Critical Height for Rotating Detonation Wave Based on the Modified ZND Model

Li Deng, Minjie Wang
Institute of Chemical Materials
Mianyang, Sichuan, China
Hu Ma
Nanjing University of Science and Technology
Nanjing, Jiangsu, China

1 Introduction

Rotating detonation engines (RDEs) have received increased attention in recent years due to the higher thermal efficiency, compact design, and one-time ignition during the operation[1]. The characteristics of RDEs have been studied extensively both in experiments and numerical simulations, including the operation map, propagation velocity, operation modes, and so on[2,3]. Four possible modes are identified by the experiments, they are single-wave, homogenous multi-wave, heterogeneous multi-wave, and longitudinal pulsed detonation, respectively[4,5].

However, there are still many fundamental problems in RDEs requiring further investigations. A rotating detonation wave(RDW) propagating around the annular chamber suffers from the nonideal mixing of fuel and oxidizer, the lateral expansion of the shocked gas in reaction zone due to the weak confinement of bounding gas products, and the curvature caused by the different diameters of inner and outer bodies. With the combination of these effects mentioned above, a large deficit in the propagation velocity of RDW is observed, and the decoupling of RDW is also likely to occur under the worst scenario. Thus, the critial propagation of RDW results from these nonideal effects is the key to the design of RDEs.

Non-premixed simulation of the propagation of RDW using CFD is a feasible way to considering the three factors simutaneously. However, the time-consumption and expensive cost of CFD are unacceptable for a systematic research[6]. Thus, some reasonable simplifications are applied in the analysis of critical propagation of RDW. The attenuation of RDW caused by the different diameters of inner and outer wall is ignored, due to the relatively small width of combustor compared to the diamer of inner body. The non-ideal mixing of fuel and oxidizer leads to the less reactive reactants compared to the premixed mixures, and we just simply treat the non-ideal reactants as the less reactive mixtures under the poor equivalence ratio case. Thus, the remanent problem is the critical propagation of RDW under the weak confinement of bounding gas, and only the effect of lateral expansion on the propagation of RDW is considered here.

Correspondence to: dengli_njust@126.com

Considering the lateral expansion of the reaction zone, a modified ZND model[7] is applied in this paper to study the critical height and the corresponding velocity of RDW. The paper is arranged as follows, the details of modified ZND model and the parameters correlating the lateral expansion are provided in section 2. The effects of H2/O2 reaction mechanism is studied based on the comparison of ignition delay time obtained by model prediction with experimental data, and the critical height under differet initial conditions are explored in section 3. Moreover, the differences between the computed cell widths and experimental data are compared, and the characteristic cell widths are selected to nondimensionalize the critical height of RDW.

2 Theoretical basis and solution procedures

Rotating detonation wave is bounded by the hot products, which exert little constraint on the shocked gas in the reaction zone, and a serious lateral expansion occurs in this region. In order to show the effect of lateral expansion on the propagation of RDW, a modified ZND model is applied, and the details are as follows

$$\begin{aligned}
\frac{\mathrm{d}\rho}{\mathrm{d}x} &= -\frac{\rho}{w}\frac{\left(\dot{\sigma}-wM^2\alpha\right)}{\eta} \\
\frac{\mathrm{d}w}{\mathrm{d}x} &= \frac{\left(\dot{\sigma}-w\alpha\right)}{\eta} \\
\frac{\mathrm{d}p}{\mathrm{d}x} &= -\rho w\frac{\left(\dot{\sigma}-w\alpha\right)}{\eta} \\
\frac{\mathrm{d}Y_i}{\mathrm{d}x} &= \frac{\dot{\omega}_i}{w} \\
\frac{dx}{dt} &= w \\
\dot{\sigma} &= \sum_{i=1}^{N}\left(\frac{W}{W_i}-\frac{h_i}{c_pT}\right)\frac{\mathrm{d}Y_i}{\mathrm{d}t}
\end{aligned} \tag{1}$$

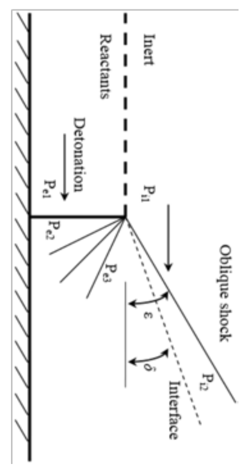

Figure 1. Sketch of the lateral expansion

where ρ is the density of gas particle, w is the local velocity in the moving shock reference, p and x are the local pressure and the distance from the shock front, respectively. Y_i represents the mass fraction of specie i, $\dot{\sigma}$ is the thermocity, and η is the Mach parameters, which is $1\text{-}M^2$. The derivation of the modified ZND model refers to Ref.[7]. The term "α" contains the information of the area expansion in the reaction zone, which is calculated as

$$\alpha = \frac{1}{A}\frac{dA}{dx} = 1 + \frac{\tan\delta}{h} \tag{2}$$

where A represents the cross-area of the reaction zone, in two dimension, the cross-area A degenerates into the detonation height of h. A sketch of the lateral expansion of detonation products is shown in Figure 1. The term "δ" is the lateral expansion angle, which can be solved by the Prantl-Meyer theory[8] based on the following assumptions:

(1) The frontal shock surface is planar.
(2) Every streamline flowing through the detonation front experiences a same lateral expansion angle.
(3) The velocity of detonation is close to the CJ value, and the reaction zone ends with a sonic plane.

The angle δ is obtained by the solution of shock expansion theory, which may needs several iterations. The solution procedure is arranged as follows.

(1) Given the initial parameters: p_{i1}, p_{e1}, T_{e1}, γ_{e1}, γ_{i1};
(2) Obtaining the CJ speed D , CJ pressure p_{e2}, and Mach number M_{i1} by the SDToolBox[7];
(3) Assuming an initial guess of angle of oblique shock wave ε_{guess}, and the angle of lateral expansion δ_{guess} can be calculated by formula (3);
(4) The pressure ratio p_{i2}/p_{i1} of the oblique shock wave is calculated by formula (5);
(5) The pressure ratio p_{e2}/p_{e3} after the expansion of products is obtained through formula (7);
(6) The Mach number M_{e3} after the expansion can be obtained according to formula (6), M_{e2} =1 (CJ state);
(7) Calculating the flow angle $\delta_{correct}$ by formula (4), and compared to the δ_{guess}, if the absolute difference $|\delta_{correct} - \delta_{guess}| < \Delta\delta$, then the correct angle of lateral expansion δ is obtained; Otherwise, using the scant method to get a new δ_{guess}, and return to step (3), until the $|\delta_{correct} - \delta_{guess}| < \Delta\delta$ is satisfied.

$$\tan\delta = 2\cot\varepsilon\left[\frac{M_{i1}^2\sin^2\varepsilon - 1}{M_{i1}^2\left(\gamma_i + \cos 2\varepsilon\right) + 2}\right] \tag{3}$$

$$\delta = \nu\left(M_{e3}\right) - \nu\left(M_{e2}\right) \tag{4}$$

$$\frac{p_{i2}}{p_{i1}} = 1 + \frac{2\gamma_i}{\gamma_i + 1}\left(M_{i1}^2\sin^2\varepsilon - 1\right) \tag{5}$$

$$\frac{p_{e2}}{p_{e3}} = \left[\frac{1 + \left[\left(\gamma_{e2} - 1\right)/2\right]M_{e3}^2}{1 + \left[\left(\gamma_{e2} - 1\right)/2\right]M_{e2}^2}\right]^{\gamma_{e2}/\left(\gamma_{e2} - 1\right)} \tag{6}$$

$$\frac{p_{i2}}{p_{i1}} = \frac{p_{e3}}{p_{e2}}\frac{p_{e2}}{p_{e1}}\frac{p_{e1}}{p_{i1}} \tag{7}$$

$$\nu\left(M\right) = \sqrt{\frac{\gamma + 1}{\gamma - 1}}\tan^{-1}\sqrt{\frac{\gamma - 1}{\gamma + 1}\left(M^2 - 1\right)} - \tan^{-1}\sqrt{M^2 - 1} \tag{8}$$

The modified ZND model is solved by the SDToolbox[7] with a slight modification, and the reaction mechanisms proposed by Li[9], Mével[10] and Burke[11]are used. The ordinary differential equations shown in (1) is boundary value problem, where the start is the condition at von Neumann point, the end point is the vanishing of both η and $\dot{\sigma}$. The standard shooting method is applied to solve the eigenvalue detonation, where the prescribed tolerance of the detonation velocity is 0.3 m/s.

The solution procedure is as follows: given a lateral expansion angle δ from (3-7), a relatively large detonation height h is substituted into formula (2), thus, an eigenvalue detonation velocity is obtained through the integration of (1). Decreasing the detonation height to a smaller value h_s to obtain a another eigenvalue velocity corresponding to h_s. Repeating this process until the condition that no eigenvalue velocity is obtained under a special height h_c, and this value h_c is the critial height of the detonaiton wave under the given initial conditions. It should be mentioned that the reactants used in the calculation throughout the paper are the stoichiometric H_2/Air mixtures at 1.0 bar and 293 K, where the bounding gas is the detonation products which expanded isentropically from the CJ state to the pressure of 1.0 bar.

3 Results and discussion

Figure 2 shows the effects of reaction mechanisms on the critical height under the lateral expansion. The ignition delay time (IDT) predicted by those mechanisms are compared to the experimental data firstly, the IDT is chosed as the time when the concentration of OH reaches its peak. It is seen that all the reaction mechanisms used in this paper have the ability to predict the ignition delay time of H_2/Air mixtures, and the IDTs predicted by the model of Mevel and Burke alomost coincide with each other.

The predicted critical heights are shown in the right part in Figure 2. It shows that the detonation velocity increases with the height, and approaches to the eigenvalue of 1974.9 m/s at sufficient large height. It is readily to find from formula (2) that a raise in height leads to a decrease of the area expansion in the reaction zone. Thus, increasing the detonation height by raising the mass flow rate reduces the velocity deficit of the RDW, and this is well proved by the experiments[12]. However, the critical heights varys with reaction mechanisms. The critical height from the Burke model is 0.0175 m, which is little bigger than those from the model of Li and Mevel. It seems that the results predicted by Mevel model and Li model are same, but the predicted IDTs show a different trend. It is obviously that the predicted critical height is closely related to the reaction mechanism we used, fortunately, the differences among these results are small. Thus, those three models are all used for comparison throughout the paper.

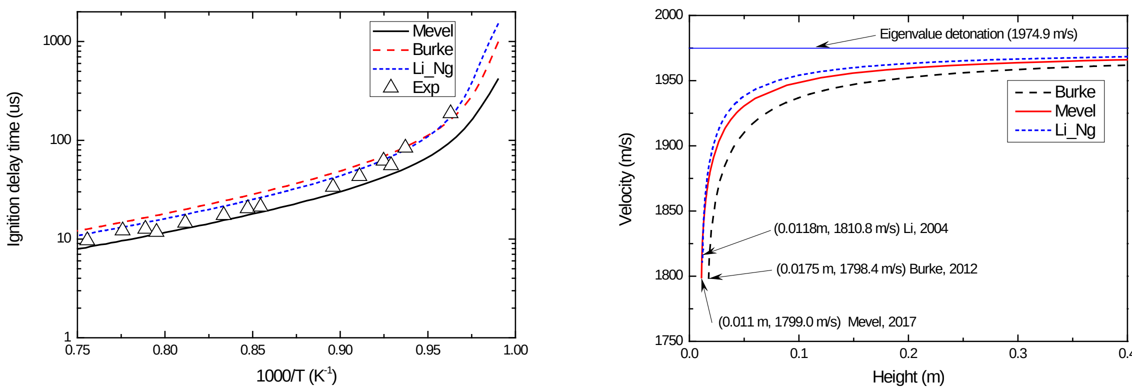

Figure 2. Effects of reaction mechanisms. Left: comparison of IDT predicted by the models with experimental data. Right: critical height under lateral expansion predicted by the different models

Figure 3 shows the comparison of predicted cell widths using the Ng correlation[13] with the experimental data from the detonation database[14] at different initial conditions. It shows that the computed cell widths exhibit a opposite trend compared to the experimental data with the increasing of initial temperature, while the predicted cell widths shows a similar trend with the experimental data at different initial pressures and equivalence ratios. Moreover, the predicted cell widths from the Burke model and Li model are almost the same except the initial pressures, which indicates that the key parameters in Ng correlation, namely the induction zone length and non-dimensinal stability paramter from those two models are similar.

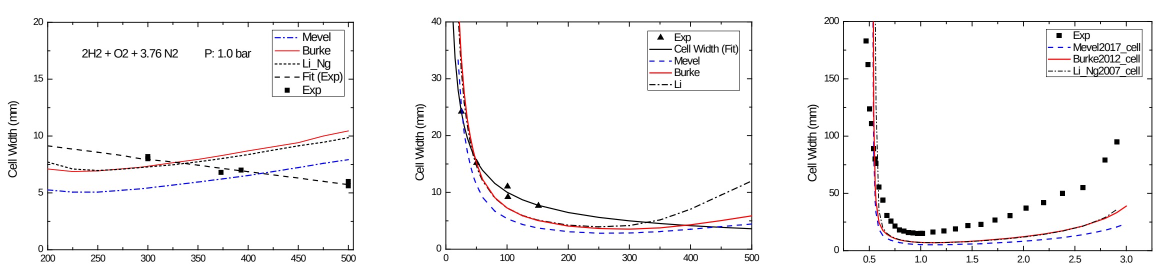

Figure 3. Comparison of computed cell widths using Ng correlation with experimental data. Left: initial temperature, Midium: initial pressure. Right: equivalence ratio.

Figure 4 shows the minimum detonation height and velocity varying with the initial temperatures ranging from 200 K to 500 K. The critical height and velocity behave a reverse trend comparing with the temperature in the left part of Figure 4. The differences between the critical velocities is small, but the differences between the critical heights of Li model and Burke model are relatively large. An interesting phenomenon is that the minimum height and velocity at 500 K are around 0.007 m and 1625.0 m/s, respectively. This may describe the steady propagation of RDW in the low mass flow rate in experiment, as shown in Ref.[12], a recirculation zone exists at the combustion zone, the initial temperature of reactants before the RDW increases at some extent. The right part of Figure 4 shows the ratios of critical height over the predicted and experimental cell widths, respectively, where the calculation cell width is based on the Ng correlations. Both of the ratios decrease with the increasing of initial temperature, and the detonation wave is prone to propagate at high initial temperature.

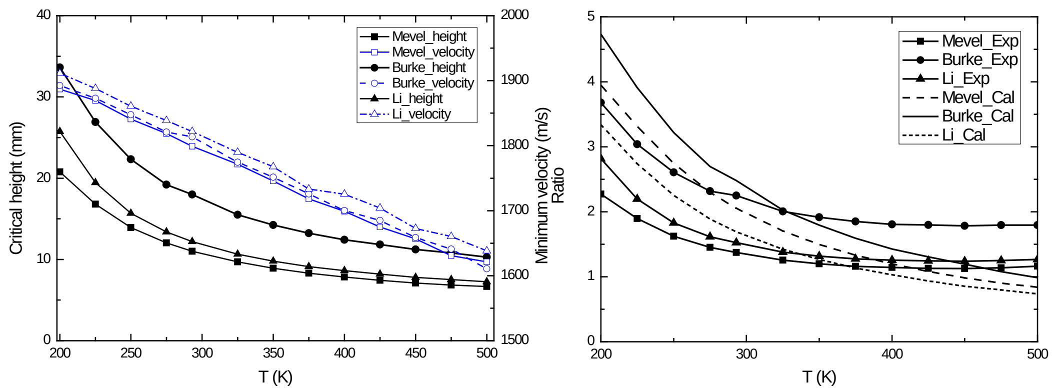

Figure 4. Critical velocity and height varying with the initial temperature. Left: critical height and velocity. Right: ratio of height to predicted cell size and experimental data.

Figure 5 shows the minimum detonation height and velocity varying with the initial pressure ranging from 0.6 bar to 2.0 bar. It is seen in the left part of Figure 5 that the critical height decreases rapidly at from 0.6 bar to 2.0 bar, and then varies slowly with the increasing of the initial pressure. The minimum propagation velocity also exhibits a rapid increase in the initial stage. Different trends of the ratios are observed in the right part of Figure 5, the ratios of height over experimental cell widths increase with the increasing of initial pressure, while the ratio of height over predicted cell widths increases first and then decreases slightly with the raising of pressure. The differences between the trend of ratios may arise in the differences between the predicted cell widths and the experimental data, which is shown in the middle part of Figure 3. It is obvious that all the ratios are smaller than 4.

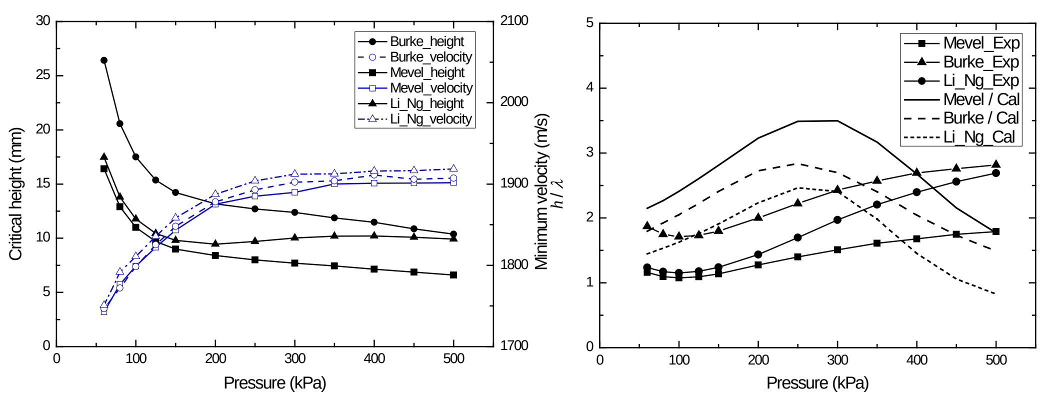

Figure 5. Critical velocity and height varying with the initial pressure. Left: critical height and velocity. Right: ratio of height to predicted cell size and experimental data.

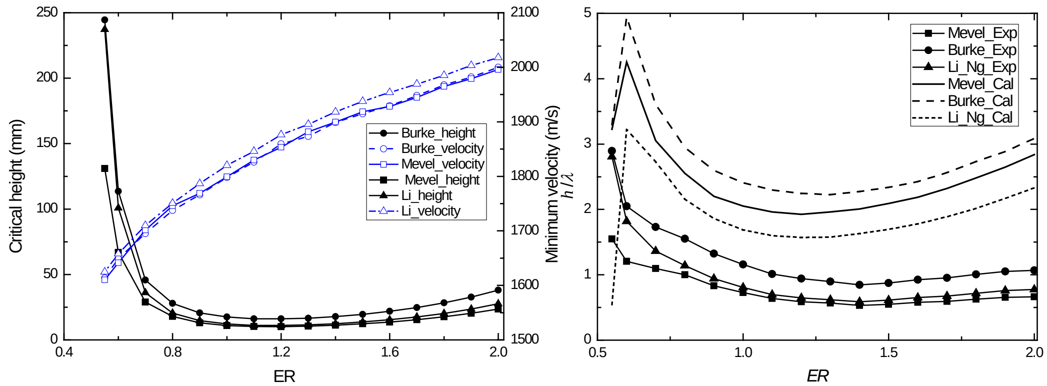

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Figure 6. Critical velocity and height varying with the equivalence ratio. Left: critical height and velocity. Right: ratio of height to predicted cell size and experimental data.

Figure 6 represents the critical velocity and the detonation height changing with the equivalence ratios. As the equivalence ratio increases from 0.55 to 2.0, the critical height of RDW decreases sharply from a large value (Mevel:0.131 m, Burke/Li: 0.244 m) to the minimal value of 0.011 m, then increases slightly to around 0.03 m at *ER* of 2.0. Thus, it speculates that the RDW is more likely to propagate stably at fuel-rich conditions. The right part of Figure 6 represents the ratios of height to predicted and experimental cell widths. The ratio of height over predicted cell width decreases from the 3.0 to around 1.0 as the equivalence ratio increases from 0.55 to 2.0, while the ratio of height over the calculated cell size ranges from 2.0 to 5.0 among the investigated equivalence ratios.

It is generally recognized that the ratio of critical height (h) over the the cell width(λ) should be a constant value in the yieding detonation tube with premixed reactants[15], namely, various initial temperatures, initial pressures and equivalence ratios. However, the results shown in Figure 4-6 violate the general recognition. The inaccurate calculations of cell size or the imperfection of the modified ZND model in descripting the RDW are the causes of the discrepancies. Whether the critical ratio h/λ changes with the operation condition in experiment requires further investigations. It can be seen in Figure 4-6 that the h/λ using the predicted cell widths in those conditions varies from 1.0 to 5.0 regardless of the reaction mechanisms, where the ratios of citical height over the experimental data varies from 1.0 to 3.0. It shows that the ratios of upper boundary based on the experimental data is similar to the experimental results of 3.0 by Murry[15]. The emperical relation of h/λ suggested by Bykovskii is around 12±5[16], however, the estimation of λ is based on the averaged combustor pressure, which is much larger than the pressure of the fresh reactants. Moreover, the results obtained by Bykovskii is under the non-premixed condition, the real cell width is much larger than the premixed one, thus, a value h/λ of around 12±5 is suggested by Bykovskii based on the extensive experiments.

Actually, from the published experimental data, it shows that a rotating detonation wave has a ability to propagate in a relatively low height of fresh reactants. Anand shows that the height over the predicted cell width near the operational lean conditions is less than one[3], which is much less than the value of 12. Here, we invoke a result from our previous study[12] to verify the calculated results. A steady RDW was observed in the combustor with inner and outer diameter of 70/80 mm using the H_2/Air mixture under the mass flow rate around 77 g/s. Considering the mass flow rate supplied by the feeding systems equals to the consumed reactants by detonation per-second, the following equation is applied.

$$\dot{m}_{feeding} = \rho u_{av} S \tag{9}$$

Where ρ, u_{av} represent the average density and injection velocity of the reactants in the combustor, respectively. S is the cross-area of the annular combustor, here, is 1178 mm^2. Considering the density is around the ambient density of air (1.259×10^{-3} g/cm^3), subsitute the density and cross-area to equation (9), and we get the value of u_{av} is around 51m/s. The operation frequency under this condition is around 6000 Hz, which results in a maximum injection time of reactants per-cycle is 1.67×10^{-4} s. Thus, the estimated detonatin height is

$$h = u_{av} \cdot \Delta t = 51 \times 1.67 \times 10^{-4} = 0.0085\text{m} = 8.5\text{mm} \quad (10)$$

As seen in (10), the detonation height is around 8.5 mm, which is less than the averaged cell width of H_2/Air mixtures. Thus, the experimental result indicates that a RDW may also propagate at relatively lower detonation height, which is around the cell width.

It can be seen from the Figure 4-6 that the ratio of critical height over cell width at different conditions is around 3±2 regardless of the reaction mechanisms used in the calculation. And the predicted ratio is similar to the results of Murry and the recent experimental results of RDE. Thus, the ratio of h/λ is suitable in the determination of the critical condition, and the safety margin is better to set as 5.0.

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