Analytical and numerical study of the expansion effect on the velocity deficit of continuous detonation waves

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1 Introduction

Detonation is a premixed combustion mode. The shock wave and a followed reaction zone form the detonation wave. Compared with deflagration, detonation generates lower entropy and thus has higher efficiency. One way to use detonation for propulsion is the continuous detonation chamber (CDC). In previous simulations of CDCs[1], it was found that the detonation propagating velocity of two-dimensional simulations is different from that of C-J theory or one-dimensional simulations. This phenomenon implies us that detonation waves in CDCs are different from C-J detonation. The difference can be derived from the expansion flow field perpendicular to the detonation propagating direction, which is pointed out by Refs[2]. The aim of this article is to extend the ideas of Fujiwara and Tsuge [3, 4] to CDCs, then we can verify and study the influence of the expansion on the detonation wave propagating velocity in CDCs. Although the real detonation waves have strong three dimension effects and the one- and two-step reaction kinetics bring a lot of error, nowadays there are also a lot of simulations performed under those conditions. So this paper can provide some references for those numerical simulation results.

2 Physical and numerical modeling

Figure 1 shows the unrolled contours of the flow field of a typical co-axial annular combustor model of CDCs with all main flow structures. One or more detonation waves propagate azimuthally in the annular combustor, each of which is combined with an oblique shock wave and a slip line. The fresh propellants are injected from the head of the combustor and the products exhaust from the exit.

When the waves propagate at a certain speed, the flow field can be considered as a steady flow in the reference frame fixed on the detonation front, allowing us to analyze the flow field with many well-developed steady supersonic flow theories. In the wave-fixed reference frame, fresh propellants flow against the detonation front at the speed of detonation wave. Gases cannot go across the slip line, so the inclination of slip line indicates the expansion direction behind the detonation wave. And the oblique shock wave is

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induced by the incline slip line. The contact surface between fresh propellants and products is an approximate slip line. As a result, it can be seen as the flow direction of fresh propellants in front of the detonation wave in the wave-fixed reference frame.

The model of Fujiwara and Tsuge [3, 4] is used here. Figure 2 shows the sketch of the steady quasi-1D ZND model. The leading shock wave is followed by an expansion reaction zone. The flow field can be understood as a detonation wave propagating in a flexible tube bounded by the slip line and the head wall. The model can reflect the expansion behind the detonation wave by the increase of cross-section (the height from head wall to slip line).

In Figure 2, line 0 is the leading shock wave. The relation between side 0 and side 1 is the Rankine-Hugoniot condition. The reaction zone stretches behind the leading shock wave. Considering the steady flow, the equations of the flow below the slip line are steady quasi one-dimensional reactive Euler equation with varying cross section area (σ). The reaction kinetics ($d\lambda/dt$) can be one-step kinetics model adopted from Ma and Yang [5]. The two-step kinetics model adopted from Taki and Fujiwara [6] can also be used here alternatively. The relation between dt and dx is $udt = dx$. The equation describing the variation of the cross-section area is necessary to close the equations. Considering the hypersonic characteristic of the oblique shock wave, the pressure field above the slip line can be approximated by the Newton model, $p = p_0 + \rho_{00} D^2 (\mathrm{d}\sigma/\mathrm{d}x)^2 / [(\mathrm{d}\sigma/\mathrm{d}x)^2 + 4\pi\sigma]$, where D denotes the velocity of detonation wave. The model is based on hypersonic theory, which will fail when zone 00 is high temperature zone. Thus an equivalent expansion slope is proposed to overcome the problem, $\mathrm{d}\sigma/\mathrm{d}x = k_{\mathrm{ex}}$. k_{ex} denotes the expansion slope. To model the expansion in CDCs, the equivalent expansion slope needs to be extracted from the numerical results, which will be discussed later in this paper. Eliminating all ρ and p in Eqs. (1-3), there exists $\mathrm{d}u/\mathrm{d}x = [u((\gamma-1)Q/c^2\, \mathrm{d}\lambda/\mathrm{d}x) - (\mathrm{d}\sigma/\mathrm{d}x)/\sigma]/(1-\mathrm{Ma}^2)$. There is no singularity in the flow field when Mach number equals to 1, So $\mathrm{d}\lambda/\mathrm{d}x = c^2/(\gamma-1)/Q/\sigma\, \mathrm{d}\sigma/\mathrm{d}x$ when Mach number equals to 1.

Concluding the steady quasi-1D model, the numerical method is guessing the detonation propagating velocity, solving flow by the ordinary differential equations and testing the non-singular condition. After serval iterations, the solution can be obtained. The ode15s function in MATLAB is used as the ODE solver, which is an implicit stiff ODE solver using adaptive integral steps. More than 3000 integral steps cover the reaction zone, confirming the resolution is sufficient. When the detonation propagating velocity is acquired, the flow field profile in front of the sonic point is known. The sonic point can stride over by an explicit step. Then the flow field profile behind the sonic point can be obtained.

3 Results by one-step kinetics model

The profiles of the flow field calculated by one-step kinetics model are shown in Figure 3. In the non-expansion case, the profiles agree well with the one-dimensional C-J theory. In the case of expansive detonation, the gases accelerate to sound speed and then exceed it in the reaction zone. Compared with the non-expansive case, the expansive detonation propagating velocity is smaller, and the strength of the detonation is weaker.

The profiles of detonation with Newton expansion model and uniform expansion model are plotted for comparison in Figure 3. A series of Newton model cases have been done, where the maximum expansion slope is approximately three times of that at the sonic point. We can take twice of the expansion slope at the sonic point of Newton model as the equivalent expansion slope. In the CDCs, the slip line slope away from the detonation wave can be seen as the slope at the sonic point. Accordingly, we can obtain the equivalent slope in the uniform expansion model through the assumption we make.

The p-v diagram of the detonation wave with and without the extra expansion process is plotted in Figure 4 for comparison. The deficit of the detonation velocity is affected by two major factors. One is that the expansion process makes the Rayleigh line no longer tangential to the Hugoniot line and reduces its slope, resulting in the gases doing more work in reaction. The other one is that the reacted gases reach sound speed before the end of the reaction, which causes the heat release behind the sonic point to lose contribution to the detonation velocity.

Figure 5 shows the normalized velocity of detonation. The expansion slope and the deficit of detonation propagating velocity are positively related. The normalized deficit of velocities reduces when the temperature in front of the detonation wave increases. That is because that in the detonation waves by the one-step kinetics model, the expansion process is the main influencing factor on the detonation velocity.

4 Results by two-step kinetics model

Except two main differences, the flow field profiles calculated by one-step and two-step kinetics model are similar, seen from Figure 6. The two differences are the existence of the induction zone and that the two-step reaction is a reversible reaction. Profiles calculated by uniform expansion model and Newton model can be compared in Figure 6. The equivalent expansion slope is set by the method discussed in 3.3, and the profiles in front of the sonic point of the two models are very close.

The normalized velocity of detonation and equilibrium reaction progress parameter is shown in Figure 7. The deficit of detonation velocity increases when the expansion slope Σ increases. The pressure and the deficit of detonation velocity are negatively related, while the temperature and the deficit of detonation velocity positively. The expansion and the shifting of reaction equilibrium are coupled. According to the equilibrium reaction progress parameter shown in Figure 7 (c) and (d), it is known that the normalized deficit of the detonation velocity is mainly controlled by chemical equilibrium.

5 Comparison with two-dimensional CDC simulation

In the simulation, the reactants are the stoichiometric hydrogen-air mixture, and the reaction kinetics is the two-step kinetics model. The convergence nozzle inflows are used as the injection condition. The other numerical setups are the same as Zhou and Wang [1]. The geometry message can be extracted from the numerical results by the discontinuity of the flow field, including the detonation propagating velocity D and the equivalent expansion slope.

A set of simulation cases with varying inlet total pressures and temperatures have been processed. Theoretical analysis of the detonation wave with and without expansion process is conducted under the corresponding pre-detonation conditions in the numerical simulation, and the results are normalized by the non-expansion theoretical results, as shown in Figure 8. When the inlet total pressure $\mathrm{P_{tot}}$ increases, the deficit of the detonation velocity will reduce, in accordance with the theoretical results. When the inlet total temperature T_{tot} increases, the deficit of the detonation velocity basically remains unchanged. The theoretical and numerical results show similar trends and the deficit of the detonation velocity are of the same order of magnitude (about 5%), which proves that the process of expansion reduces the detonation wave velocity of the rotating detonation waves, and the effect can be described by the model in this article.

6 Conclusions

Based on the quasi-1D ZND model, a detonation wave model considering the expansion process is used to investigate the deficit of the detonation velocity with the one- and two-step kinetics models.

(1) The expansion in the reaction zone of detonation reduces the propagating velocity of detonation waves. The expansion slope and the deficit of detonation propagating velocity are positively related.

(2) The deficit of the detonation velocity is affected by two major factors. One is that the expansion process makes the Rayleigh line no longer tangential to the Hugoniot line and reduces its slope, resulting in the gases doing more work in reaction. The other one is that the reacted gases reach sound speed before the end of the reaction, which causes the heat release behind the sonic point to lose contribution to the detonation velocity.

(3) For the one-step kinetic model, the deficit of the detonation velocity is mainly controlled by the expansion process. For the two-step kinetic model, the deficit of the detonation velocity is mainly controlled by the heat release behind the sonic point.

(4) The expansion process in RDEs reduces the speed of the detonation wave by approximately 5%, which is an important factor of the deficit of detonation velocity in two-dimensional simulations.

Acknowledgments

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Figures

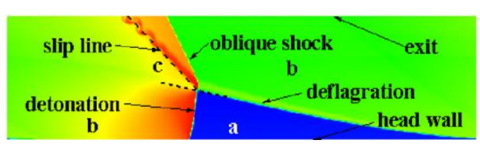

Figure 1 Typical CDC flow field a-fresh propellants; b- products, c-reaction products from the previous cycle

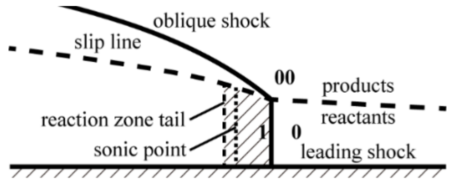

Figure 2 ZND model in the steady quasi-1D analysis

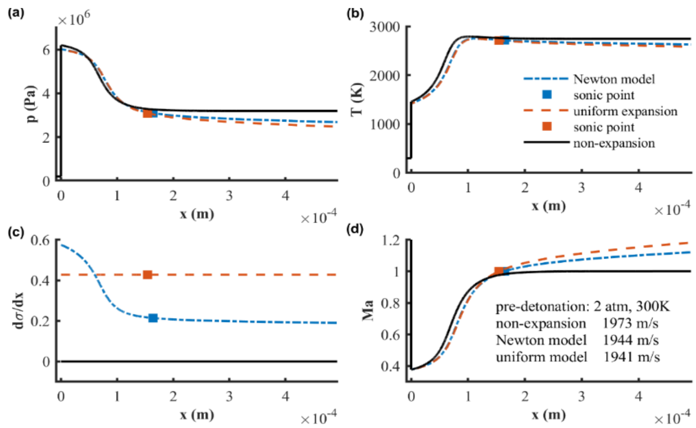

Figure 3 Profiles of the flow field calculated by one-step kinetics model (a) pressure; (b) temperature; (c) expansion slope; (d) Mach number

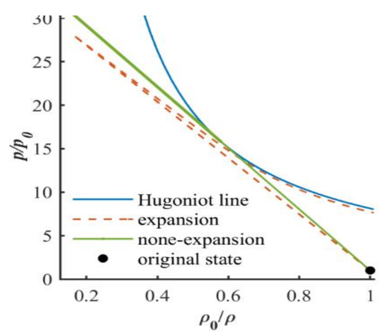

Figure 4 Comparison of p-v diagram between expansive and non-expansive detonation waves

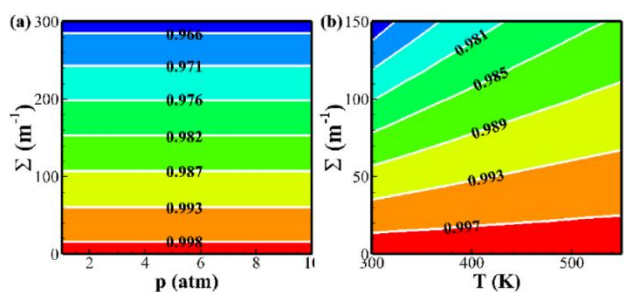

Figure 5 Normalized velocity of detonation $D_{\mathrm{ex}}/D_{\mathrm{non-ex}}$ (color and line label) under the variation of pre-detonation state, where D_{ex} and $D_{\mathrm{non-ex}}$ represent the detonation velocity with and without expansion and Σ denotes the expansion slope $(\mathrm{d}\sigma/\mathrm{d}x)/\sigma_0$ (a) with constant temperature T = 450 K; (b) with constant pressure p = 2 atm

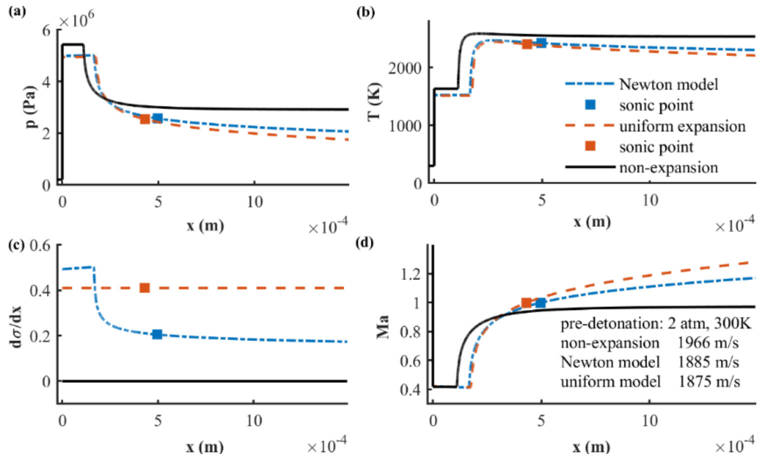

Figure 6 Profiles of the flow field calculated by two-step kinetics model with pre-detonation (a) pressure; (b) temperature; (c) expansion slope; (d) Mach number

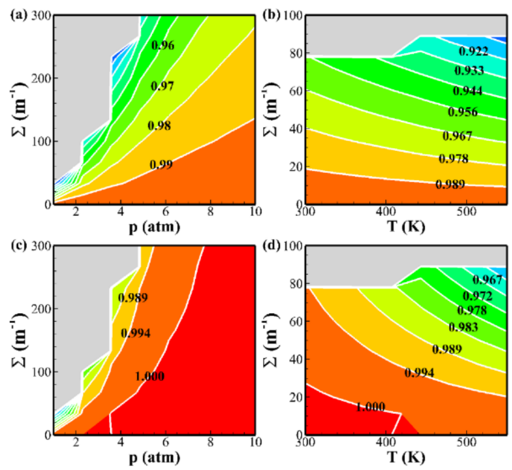

Figure 7 Normalized velocity of detonation $D_{\mathrm{ex}}/D_{\mathrm{non-ex}}$ and equilibrium reaction progress parameter λ (color and line label) under the pre-detonation state variation, where D_{ex} ,$D_{\mathrm{non-ex}}$, Σ, T, p are the same as those in Figure 5 (a) $D_{\mathrm{ex}}/D_{\mathrm{non-ex}}$, T = 450 K; (b) $D_{\mathrm{ex}}/D_{\mathrm{non-ex}}$, p = 2 atm; (c) λ, T = 450 K; (d) λ, p = 2 atm

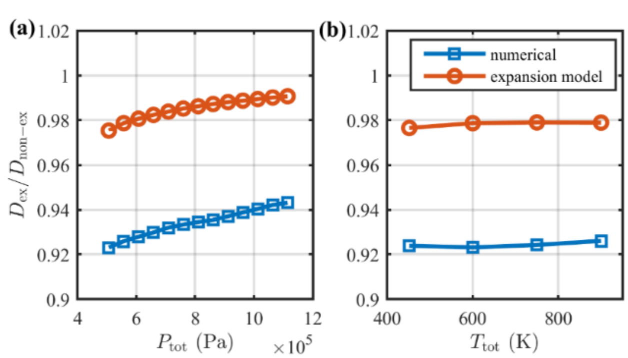

Figure 8 Comparison between numerical and expansion model about the deficit of detonation velocity when the inlet stagnation state changes (a) with the constant total temperature of 450 K; (b) with the constant total pressure 5 atm