Effect of Longitudinal Concentration Gradient on 1-D Double-Period Detonation

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1 Introduction

A detonation wave manifested pulsations in one dimension [1] and cellular instability in multiple dimensions [2], depending on the initial conditions and mixture properties. In uniform media, an unstable 1-D detonation presents pulsating mode. Regarding pulsating instability, extensive experiments have shown longitudinal oscillation of the detonation front when a blunt body travels through a reactive gas at near-Chapman-Jouguet (C-J) velocities [3, 4], while extensive theoretical analyses and numerical simulations have also been performed on the propagating instability [5]. In previous simulations, 1-D detonation instability usually was described by using one-step [1, 6], two-step [7] models. Subsequently, some numerical studies of 1-D detonation were carried out by using real chemistry [8, 9].

However, for detonations propagating in inhomogeneous media, Thomas et al. [10] found that for a steeper gradient, the detonation is less likely to survive because it has less time to adapt to the new environment. Kuznetsov et al. [11] found that propagation and quenching depended significantly on the sharpness of concentration gradient. Recently, Mi, Timofeev & Higgins [12] studied numerically gaseous detonation behavior in a spatially inhomogeneous medium by using one-step model, and found interestingly that detonation velocity is higher than the CJ speed. However, numerical study of 1-D detonation in inhomogeneous media still are few by using real reaction mechanism.

The present work carried out simulations to study the propagation of a 1-D detonation in the media with periodical concentration gradient and to address the effects of longitudinal concentration gradient on a 1-D double-period detonation.

2 Numerical method and specifications

The governing equations are the one-dimensional, reactive, compressible N-S equations. The mixture properties are evaluated using the CHEMKIN [13] and TRANSPORT [14] packages. We adopt the San Diego mechanism [15] which comprises the eight species H_2, O_2, OH, O, H, H_2O, HO_2 and H_2O_2. The spatial discretization of the advection term by the 5th-order WENO scheme [16]. To solve the stiffness problem,

an explicit-implicit Additive Runge-Kutta scheme [17] was used in the time discretization. Eventually, the method based on conservation variables was used to solve the equations, which guarantees conservation and also yields good solution with the shock speed evaluated accurately [18].

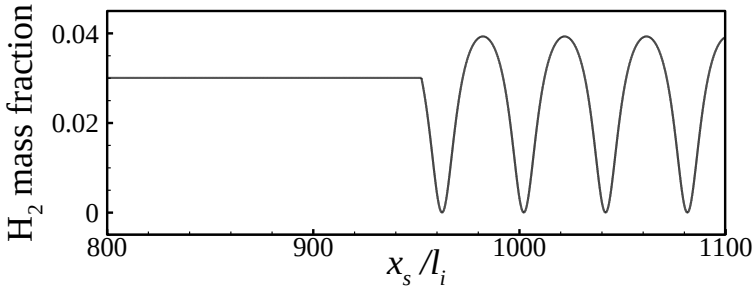

Fig. 1 Variation of hydrogen mass fraction.

The stoichiometric H_2-O_2 mixture with 45%Ar dilution has constant initial pressure and temperature of p_0 = 1atm and T_0 = 298 K, respectively. A periodical disturbance determined by H_2 mole fraction is set at x/l_i >945, where l_i is the induction length and is 3.78×10^{-5}m; the H_2 mole fraction is given by X_{H2}=0.3667sin($z\pi x/L$), where $z\pi$ denotes the frequency of disturbance and L is the length of domain; and $z\pi$ is 4π, 40π and 400π in the present simulations, respectively. This gradient can hold the overall reactivity and exothermicity fixed the same as that in the uniform region. The physical model is shown in Figure 1.

3 Results and discussions

For 45%Ar dilution, the detonation takes on a multi-period pulsation in uniform region, as shown in fig 2. As it goes into the nonhomogeneous region the mode is influenced. This influence depends significantly on the frequency of concentration disturbance. For the gradients with the frequencies of 4π and 40π, as the detonation goes into the nonuniform media, it undergoes a long transition to reestablish to a new propagation mode. Nevertheless, for the lower frequency the double-period mode is destroyed significantly and the reinitiated detonation propagates in highly unstable mode, with chaotical pulsation. As the frequency increases, the detonation in the inhomogeneous mixture becomes regular, showing that the effect of periodical gradient weakens.

To explain the effect of gradient on pulsating instability, the detonation front structures are inspected. Since for lower frequency the wave length of disturbance is close or larger than the induction length. Hence, we take a point where detonation is close to be steady ZND solution to examine effect of the gradient. Figure 3 shows typically front structure for the cases with 4π and 40π. It is seen that for 4π case the wave length of disturbance indeed is much larger than the induction length and therefore the global detonation wave passes over concentration gradient, shown in Fig. 3(a). Although the global front structure is not affected significantly by the gradient, the induction and reaction zones are modified by the interaction of leading shock with gradient, leading to the change of pulsating instability. This interaction is substantiated by bump along the profile of H_2 mass fraction; see the upper panel in Fig. 3(a). The bump is reasonable because the H_2 concentration increases locally due to interaction of the leading shock with the gradient. The excess H_2 fuel cannot be burnt immediately through shock induction so that it is left downstream to form unreacted matter. Delay of burning the unreacted matter also modifies original pulsating mode in the uniform media. However, for 40π case the shock can compress the gradients into the induction zone due to the relatively short wave length of disturbance; local bump of H_2 mass fraction however is not observed; see the top panel

in Fig. 3(b). Hence, the gradient produces fluctuations of physical variable in the internal front, leading to the H_2 fuel left in the downstream.

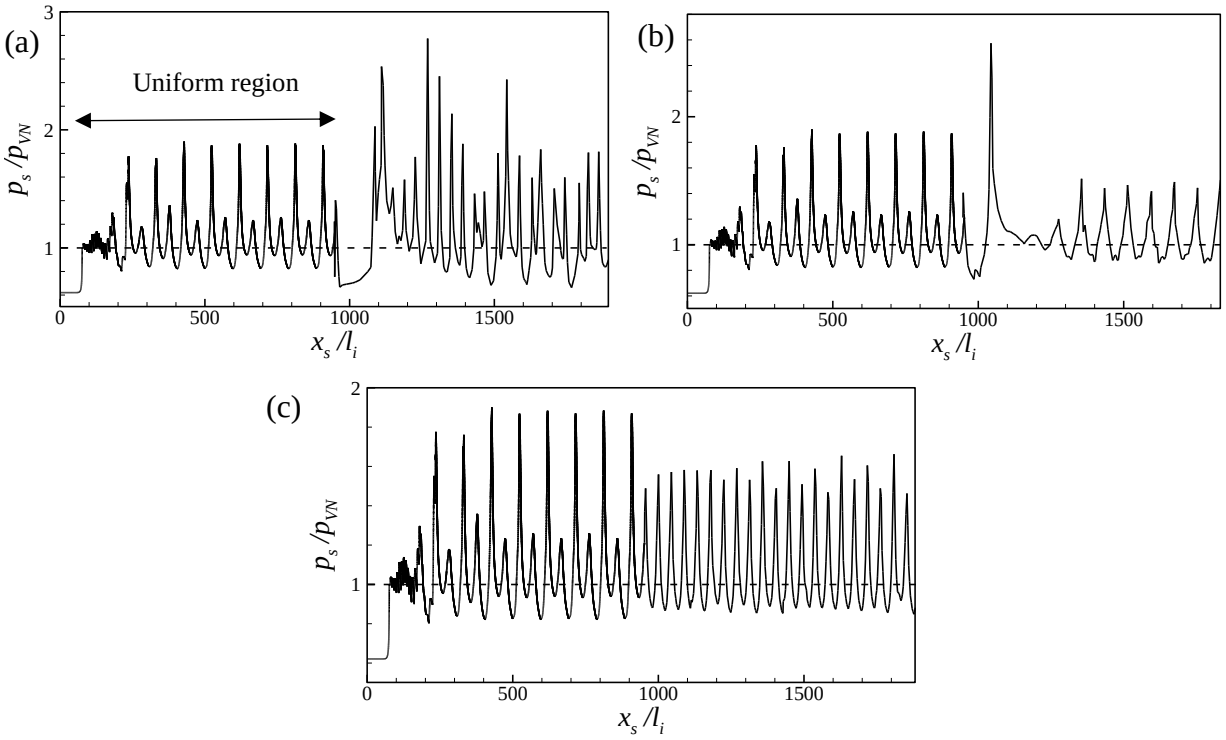

Fig. 2 Maximum pressure histories : (a)4π, (b)40π, (c)400π.

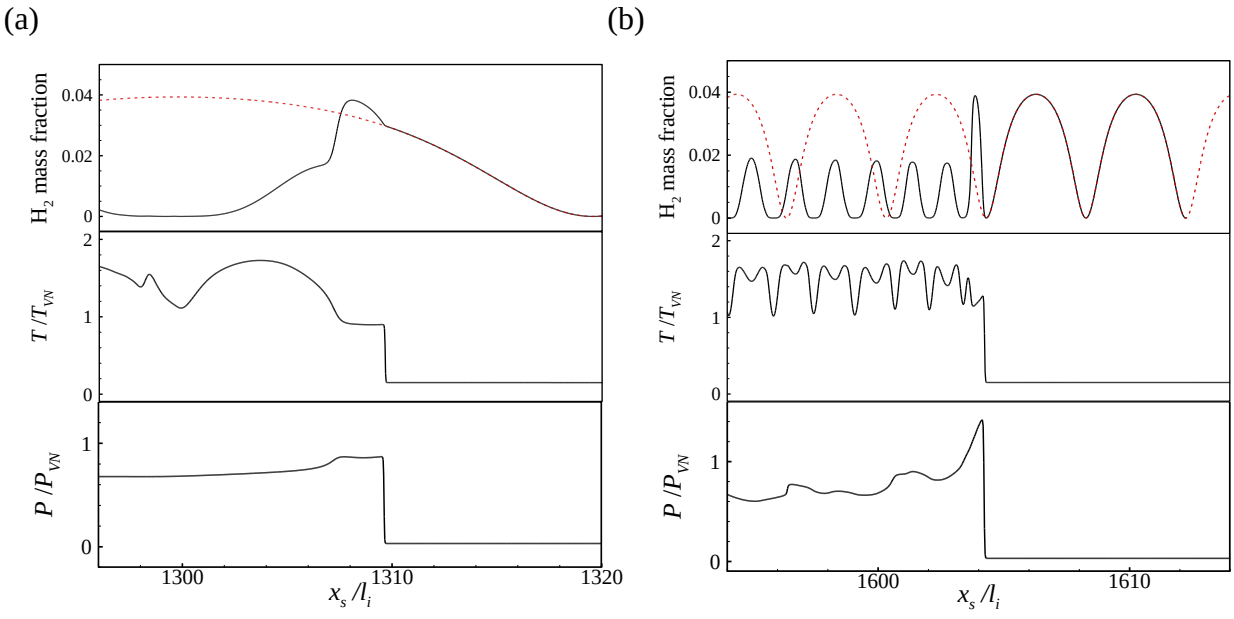

Fig. 3 Detonation front structures for frequencies of 4π (a) and 40π (b): red dash line is initial gradient.

Figure 4 shows the evolution of pressure, mass fraction and temperature profiles for cases with 4π and 40π during a typical pulse. It is seen that when shock climbs from a low to high H_2 concentration, H_2 mass fraction is lowered locally. As such, H_2 fuel entering the front is burnt fully. However, as the shock goes downs along the gradient, local H_2 bump is produced due to the shock-gradient interaction. The bump is more obvious at the place with larger gradient. The excess H_2 fuel entering the front cannot be burnt and left downstream, as shown in the top panel of Fig. 4(a). During the phase, the pressure and temperature profiles show the changes of induction and reaction zone in the expansion and compression stages are globally similar to characteristics in uniform media. For 40π case, the global gradient is able to enter the detonation structure and causes lots of fluctuations in both induction and reaction zones due to compression role. In the compression phase, periodical gradients are compressed into the front; small disturbances in the temperature profile appear in induction and reaction zones. Due to the reaction sensitive to temperature fluctuations, the reaction and induction zones are modified substantially so that the propagation mode is significantly modified for the case with 40π; see the middle panel in Fig. 4(b). As the frequency increases to 400π, the small fluctuations along both temperature and pressure profiles in the induction and reaction regions are caused, while the global structure is not affected significantly. Hence, for the gradient the detonation still is relatively regular (see Fig. 5), although the global propagation mode is changed substantially.

Figure 6 shows the average detonation velocity as a function of frequency of periodical concentration gradient. It is seen that the concentration gradient leads to deficit of the detonation velocity. The deficit is related to the frequency of gradient. The lower frequency causes more velocity deficit that is by12%CJ value, while increasing the frequency decreases the deficit.

In summary, periodical and longitudinal gradient in terms of concentration disturbance will cause the propagation mode to change. The reestablished mode depends on the frequency of the gradient. As the frequency of gradient increases, the influence on the detonation behavior weakens and the front structure does not change significantly. It is found that the periodical gradient leads to the deficit of propagation velocity and the lower frequency leads to more deficit of detonation velocity.

(a) (b)

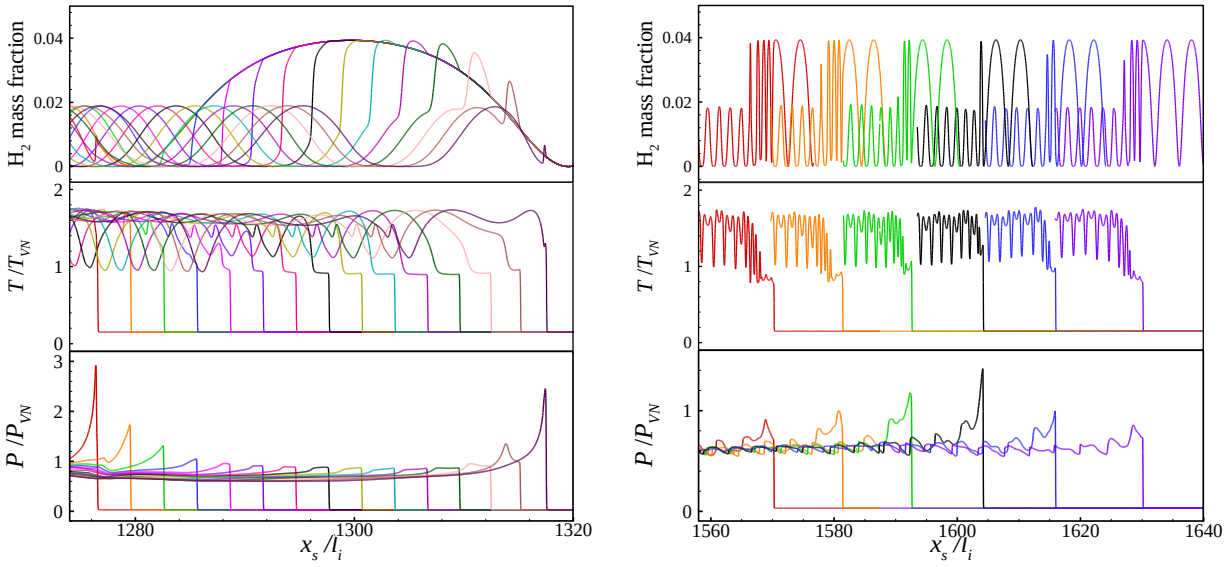

Fig. 4 Evolution of detonation structure for 4π and 40π: (a) t = 23.665, 23.712, 23.768, 23.828, 23.888, 23.948, 24.006, 24.064, 24.123, 24.181, 24.240, 24.299, 24.358, 24.415, 24.465 μs; (b) t = 22.878, 23.124, 23.358, 23.572, 23.795, 24.097 μs.

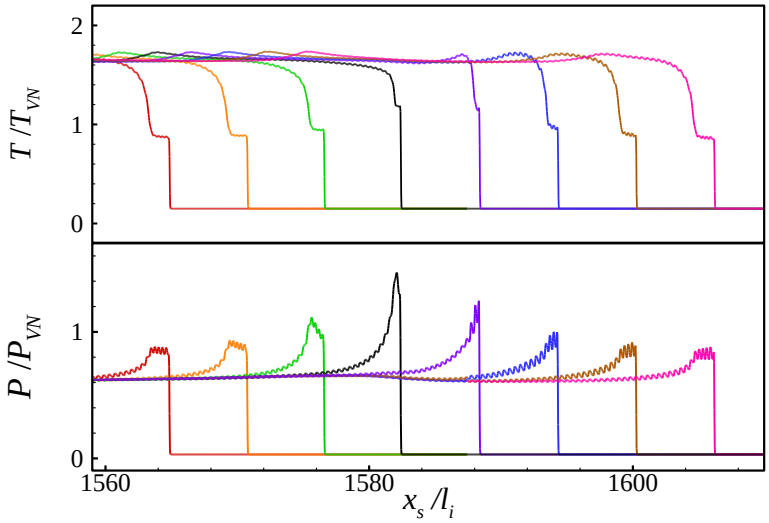

Fig. 5 Evolution of detonation structure for the case with 400π during t = 22.266, 22.392, 22.514, 22.625, 22.727, 22.842, 22.965, 23.092 μs.

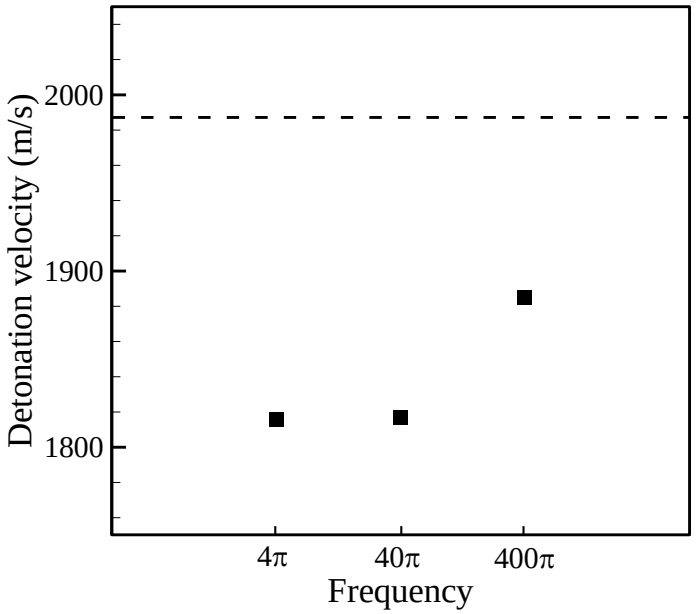

Fig. 6 Average detonation velocity.

References

[1] J.H.S. Lee, The Detonation Phenomena, Cambridge University Press, Cambridge, New York, 2008.

[2] P. Clavin, G. Searby, Combustion waves and fronts in flow, Cambridge University Press, ISBN: 978-1-107-09868-8, 2016.

[3] J.B. McVey, T.Y. Toong, Mechanism of instabilities of exothermic hypersonic blunt body flows, Combust. Sci. Tech. 3(1971) 63-76.

[4] P. Clavin, F.A. Williams, Dynamics of planar gaseous detonations near Chapman-Jouguet conditions for small heat release, Combust. Theor. Model. 6 (2002) 127.

[5] J.J. Erpenbeck, Stability of steady-state equilibrium detonations, Phys. Fluids 5 (1962) 604.

[6] G.J. Sharpe, S.A.E.G. Falle, One-dimensional numerical simulations of idealized detonations, Proc. R. Soc. Lon. 455(1999) 1203-1214.

[7] M. Short, G.J. Sharpe, "Pulsating instability of detonations with a two-step chain-branching reaction model: Theory and numerics," Combust. Theory Modell. 7(2003) 401-416.

[8] M.I. Radulescu, H.D. Ng, J.H.S. Lee, B. Varatharajan, The effect of argon dilution on the stability of acetylene-oxygen detonations. Proceedings of the Combustion Institute, 29(2002) 2825-2831.

[9] S. Yungster, & K. Radhakrishan, Pulsating one-dimensional detonations in hydrogen-air mixtures. Combust. Theor. Model. 8 (2004) 745-770.

[10]Thomas, G.O., Sutton P. & Edwards D.H. 1991 The behavior of detonation waves at concentration gradients. Combust. Flame. 84, 312-322.

[11]Kuznetsov, M.S., Alekseev, V.I., Dorofeev, S.B., Matsukov, I.D. & Boccio, J.L. 1998 Detonation propagation, decay, and reinitiation in nonuniform gaseous mixtures. P. Combust. Inst. 27, 2241-2247.

[12]Mi, X.C., Timofeev, E.V. & Higgins, A.J. 2017 Effect of spatial discretization of energy on detonation wave propagation. J. Fluid Mech 817, 306-338.

[13] R.J. Kee, F.M. Rupley, J.A. Miller, Chemkin II: a Fortran chemical kinetics package for the analysis of gas phase chemical kinetics. Tech. Rep. SAND89-8009B. Sandia National Laboratories. 1992.

[14] R. J. Kee, G. Dixon-Lewis, J. Warnatz, M.E. Coltrin, J.A. Miller, A Fortran computer code package for the evaluation of gas-phase multi-component transport properties. Tech. Rep. SAND86-8246. Sandia National Laboratories. 1991.

[15] A.L. Sánchez, F.A. Williams, Recent advances in understanding of flammability characteristics of hydrogen, Prog. Energ. Combust. 41 (2014) 1-55.

[16] G.S. Jiang, C.W. Shu, Efficient Implementation of Weighted ENO Schemes, J. Comput. Phys. 126 (1996) 202-228.

[17] C.A. Kennedy, M.H. Carpenter, Additive Runge-Kutta schemes for convection diffusion reaction equations, Appl. Numer. Math. 44(2003) 139-181.