Numerical Study of Detonation Structure in a Channel with Porous Wall

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1 Abstract

To study the propagation of gaseous detonations in a channel with porous wall, 2-D Euler equations with a single step Arrhenius kinetics model are integrated in the present study. Different mixtures with both high and low activation energy, characterized by their irregular and regular detonation structure, are studied. It is found that the failure mechanisms of a detonation wave, propagating in a porous channel, are attenuation of transverse wave and mass divergence into the permeable wall. However, mass divergence has major role in detonation failure. The present results reveal that, as activation energy increases, higher number of transverse waves in the channel width are required to re-generate new triple points, in order to overcome the effect of mass divergence into the porous wall and support the self-sustenance propagation of detonation waves. The results also depict that close to the porous wall the front curvature increases. If the curvature extends to all the channel width, the wave fails to propagate. In contrast to the previous observations, this effect is seen for both regular and irregular structures. For unstable detonations, the critical limit, d/λ, is found to be higher than that of stable detonations, while previous experimental investigations reported that in high activation energy mixtures the critical limit is lower. It is suggested that this significant discrepancy manifests the effect of turbulent mixing in controlling the reaction rate in highly unstable detonations, which is not considered in the present simulation due to low grid resolution.

2 Introduction

Experiments in reactive mixtures reveal that detonation fronts exhibit complicated three-dimensional time-dependent cellular structure consist of an ensemble of interacting triple points, turbulent shear layers and strong transverse shocks [1]. There is strong evidence that the shock compression cannot ignite all the gases that pass through the shock front and hydrodynamic instabilities play significant role in detonation propagation in high activation energy mixtures [2-3]. It has also been postulated that more insight on the detonation propagation mechanism is achieved by studying the response of the detonation wave to external perturbations near the failure or initiation limits [4-5]. Porous walls may be used as the external perturbation for studying the structure of detonation waves. The exact failure mechanism of detonation waves propagating in porous channels is not well recognized. Dupre et al. [4] and Vasilev et al. [6] showed that porous wall causes the attenuation of transverse shocks and consequently the failure of the detonation. Guo et al. [7] in an experimental study, showed that

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increasing the porosity of the porous wall increases the transverse shocks attenuation. Radulescu and Lee [5] used the porous wall to further elucidate the effect of porous wall on the detonation structure. They found that the transverse waves do not play essential role in the propagation of detonation in mixtures diluted with argon, which is characterized by regular cellular structure. The mass divergence of gas into the porous wall was suggested as the failure mechanism for such mixtures. They also proposed the attenuation of transverse waves as the failure mechanism for mixtures with irregular structure. Therefore, the transverse waves have significant role in the propagation of detonation in these mixtures. They also found that a channel width smaller than a critical value causes the failure of detonation in medium with porous wall. The critical channel width for detonations with irregular structure was about $d/\lambda \approx 4$, where d is the channel width and λ is the characteristic cell size. However, for regular cellular structure there was not a unique failure limit. For highly argon diluted acetylene-oxygen mixtures, the limit was about $d/\lambda \approx 11$ and for H_2-O_2 mixture, the critical limit was found to be $d/\lambda \approx 6$-8. Pintgen et al. [8] attempted to find the role of transverse waves in structure of detonation in different Fuel-O_2 mixtures. They concluded that the detonations in mixtures diluted by argon and nitrogen the transverse waves do not have essential role in propagation of detonation in these mixtures. Unfortunately, very little numerical modeling of the propagation of detonation waves in channels with porous walls has been reported. The most prominent one is done by Reddy et al. [9] who used a relatively low grid resolution. They showed qualitatively the attenuation of detonation in channels with porous walls. Using the same numerical model as Reddy et al., the present work aims to study the problem of the propagation and failure of detonation waves in a channel with porous wall.

3 Problem description and governing equations

For simulating the flow inside the porous wall it is assumed that a large number of thin circular capillary tubes are inserted on the channel walls. The tubes are open in one side that is in contact with the channel flow, while the other side is sealed. Therefore, the entire flow can be treated as two-stream fluid flow, with the main reactive flow inside the channel and the capillary flow in the tubes. The governing equations for flow inside the porous tube are given in [9-10]. The two-dimensional reactive Euler equations with a single step Arrhenius kinetics model and the assumption of perfect gas are integrated to simulate the structure of gaseous detonation. A simple version of the "Adaptive Mesh Refinement" of Berger and Colella [11] is utilized to use fine meshes in the region close to the shock. The details of the governing equations and nondimensionalizing were discussed in depth in [12]. The characteristic length scale is the length traveled by a fluid particle from the leading shock to position where β=0.5 in a ZND structure, the so-called half-reaction length (hrl). This length scale calculated for a mixture with $Q/RT_0=50$, $E_a/RT_0=25$, and $\gamma=1.2$.

4 Attenuation of detonation in low activation energy mixtures

To demonstrate the effect of porous wall on the detonation structure in low activation energy mixtures, a porous wall with the porosity of Dc=0.0001 is inserted at the lower boundary of a channel from x=300 to the end, where the detonation structure is not affected by the initial disturbances. The activation energy of the mixture is considered to be $E_a/RT_0=15$. The maximum pressure history in the channel is shown in Fig. 1. This figure shows very regular cellular structure of the detonation in such mixture before the porous section. Figure 1a is produced for the detonation propagation in a channel with W (channel width)=10. This figure shows significant difference between the cellular structure in the porous section and in the solid wall section. The cells are regular in solid wall section, but irregular structure with the enlarged cells are clearly visible in porous section. Increasing the cell width at the porous section is an indication of the lower chemical reaction in the porous section. In addition the detonation does not fail in the porous wall for channel with W=10. Qualitatively these results are in agreement with the results reported by Radulescu [5] and Guo et al. [7]. As the detonation enters the porous wall section, the weakening of the transverse waves and triple points upon reflection on the porous wall are evident. This effect is found by tracing the light lines which represent the track of the triple points. At x=320, tracing the light lines shows that after the collision of the triples point with the porous wall the light lines are disappeared. The strong transverse shocks move towards the porous wall, and the weak transverse shock traveling toward the solid wall. These strong and weak shocks get reflected from the porous and solid walls respectively as a weak and strong transverse waves, respectively. These two reflected shocks that are moving toward the center of the channel collide with each other and generate new triple points. This will be explained further by comparing the maximum pressure at two cross section of the channel at the vicinity of the porous wall and upper solid wall. Figure 1b shows the effect of the porous wall on the detonation structure in a channel with W=5, where only one cell exists in channel width before the porous wall section. As the detonation enters the porous section, there is a competition between the triple point weakening at the porous wall and the re-amplification of the triple point at the detonation structure. Re-amplification occurs close to the lower porous wall and far from the upper solid wall. The interaction of the weakened transverse waves and the strong transverse waves, reflected from the solid upper wall, causes the re-amplification of the triple points.

(a) W=10

(b) W=5

(c) W=3

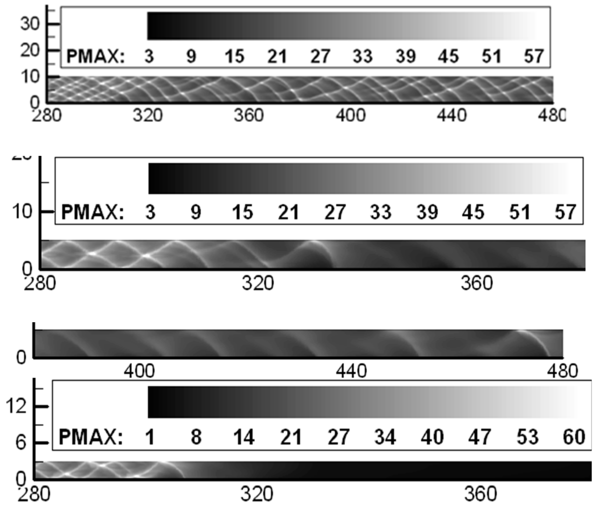
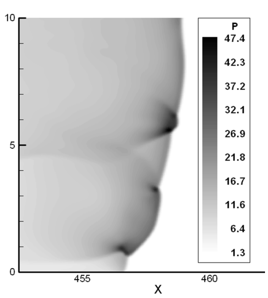
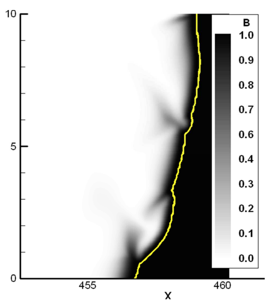


Figure 1. Cellular structure in the channel for E_a/RT_0=15. Porous wall is inserted from x= 300 to the end.

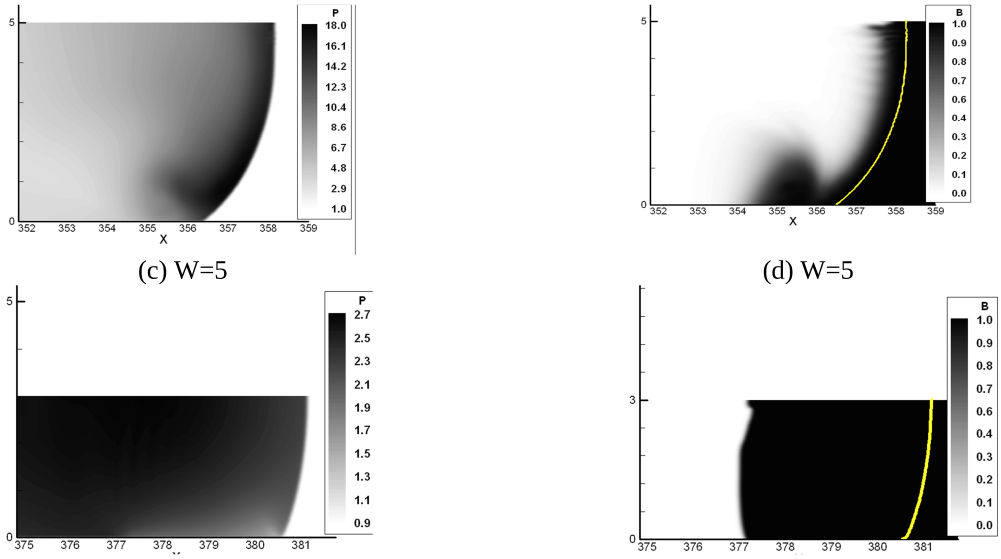
Thus, as the channel width decreases from W=10 to W=5, the detonation fails to propagate in W=5.Hence, W=5 may be considered as a critical channel width for propagation of detonation in a channel with porous wall at lower boundary. Therefore, to prevent the detonation from failure, more than two transverse waves should be formed in channel width. In other word, the critical channel width limit is at least d/λ≈2 for the mixture with E_a/RT_0=15. Figure 1c illustrates that the detonation completely fails in porous section in the channel with W=3. To further clarify the effect of the porous wall on the structure of the detonation, the contours of reaction progress variable and pressure are shown in Fig. 2 for mixture with E_a/RT_0=15 and for different channel width. Figures 2a to 2f show that as the channel width decreases the curvature in the detonation front at the vicinity of the porous wall increases and extends over the whole channel width.



(a) W=10



(b) W=10



(c) W=5 (d) W=5

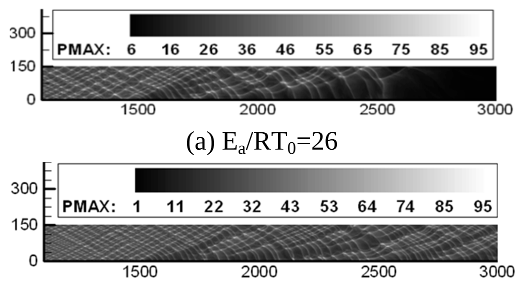
(e) W=3 (f) W=3

Figure 2. The reaction progress and presuure countors in mixture with E_a/RT_0=15 in porous section of the channel with different channel width. Solid lines marks the position of the shock front

Although the transverse waves weakened upon reflection from the porous wall, the shock front is still strong enough to sustain the detonation propagation in channel with W=10. As the channel width reduces to W=5, the curvature caused by the porous wall affects the whole detonation structure and results in the global wave curvature, Figs. 2c and 2d. The pressure contour shows that the pressure of the shock front is about 18 for W=5, which is much lower than the pressure in channel with W=10 (p≈47). Therefore, at W=5 the shock front is not strong enough to compress the gas and prevent the detonation attenuation. Comparison of Figs. 2b with 2d shows that the reaction zone length in channel with W=5 is larger than that in the wider channel. By decreasing the channel width to W=3 (Figs. 2e and 2f) the reaction zone is decoupled from the detonation front and the detonation fails.

5 Attenuation of detonation in high activation energy mixtures

Increasing the activation energy of the mixture, increases the irregularity of the detonation structure and causes more instability in the detonation front. Figures 3a and 3b show the cellular structure of detonation that produced by numerical sooted foil for two mixtures with activation energies E_a/RT_0=26 and E_a/RT_0=24 in a channel with W=150. The porous wall inserted from x=1500 to the end of the channel on lower boundary. The figures reveal that the cellular structure is more irregular in the porous section than that in the solid wall section. The cells are enlarged and the transverse waves and triple points are weakened after the reflection upon the porous wall.



(a) E_a/RT_0=26

(b) E_a/RT_0=24

Figure 3. Detonation attenuation in a channel with W=150. porous wall inserted from x=1500 to the end

It is clear that the detonation fails to propagate in porous wall section for E_a/RT_0=26. Figure 3a also shows that before entering the porous section the front involves about 7 cells in channel width. Therefore, considering that the simulation is carried out for half width of the channel (due to symmetry), it can be concluded that for preventing the failure in this case, more than 14 cells in channel width are needed. In other word, if porous wall is inserted on both upper and lower boundary the critical channel width limit is $d/\lambda \approx 7$ for the mixture with E_a/RT_0=26. Comparing the critical channel width for the mixture with E_a/RT_0= 15 ($d/\lambda \approx 2$), with the mixture with activation energy 26, Fig. 3, reveals that mixtures with high activation energy need much more transverse wave (across the channel) to support a self-sustained detonation in a channel with porous wall. This is an indication of the essential role of the transverse waves in detonation propagation in high activation energy mixtures.To study the effect of porous wall on the detonation structure in high activation energy mixtures, the structure in three different axial positions of shock front are shown in Figs. 4a to 4f. Figures 4a and 4b show the contours of reaction progress variable and pressure before the failure. Maximum pressure is about 89 around the triple point at the vicinity of the solid upper wall. It is clear that the global curvature of the detonation covers almost the whole channel width from Y=0 to Y=120, and the region close to the upper wall is not affected by the wave curvature, (Y=120 to Y=150).

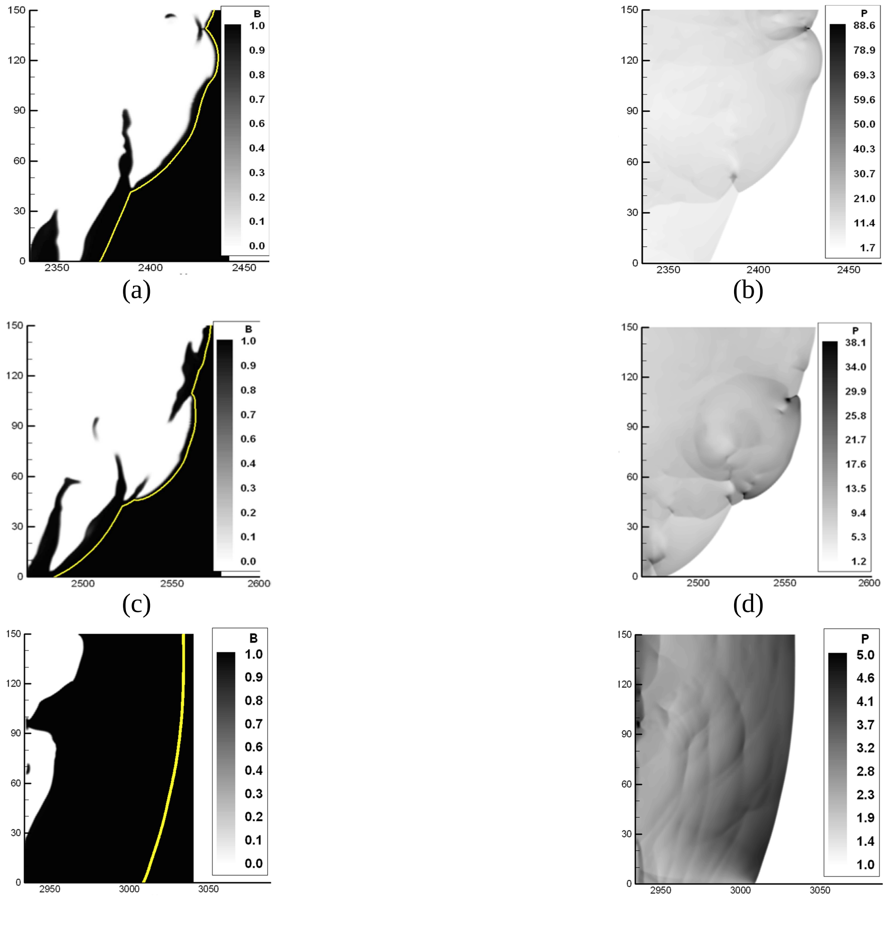


Figure 4. Shock front in three different position for channel with W=150 for mixture with E_a/RT_0=26, Left and right figures show reaction progress variable and pressure, respectively.

Therefore the influence of porous wall on the detonation wave does not affect the front wave at the vicinity of the upper wall and the detonation does not fail at this position. However, Fig. 4a shows that the reaction zone length increases at the vicinity of the porous wall. As the detonation travels, the wave curvature covers the whole channel width, Figs. 4c and 4d. Figure 4d shows that although the detonation does not fail in this position, but the maximum pressure of the shock is decreased to about 40 around the triple point. Eventually, as the detonation propagates more in the porous wall region (Figs. 4e and 4f), the transverse waves are eliminated, the reaction zone is decoupled from the shock front, and the detonation is quenched. The maximum pressure in this position is about 5. Present results reveal that, for the mixture with $E_a/RT_0=26$**,** the local wave curvature close to porous wall section is extended to the whole channel width before the complete failure of the front. Qualitatively, the present results are in agreement with the experimental results of Guo et al. [7].

6 Conclusion

In the present work, a two-dimensional numerical simulation of the structure of gaseous detonations propagating in a channel with porous wall has been performed. It is observed that the detonation failure in a porous channel is mostly due to the wave curvature, rather than the attenuation of transverse waves. The extension of local wave curvature close to the porous wall to the whole channel width causes the attenuation and failure of detonation in both low and high activation energy mixtures. Previous experimental observation reported that the effect of mass divergence (wave curvature) is the mechanism of failure only for regular structure detonations. In experiment, it was also found that for unstable detonations the critical limit is lower than that in stable detonations. The significant discrepancy between the experiments and the present numerical simulation manifests the important role of hydrodynamic instabilities and turbulent mixing which should be considered in future numerical investigation of detonations in high activation energy mixtures.

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