r-r_0)\dfrac{dT_0}{dr} & \text{for} \quad 0\le r\le r_0 \\ T_0 & \text{for} \quad r_0\le r\le R_W \end{cases} \tag{1}$$

where t and r are respectively the temporal and spatial coordinates; r_0 the hot spot size; R_W=5 cm the radius of the spherical chamber; dT_0/dr the temperature gradient to be specified; and T_0 the initial temperature of the mixture outside of the hot spot. The computational domain is initially filled with static hydrogen/air mixture with uniformly distributed pressure and equivalence ratio. At both boundaries (i.e., r=0 and r=R_W), zero flow speed and zero gradients of temperature and mass fractions are enforced.

The in-house code, A-SURF [12-14], is used to simulate the autoignitive reaction front propagation induced by a hot spot in hydrogen/air mixture. A-SURF solves the conservation equations for a multi-species reactive mixture using the finite volume method. Ideal gas is assumed and the non-ideal gas behavior, which is important at very high pressure, is not considered here. The CHEMKIN packages are incorporated into A-SURF to calculate the reaction rates and the temperature- and component-dependent thermodynamic and transport properties. The hydrogen mechanism developed by Keromnes et al. [15] is used. The mixture-averaged model is used to evaluate the mass diffusivities. The readers are referred to Refs. [12-14] for details on numerical schemes and code validation of A-SURF. In simulation, dynamically adaptive mesh refinement algorithm is used to efficiently and accurately resolve the reaction front, pressure wave, shock wave and detonation. The finest mesh size is 2 μm and the corresponding time step is 0.4 ns. Numerical convergence has been checked and ensured by further decreasing the time step and mesh size in simulation.

3 Results and discussion

3.1 Different regimes for autoignitive reaction front propagation from a hot spot

According to the SWACER mechanism [4] and reactivity gradient theory [5], different modes of reaction front propagation can be observed depending on the magnitude of temperature gradient. The reaction front propagation speed, u_a, is inversely proportional to the gradient of the ignition delay time [6, 7]:

$$u_a=\left(\frac{d\tau_{ig}}{dr}\right)^{-1}=\left(\frac{d\tau_{ig}}{dT_0}\cdot\frac{dT_0}{dr}\right)^{-1} \tag{2}$$

When the reaction front speed, u_a, is equal to the local sound speed, a, chemical reaction and pressure wave can be coherently coupled to form a developing detonation [6, 7]. The requirement of u_a=a determines the critical temperature gradient as [6, 7]

$$\left(\frac{dT_0}{dr}\right)_c=\left(a\frac{d\tau_{ig}}{dT_0}\right)^{-1} \tag{3}$$

Based on the critical temperature gradient, the non-dimensional temperature gradient is defined as [6, 7]:

$$\xi = \frac{dT_0}{dr} \Big/ \left(\frac{dT_0}{dr} \right)_c = \frac{a}{u_a} \tag{4}$$

in which the second equation is obtained by using Eqs. (2) and (3).

To quantify the detonation development regime, two non-dimensional parameters were introduced by Bradley and coworkers [6, 7]. One is the normalized temperature gradient, ξ, which represents the ratio between local sound speed and reaction front propagation speed according to Eq. (4). The other is the non-dimensional time, ε, which is the ratio of acoustic time (r_0/a) to excitation time τ_e (defined as the time interval between 5% and maximum heat release rate):

$$\varepsilon = \frac{r_0}{a\,\tau_e} \tag{5}$$

In simulation, different temperature gradients and hot spot sizes are considered so that different values of ξ and ε can be reached.

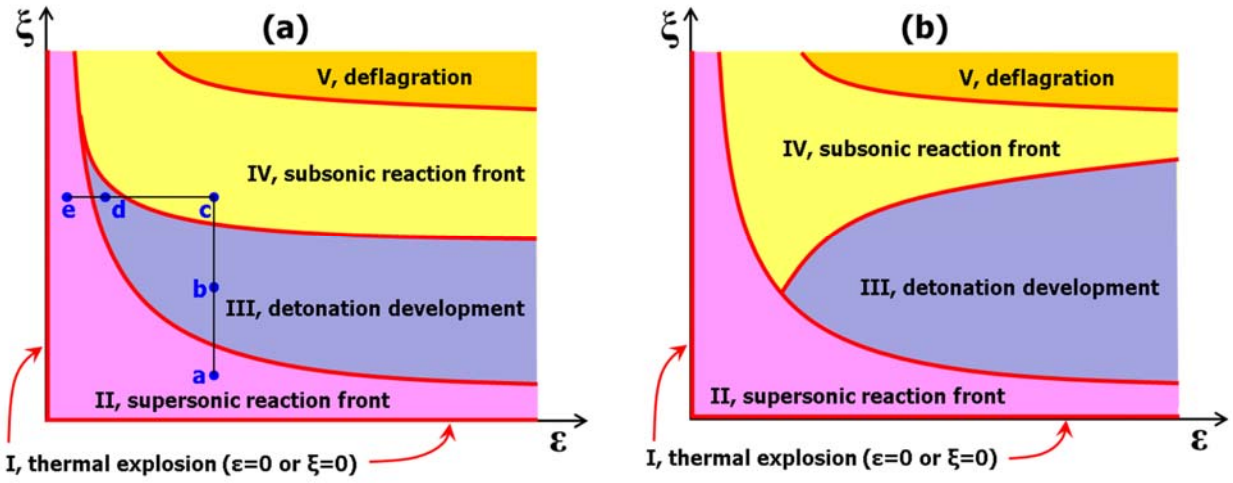

Figure 1. Schematics for different regimes of autoignitive reaction front propagation induced by a hot spot in hydrogen/air mixtures.

Figure 1 summarizes the five possible autoignition modes in the plot of ξ versus ε. These modes are: I, thermal explosion; II, supersonic reaction front; III, detonation development; IV, subsonic reaction front; and V, deflagration. Modes I and V occurs for zero and very large temperature gradients, respectively. It is note that unlike the detonation peninsula of Bradley and coworkers [6, 7], detonation development regime for hydrogen/air has different shapes as shown in Figs. 1(a) and 1(b). This indicates that the detonation development regime is fuel dependent and thereby the detonation peninsula might not work for different fuels. To achieve quantitative prediction of engine knock, we need use the detonation development regime for specific fuel rather than that for syngas. It is noted that in previous studies, only the detonation development regime was obtained while the line between regimes II and IV was not obtained. Besides, it is expected that regime V will be affected by the boundary conditions used at $r=R_W$ or chamber size.

The typical detonation development processes are shown in Fig. 2. For case b, dT_0/dr=-0.379 K/mm, r_0=1.5 mm, ξ=15, and ε=20.1; while for case d, dT_0/dr=-1.059 K/mm, r_0=0.37 mm, ξ=42, and ε=5. Results for cases

a, c and e are not presented here due to paper length limit. It is observed that the peak pressure is above 20 MPa when detonation development occurs. Detailed analysis indicates that the positive feedback between pressure wave and chemical reaction/autoignition induces detonation development, and this can be explained by the SWACER mechanism [4] and reactivity gradient theory [5]. More details on the detonation development caused by SWACER mechanism will be presented in the revision of this extended abstract.

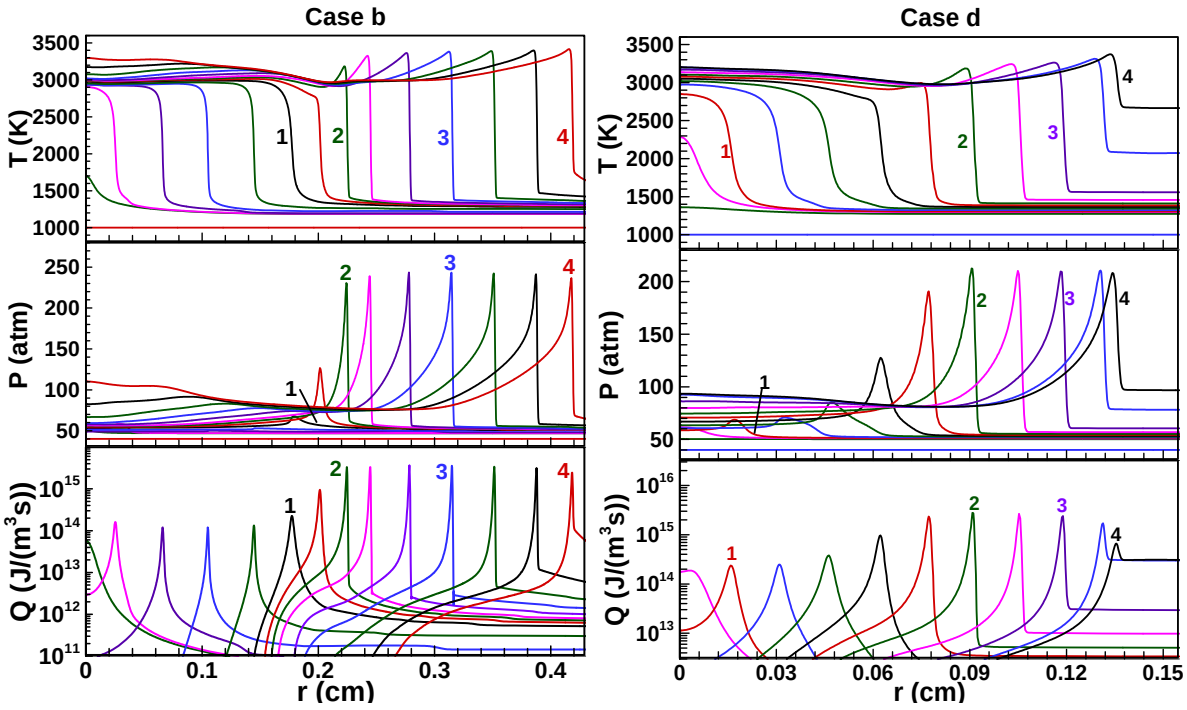

Figure 2. Temporal evolution of temperature, pressure and heat release rate distributions for cases b and d indicated in Fig. 1(a). The mixture is stoichiometric hydrogen/air initially at 1000 K and 40 atm. The time sequence of case b is 1: 2574.50 μs, 2: 2574.87 μs, 3: 2575.35 μs, 4: 2575.91 μs; and that for case d is 1: 2575.22 μs, 2: 2575.96 μs, 3: 2576.12 μs, 4: 2576.21 μs.

3.2 Effects of initial temperature, pressure and equivalence ratio on detonation development regime

Figure 3 shows the detonation development regime for hydrogen/air mixture at different initial temperatures, initial pressures, and equivalence ratios. Comparison among these regime maps indicates that the initial temperature, initial pressure, and equivalence ratio all can affect the detonation development regime. By comparing the results at 40 atm and 20 atm, we find that the detonation development regimes in the ξ-ε plot are similar. Therefore, the initial pressure has weak influence on the detonation development regime. With the increase of the initial temperature from 1000 K to 1200 K, the energy density of the mixture decreases. Therefore, the upper bound of detonation development regime moves upward and a C-shaped detonation development regime is observed in Fig. 3(c). When the equivalence ratio decreases from 1.0 to 0.5, a much wider detonation development regime is obtained and it is similar to the detonation peninsula proposed by Bradley and coworker [6-8]. Figure 3 shows that under different initial conditions different shapes of

detonation regime can be observed including detonation peninsula [6-8], C-shape and Rhino-Horn-shape. Therefore, the initial conditions play an important role in the formation of detonation regime, and we cannot use the same detonation development regime map for different initial conditions and different mixtures.

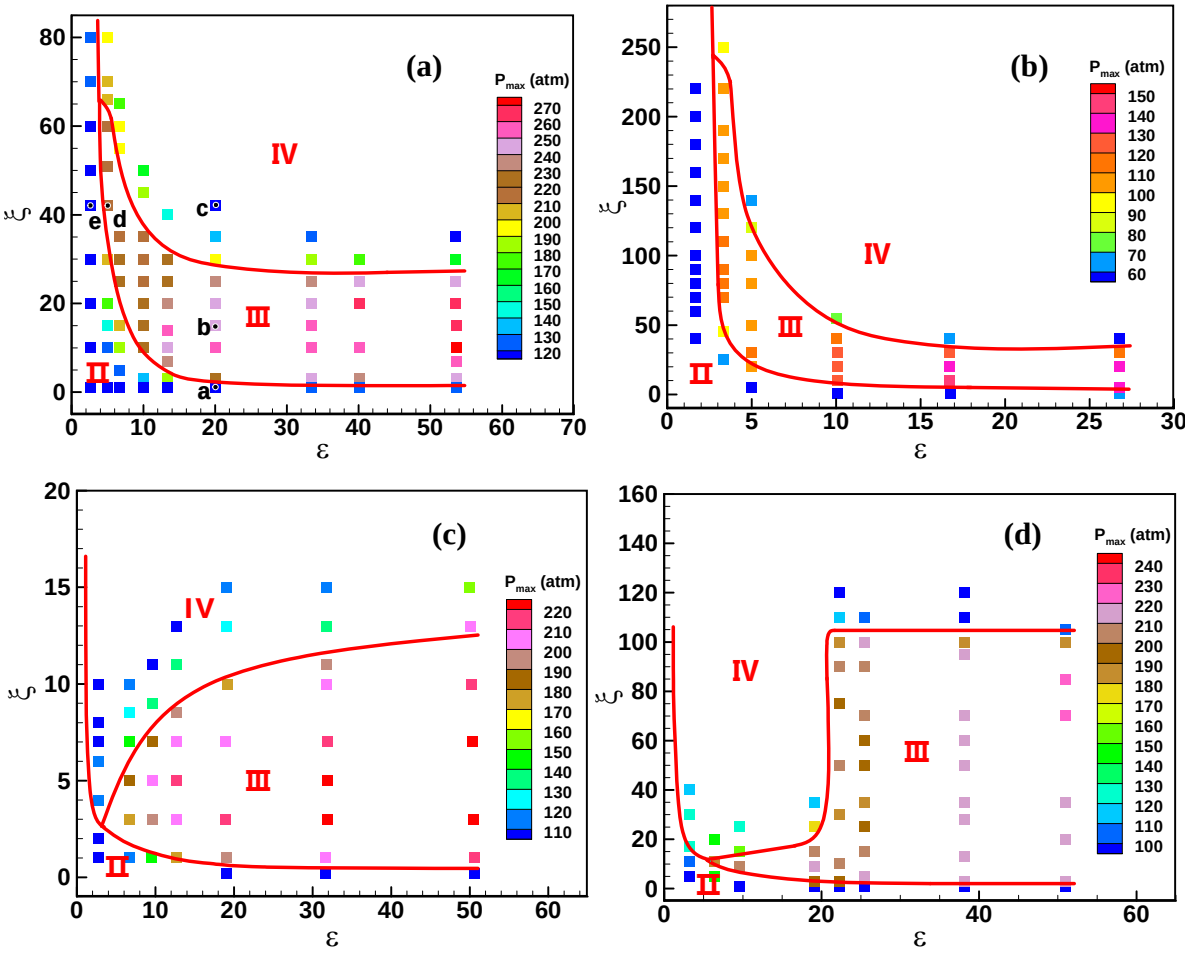

Figure 3. Maximum pressure and detonation development regime in the ξ-ε diagram for H_2/air mixture at (a), T_0=1000 K, P_0=40 atm, ϕ=1; (b), T_0=1000 K, P_0=20 atm, ϕ=1; (c), T_0=1200 K, P_0=40 atm, ϕ=1; (d), T_0=1000 K, P_0=40 atm, ϕ=0.5. Three modes of reaction front propagation are identified: II, supersonic reaction front; III, detonation development; and IV, subsonic reaction front.

4 Conclusions

Autoignitive reaction front propagation and detonation development from a hot spot in hydrogen/air mixtures are investigated numerically. Five different modes are identified in the plot based on two non-dimensional parameters, ξ and ε. The detonation development is induced by the coherent coupling between pressure wave and chemical reaction, which can be explained by the SWACER mechanism and reactivity gradient theory. It is found that detonation development regime is fuel-dependent and thereby the detonation peninsula might not work for different fuels. Besides, different shapes of detonation development regime are observed for different values of initial pressure, temperature and equivalence ratio. The initial

temperature, initial pressure, and equivalence ratio all can affect the detonation development regime. Therefore, to achieve quantitative prediction of engine knock, we need use the detonation development regime for specific fuel at specific initial temperature, initial pressure, and equivalence ratio.

Acknowledgements

This work was supported by National Natural Science Foundation of China (Nos. 91541204, 51322602).

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