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Effect of wall curvature on detonation reflection in combustion chambers

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Abstract

This study investigates the impact of curvature on the reflection of detonation waves in a detonation engine. The reflection of detonation waves in the combustion chamber is inevitable and therefore requires investigation. This paper focuses on the reflection of curved detonation waves on convex and concave walls. It has been determined that there are two mechanisms by which curvature affects the stability of the waves: firstly, curvature affects the angle of the wave, leading to the appearance of a subsonic and high-temperature/high-pressure region behind the wave, which affects stability; secondly, curvature affects the mutual positioning of the wave systems, leading to mutual interference and stability. In addition, analysis of the detonation wave flow field has revealed the important influence of curvature. Therefore, a relationship between the gradient of wave parameters and curvature has been established, which can be used for detonation reflection analysis and generally regulate gradient effects of curved walls. Comparison with simulation results shows that this relationship can effectively predict the gradient of the reflected wave and provide a higher-order analysis tool for detonation reflection.

Keywords: *Detonation, Reflection, Curvature*

Nomenclature

H_1 – Height of inlet in the geometric model
H_2 – Height of outlet in the geometric model
L – Length of geometric model
p_1 – pressure of incoming flow
T_1 – temperature of incoming flow
u_1 – velocity of incoming flow
U – the conservation variable
F – the convective flows in the x direction
G – the convective flows in the y direction
S – the source term
t – time
ρ – density
v – velocity in the y-direction
e – total internal energy per unit mass
Y_i – mass fraction of component i
$\dot{\omega}_i$ – mass production rate of component i
ns – the number of components
v'_{ir}– the stoichiometric coefficients of forward reaction
v''_{ir} – the stoichiometric coefficients of reverse reaction
k_{fr} – the forward reaction rates
k_{br} – the reverse reaction rates
M_i – the molar mass of component i
x_j – the molar concentration of component j
$Coef_{ir}$ – the three-body enhancement factor
β – the detonation angle
S – the curvature

1. Introduction

Detonation, a phenomena characterized by shock-induced extreme combustion, has garnered significant attention as an ideal propulsion technology due to its supersonic propagation, nearly isovolumetric combustion, and short combustion time [1]. Consequently, detonation and detonation engines have been extensively studied. Research efforts have primarily focused on elucidating the characteristics of the detonation wave itself, including the solution of the detonation [2], the morphology and standing region of the detonation wave [3], and the cellular structure of the detonation [4]. Concurrently, research has also centered on the design and development of novel detonation engines. Depending on the type of detonation wave, these engines can be categorized as rotating detonation engine (RDE) [5], pulse detonation engine (PDE) [6], and oblique detonation engine (ODE) [7]. Among these, ODE holds promise for its simpler construction and effective application. Therefore, it is imperative to delve deeper into the structure and dynamics of the detonation wave within the combustion chamber specific to ODE. Unlike detonation waves that develop freely in open space, oblique detonation waves (ODWs) within the combustion chamber are bound to undergo reflection. The type and nature of these reflections can significantly impact the propulsive performance of ODE. ZHANG conducted a comprehensive investigation into the influence of reflections at varying positions on the nature of the reflection itself. This study revealed the reasons why Mach reflections do not occur in this context and provided a formula for determining the stable position of the Mach stem [8]. WANG conducted a study on the structural changes of the reflected wave system from ODW on the upper wall of the combustion chamber, considering the influence of the expansion nozzle using a simplified ODE model. The results reveal that the merging of subsonic regions, resulting in thermal choking, significantly impacts the stability of the reflected structure [9].

Given the close relationship between detonation and shock waves, it is crucial to consider shock wave reflection prior to the study of detonation waves. In 1878, Mach reported the discovery of shock wave reflection and documented two distinct structures of shock wave reflection: regular reflection (RR) and Mach reflection (MR) [10]. Subsequently, Von-Neumann further developed the two-wave theory and triple-wave theory, leading to the Von-Neumann's criterion for the transformation of RR and MR and the detachment criterion [11][12]. This established the theoretical framework for shock wave reflection research. Since then, research on shock wave reflection has deepened, and its application fields have gradually expanded. Hornung and Robinson conducted experiments to investigate the variation of Mach stem height with incident shock angle and derived an equation to describe it [13]. Subsequently, Li and Ben-Dor proposed an approximate analytical model of Mach stem shape with first-order accuracy [14].

The study of shock wave reflection is crucial and worthwhile for understanding detonation wave reflection, as both share a similar composition of incident wave, reflected shock, and Mach stem. This shared composition leads to numerous similarities that can be explored through similar methods. However, in contrast to shock wave reflection, detonation wave reflection involves a chemical reaction, resulting in both the incident wave and Mach stem being reactive shock waves. Thomas studied the reflection of detonation waves on wedge surfaces, curved channels, and cylindrical pipes, exploring the changes in cellular lattice structure through experimental methods [15]. Guo experimentally investigated the relationship between the critical angle of RR to MR transition and wedge angle for detonation wave reflection [16]. LI utilized numerical methods to simulate Mach reflection of ZND detonation waves on wedge surfaces [17]. The results indicate that the process of Mach reflection is no longer self-similar due to the presence of the reaction zone thickness, and the variation of Mach stem height with distance differs from the straight line prescribed by the triple-wave theory. This conclusion that the triple-wave point trajectory is no longer straight was also observed in the study by Ohyagi [18]. LI conducted simulations to investigate the reflection of positive detonation waves on various curved walls, focusing on the law governing the effect of curvature on RR and MR transition angles and Mach stem height [19].

The aforementioned studies primarily focus on oblique detonation waves and engines, with fewer investigations on curved detonation waves (CDWs) and curved detonation engine (CDE). CDWs is more complex than ODWs, potentially increasing the challenges in theoretical modeling and analysis. This paper examines the reflection of CDWs in a combustion chamber, particularly the influence of curvature on detonation reflection. We present two combustion chamber structures with curved walls and calculate the structure of detonation wave reflection using simulation methods. A small difference allows the Mach reflection to be stationary, while a large difference prevents it. Additionally, we investigate the influence of curvature on post-wave parameters of detonation reflections. Simulation results show that curvature significantly alters the post-wave flow situation. Therefore, the relationship between curvature and post-wave parameters requires further investigation. Overall, this study provides valuable insights into curved detonation waves and engines, highlighting the importance of wall curvature and other factors in detonation reflection. Future work could explore further the relationship between curvature and post-wave parameters to better understand their effects on engine performance and efficiency.

2. Numerical methods and computational model

The schematic diagram of the curved detonation engine is shown in **Fig. 1(a)**, which is based on the oblique detonation engine by replacing the oblique wedge with a curved wall. Considering the curved detonation wave has features that are not present in the oblique detonation wave, the curved detonation engine has the value of theoretical research and potential for applications.

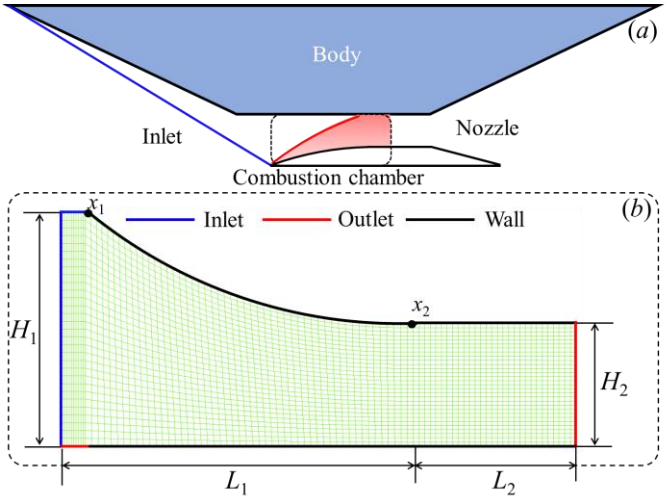

Fig 1. Schematic diagram of curved detonation engine: (a) vehicle with engine, (b) grids and boundary conditions.

Fig. 1(b) presents the computational domain and the boundary conditions set in this study. For ease of observation, the entire computational domain is inverted vertically. The left boundary is set as the incoming flow condition, while the right boundary is defined as the exit. As viscosity is neglected, the upper and lower walls are set as inviscid walls. The geometrical parameters are set to $H_1 = 100\,mm$, $H_2 = 52/62\,mm$, $L_1 + L_2 = 210\,mm$, and the wall curvature and x_2 will be changed as needed in different cases. Fuel is a mixture of hydrogen and air with an equivalent ratio of 0.34. The incoming flow parameters are kept constant at $p_1 = 100\,kPa$, $T_1 = 700\,K$, and $u_1 = 3000\,m/s$. The above geometric parameters and incoming flow conditions were obtained by simulating real flight conditions, and the specific computational process was ignored.

The numerical solution strategy adopted in this paper is described next. Considering that detonation is a shock-induced chemical reaction process, and this article mainly focuses on detonation in the absence of viscosity, the influence of viscosity has not been considered for the time being. Therefore, the control equation adopted in this article is the Euler equation coupled with the chemical reaction source term. In the Cartesian coordinate system, the two-dimensional Euler equation is:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = S \tag{1}$$

Where, U is the conservation variable; F and G are the convective flows in the x and y directions, respectively; and S is the source term. The above variables are expressed in the form of:

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho e \\ \rho Y_1 \\ \cdots \\ \rho Y_{ns-1} \end{bmatrix}, F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (\rho e + p)u \\ \rho u Y_1 \\ \cdots \\ \rho u Y_{ns-1} \end{bmatrix}, G = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (\rho e + p)v \\ \rho v Y_1 \\ \cdots \\ \rho v Y_{ns-1} \end{bmatrix}, S = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \dot{\omega}_1 \\ \cdots \\ \dot{\omega}_{ns-1} \end{bmatrix} \tag{2}$$

Where, ρ , u , v , p, and e are the density, velocity in x and y directions, pressure, and total internal energy per unit mass of the gas mixture, respectively; Y_i and $\dot{\omega}_i$ are the mass fraction and mass production rate of component i, respectively, and ns is the number of components in the gas mixture. The chemical reaction model adopted in this paper is the 9-component, 19-step primitive reaction model of Jachimowski [20] modified by Wilson [21]. This model has been well demonstrated to conform well to experimental data and is not widely used in detonation studies [22]. In particular, the chemical reaction equation can be expressed generally in the following form:

$$\sum_{i=1}^{ns} v'_{ir} x_i \underset{k_{br}}{\overset{k_{fr}}{\rightleftarrows}} \sum_{i=1}^{ns} v''_{ir} x_i \, , r = 1,2, \dots , nr \tag{3}$$

where, x_i is the component i; v'_{ir} and v''_{ir} are the stoichiometric coefficients of component i in the reactants and products of the r reaction, respectively; k_{fr} and k_{br} are the forward and reverse reaction rates of the r reaction, respectively. Further, $\dot{\omega}_\iota$ the mass production rate per unit volume of component i is as follows:

$$\dot{\omega}_\iota = M_i \sum_{r=1}^{nr} \left\{ \Gamma_r (v''_{ir} - v'_{ir}) \left[k_{fr} \prod_{j=1}^{ns} [x_j]^{v'_{jr}} - k_{br} \prod_{j=1}^{ns} [x_j]^{v''_{jr}} \right] \right\}, i = 1,2 \dots , ns \tag{4}$$

where, M_i is the molar mass of component i and $[x_j]$ is the molar concentration of component j. For non-trimeric effects, $\Gamma_r = 1$; if the r reaction is trimeric, then we have:

$$\Gamma_r = \sum_{i=1}^{ns} Coef_{ir} [x_i] \tag{5}$$

Where, $Coef_{ir}$ is the three-body enhancement factor for the r-th primitive reaction component i. The forward reaction rate is given by the Arrhenius formula:

$$k_{fr} = A_r T^{\beta_r} exp\left(\frac{-Ea_r}{R_u T}\right) \tag{6}$$

The reverse reaction rate k_{br} is calculated from the corresponding forward reaction rate k_{fr} and the concentration equilibrium constant of the chemical reaction K_{cr}.

$$k_{br} = \frac{k_{fr}}{K_{cr}} \tag{7}$$

The relationship between the concentration equilibrium constant of a chemical reaction K_{cr} and the pressure equilibrium constant of the reaction K_{pr} is as follows:

$$K_{cr} = K_{pr} exp\left[\sum_{i=1}^{ns} (v''_{ir} - v'_{ir}) ln\left(\frac{p_{atm}}{R_u T}\right) \right] \tag{8}$$

Where the pressure equilibrium constant is obtained from the relevant thermodynamic parameters. In order to verify that the grid sizes adopted in this paper are appropriate, the simulations for three different grid sizes are given in this paper as shown in **Fig. 2**.

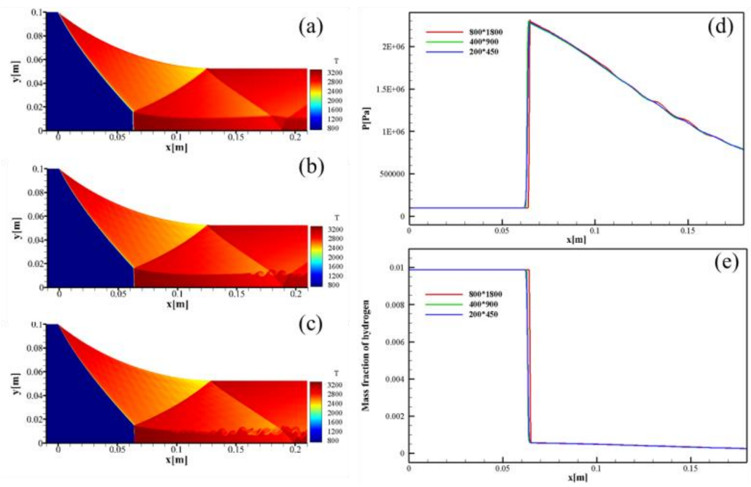

Fig 2. Verification of grid-independence: (a) temperature contour for a grid size of 200*450, (b) temperature contour for a grid size of 400*900, (c) temperature contour for a grid size of 800*180, (d) variation of pressure at y=0 for three grid sizes. (e) variation of hydrogen mass fraction at y=0 for three grid sizes.

In this case, the smallest grid size has 200*450 grids in two directions respectively, the moderate grid size is 400*900 and the fine grid size has 800*1800 grids. In terms of the temperature field, the larger the grid the clearer the calculated flow field, although all three remain similar in the overall structure of the flow field. The pressure and hydrogen changes at the bottom wall surface also indicate that the calculation results are similar under different grid sizes. Considering both the computational performance and the cost, this paper selects the 400*900 grid size for the calculation.

3. Curved detonation reflection with different curvatures

Under different curved walls, different types of reflections of the detonation wave occur. In this paper, the curved detonation reflected flow fields are calculated for a variety of different curved wall surfaces, and the standing Mach reflected flow fields are demonstrated for each of the two types of concave and convex wall surfaces. Firstly, the convex detonation wave is used as an example, and in this part of the study, the curvature of the curved wall surface is varied by the x coordinate of x_2. A wall with curvature is taken and the wall function is set to $y = 0.0085x^2 - 1.2531x + 100$. The mean curvature is -0.0045. Negative values indicate a decrease in the wave angle. To observe the process of reflection, non-constant calculations were taken and the results are shown in **Fig. 3**.

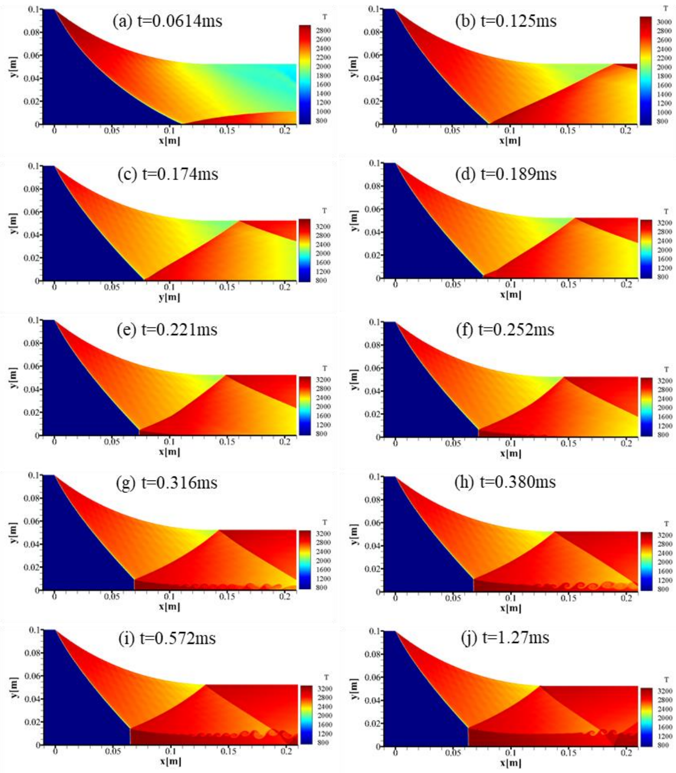

Fig 3. Stationary Mach-reflected detonation waves flow field in the case of convex wall surfaces

In **Fig. 3**, at t=0.0614 ms, the curved detonation wave is reflected by contacting the wall, and then with time, at t=0.125 ms, the reflected shock wave contacts the upper wall and produces a secondary reflected shock wave near the exit. Then, with the forward propagation of the detonation wave, the Mach stem gradually appeared, and from t=0.174 ms a tiny Mach stem began to appear, and at t=0.189 ms the shape of the Mach stem became clearer. Thereafter, the Mach stem grows while propagating forward, and the motion in both directions gradually slows down until it stabilizes at t=1.27 ms.

After studying the convex curvature, the concave curved wall is the next case to be discussed. Since this concave curved wall results in a particularly pronounced induced zone and a relatively farther back reflection position, using the same exit height as for the convex curved wall combustion chamber would not yield consistent reflection results. Therefore, H_2 is increased to 62.

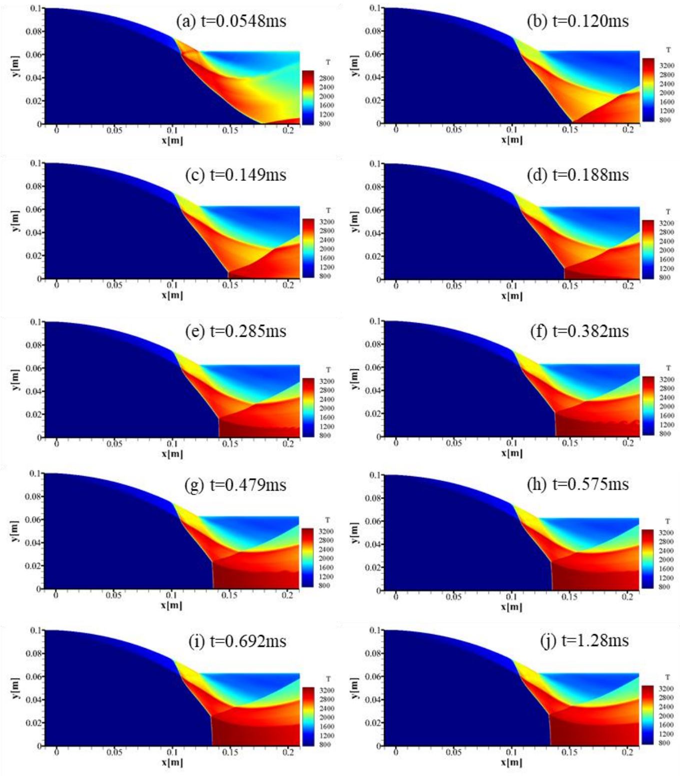

Fig 4. Stationary Mach-reflected detonation waves flow field in the case of concave wall surfaces

In **Fig. 4,** at t=0.0548 ms the detonation wave produces a reflected shock with the lower wall surface, followed by a gradual growth to the exit height. Then at t = 0.188 ms produces a secondary reflection at the same time the structure of the Mach stem appears, followed by a gradual increase in the height of the Mach stem, the position is also moving forward. With the continuous advance of time, at t = 0.692 ms curved detonation wave eventually completely transformed into a Mach stem.

In order to further understand the effect of curvature on the detonation reflected flow field, the streamlines on the detonation reflected flow field in the case of concave and convex wall surfaces are selected and analysed in the following. Firstly, the two streamlines in the convex wall reflected flow field are shown in **Fig.5**.

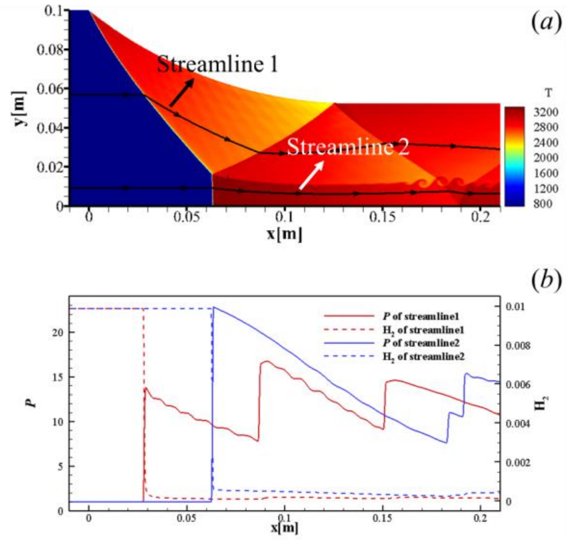

Fig 5. Mach reflection of the curved detonation in convex wall condition: (a) temperature contour, (b) parameters on the streamline.

By observing **Fig. 5 (a)**, it can be found that the overall structure of the flow field is similar to oblique detonation, and the effect caused by curvature is not obvious. However, by extracting the data on the streamline it can be found that the curvature of the wall causes a significant change after the incident detonation wave. Compared with oblique detonation, similar flow field structure, the difference in the airflow variation is mainly caused by the curvature. This also proves that even a small curvature can have a large effect on the post-wave flow. Specifically taking streamline 1 as an example, the existence of curvature on the one hand causes different wave angles at different wave positions, which results in a change of aerodynamic parameters. On the other hand, the curved wall will lead to a non-uniform flow field after the post-wave of the detonation, and the aerodynamic parameters will be continuously changed. The mechanism of this effect and the specific effect size need to be further analysed and calculated by theory.

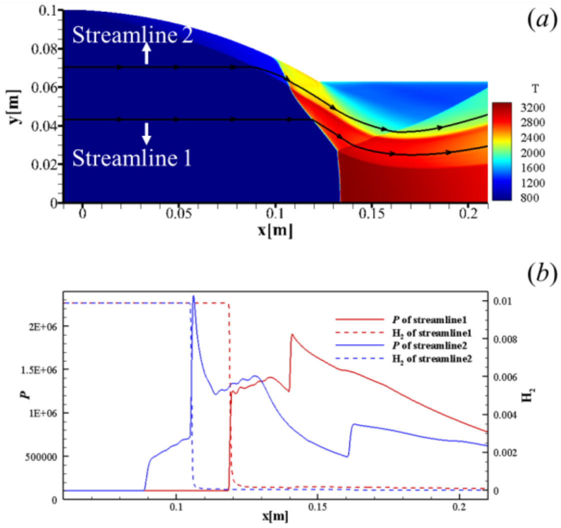

Fig 6. Mach reflection of the curved detonation in concave wall condition: (a) temperature contour, (b) parameters on the streamlines.

According to **Fig. 6 (a)**, it is easy to see that the secondary curved detonation wave (SCDW) undergoes a curved shock (CS) and multiple compressional wave actions before combustion. These may affect the strength and shape, to further study, the difference between the two detonation waves, respectively, two streamlines are extracted as shown in **Fig. 6 (b)**. The detonation waves of streamline 1 undergoes the action of CS and compression waves, resulting in a non-uniform incoming flow of the detonation wave and a large increase in pressure. The CDW is straight because the incoming flow is uniform, and the pressure after the wave is lower than that of the SCDW. However, it is worth noting that the mass fraction of hydrogen increases in streamline 2 as the flow goes through the RS. This phenomenon implies that the chemical reaction proceeds in the reverse direction due to the pressure and temperature increase caused by the RS and the presence of water decomposition.

4. Theoretical study of the curvature effect on curved detonation reflection

The curvature will not only determine the stability of the Mach stem, but also significantly affects the flow parameters behind the wave. In the flow field of oblique detonation/shock waves, the post-wave parameters are essentially the same at different locations along the wave. However, in curved detonation/shock, the flow parameters are different at different locations on the wave. Therefore, it is necessary to study the effect of curvature on the post-wave parameters. For curved shock waves with constant specific heat, if the shape function of the curved shock wave can be expressed as a quadratic function:

$$y = ax^2 + bx + c \tag{9}$$

Therefore, the shock angle can be found using the slope:

$$\beta = arctan(y') \tag{10}$$

Where, the derivative of the wave angle concerning the coordinate x is related as follows:

$$\frac{\partial \beta}{\partial x} = \frac{y''}{1+(y')^2} \tag{11}$$

The geometric relationship leads to the expression for the curvature as:

$$S = \frac{y''}{1+((y')^2)^{1.5}} \tag{12}$$

Therefore,

$$\frac{\partial \beta}{\partial x} = S\sqrt{1+(y')^2} \tag{13}$$

According to the RH relationship, the derivative relationship between pressure and shock angle can be found:

$$\frac{\partial p_2}{\partial \beta} = 2p_1 \frac{2\gamma}{\gamma+1} M_1^2 sin\beta cos\beta \tag{14}$$

The derivative relationship between the pressure and the coordinate x can be found according to the formula for the derivative of the composite function:

$$\frac{\partial p_2}{\partial x} = \frac{\partial p_2}{\partial \beta}\frac{\partial \beta}{\partial x} = 4p_1 \frac{\gamma}{\gamma+1} M_1^2 sin\beta cos\beta S\sqrt{1+(y')^2} \tag{15}$$

For the detonation of variable specific heat, the shock of the RH relationship is to be rewritten as the detonation of variable specific heat relationship, the specific derivation have been overlooked, the results are as follows:

$$\frac{\partial p_2}{\partial \beta} = 2p_1\gamma_1 M_1^2 sin\beta cos\beta(1-X) - p_1\gamma_1 M_1^2 sin^2\beta \frac{\partial X}{\partial \beta} \tag{16}$$

In order to verify the accuracy and validity of the above calculations, the data of the flow field of the detonation reflection on the convex wall surface is selected for verification in this paper. As shown in the **Fig.7**, the streamline pressure can be obtained by extracting the pressure data from the numerical simulation results. It is not difficult to see through observation that the pressure shows regular changes on the curved wavefront.

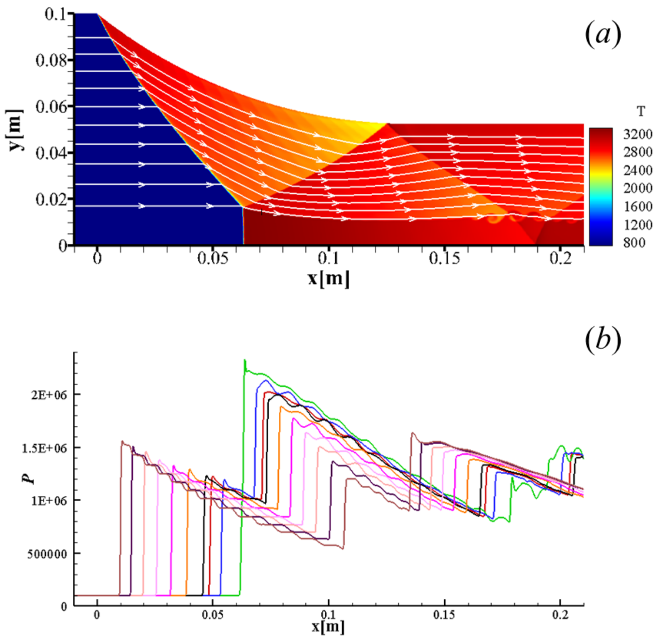

Fig 7. Curved detonation reflection flow field and parameters on streamlines: (a) temperature contour, (b) pressure on the streamlines.

In order to verify the correctness of the above theoretical calculation points, this paper plots the pressure and its gradient change curve obtained by numerical simulation together with the numerical simulation results in **Fig.8**. The black circular data points indicate the pressure on the streamline in the above **Fig.7**, the red curve is the change rule of pressure, and the blue curve is the change of pressure gradient. The negative value of the blue curve indicates that the pressure along the x-direction is gradually decreasing, which is also consistent with the law of numerical simulation, which is because the wave angle is gradually decreasing.

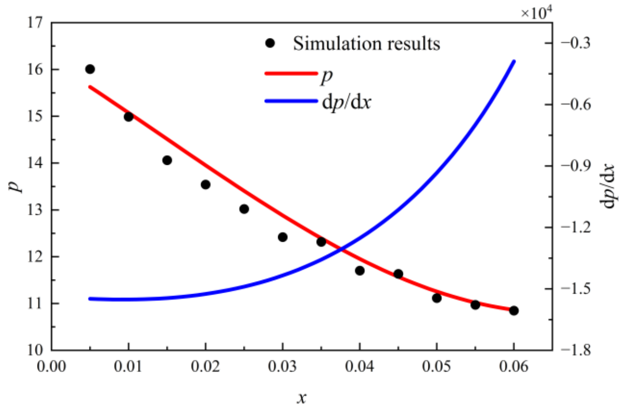

Fig 8. Comparison between theoretical and simulation results.

5. Conclusion

In this paper, the reflection of curved wall-induced detonation waves in combustion chambers is investigated, and numerical simulations are conducted mainly for the flow field structure, and aerodynamic parameter variations in curved detonation reflections. In terms of the overall structure of the flow field, the curvature leads to the appearance of expansion/compression waves, which in turn affects the post-detonation wave aerodynamic state or pre-wave flow conditions. In terms of specific aerodynamic parameters, the curvature can lead to significant changes in the aerodynamic parameters after the detonation wave, and in order to quantitatively express this effect, the relationship between the pressure gradient and the curvature of the detonation wave is derived from the theoretical analysis in this paper. The correctness of the theoretical derivation is verified by comparison with the numerical simulation results.

6. References

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