Diffusion in Gaseous Detonations

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1 Abstracts

To clarify the role of diffusion on detonation structure a two-dimensional numerical simulation is performed by solving the Navier-Stokes equations and considering the single step Arrhenius kinetic as reaction model. The effect of diffusion on the generation of vortices produced by hydrodynamic instabilities (RM and KH instabilities) is investigated in this study. All the computations are performed with resolution of 300 cells per hrl. Mixtures with both low and high activation energies, characterized by their regular and irregular detonation structures, are considered. Results provided by very high resolution reveal that the structure obtained for irregular structure by solving the Euler equations differ from that obtained by solving the Navier-Stokes equations. However, in lowresolution simulations, the irregular structure obtained by solving both the Euler and Navier-Stokes equations are very the same. The major effect of diffusion occurs at shear layers and unburned pockets boundaries. Diffusion suppresses the small-scale vortices produced by KH instabilities and decreases the mixing rate of hot and cold gases at shear layers. However, behind the shock front where less concentration of small scale vortices exist, the diffusion of heat and mass from neighboring hot regions of burned material to the un-reacted gases increases the burning rate of the un-reacted pockets. In addition, the solution of Navier-Stokes equations shows that, the diffusion increases the strength of the shock front while decreases the strength of the transverse waves. Due to the absence of hydrodynamic instabilities and un-reacted gas pockets behind the main front of regular structure detonations, the results obtained by solving the Euler equations and Navier-Stokes equations are similar for detonations with regular structure even in high resolution simulations.

2 Introduction

The detonation shock front consists of Mach stem and incident wave. The detonation structure is also contains transverse shocks that moves laterally behind the front. Triple points are formed at the intersection of detonation leading shocks and transverse waves. The trajectory of a triple point on smoked foil is called cellular structure[1]. Based on the cellular structure regularity, detonation waves are classified as regular and irregular structure detonations. Numerical [2] and experimental [3] observations, indicate the existence of two different types of detonation structure. Smoked foil patterns of mixtures with high activation energy display a very irregular structure of interacting pressure waves at the detonation front, while regular structures are observed in low activation energy mixtures[4]. Schlieren visualizations of the reaction zone structures in regular structure detonations indicates smooth front with very little evidence of turbulence. On the other hand, in highly unstable detonations rough front with irregular spacing of transverse wave is observed and the shear layer in such

detonation is Kelvin-Helmholtz (KH) unstable [5]. The possible role of diffusion in detonation waves has been previously addressed in several investigations. Gamezo et al. [6], using 2-D Euler equations, estimated the importance of diffusion in consuming un-reacted gas pockets some distance downstream of the lead shock. Arienti and Shepherd [7], using detailed chemical kinetics and a simplified mixing rule in a one-dimensional model, showed that the effect of diffusion at shear layer in the decaying portion of the cell cycle depends on the mixture activation energy. Diffusion was negligible for modest activation energy mixtures, while decreased the induction time in high activation energy mixtures. Lindstrom [8] observed that at low gird resolution (about 3 cells per hrl) the solutions of Euler and Navier-Stokes equations were similar. However, as the resolution increased (22 cells per hrl), due to low numerical diffusion, unphysical structures appeared in numerical solution of Euler equations. Singh et al. [9], using two-dimensional simulation of Euler equations, pointed out that physical diffusion is important in high-resolution simulations (24 points per half reaction length), where the numerical diffusion is low. Previous research did not elaborate the effect of diffusion on the growth of hydrodynamic instabilities inside the structure. Besides, the role of diffusion in consumption of unreacted gas pockets is an important issue that has not been addressed yet. The present investigation focuses on the role of diffusion on the appearance of vortices associated with hydrodynamic instabilities, with the aim of exploring the mechanism of consumption of unburned gas pockets, both in low and high activation energy mixtures. Moreover, the role of transport phenomena on the propagation mechanism of gaseous detonation with both regular and irregular structures is addressed in the present study.

3 Governing equations and numerical issues

The two-dimensional reactive Navier-Stokes equations with a single step Arrhenius kinetics model with 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 [10] is utilized to use fine meshes in the region close to the shock. The details of the governing equations, non-dimensionalizing, and the numerical methods were discussed in depth in [11]. The half reaction length (hrl) of the steady structure of ZND detonation is considered as the length scale in all computations reported in this study. The thermo-physical properties of the mixtures are chosen as follows:non-dimensional activation energies $E_a/RT_0=20$ and $E_a/RT_0=10$, for high and low activation energy mixtures respectively, the dimensionless heat release $Q/RT_0=50$, and $\gamma=1.2$. The kinematic viscosity is 1.59×10^{-5} (m²s⁻¹) and the conductivity coefficient set to 3.179×10^{-2} (w m⁻¹K⁻¹). The detonation runs from left to right in the positive *x*-direction in a two-dimensional channel. Since the fluid ahead of the detonation is in its quiescent state, the right-hand boundary condition is irrelevant. The boundary conditions imposed on the lower and the upper sides of the channel are reflecting or free-slip solid wall boundary conditions. To reduce the computational time a non-reflecting boundary condition is imposed on the left side of the domain. A scalable parallel code is developed to carry out the heavy two-dimensional computations.

4 Detonation with irregular structure

To demonstrate the effect of diffusion and hydrodynamic instabilities in turbulent mixing behind the front, the computations are performed for very high resolution of 300 points per hrl and $E_a/RT_0=20$ The computational domain is considered such that half a cell (one mode) is formed in the channel width. All results are obtained after a very long time, when the structure of detonation becomes independent of the initial perturbation. Figures 1 and 2 illustrate the detonation structure where a primary triple point moves upward. Figure 1a represents the density contour corresponds to the solution of Euler equations for resolution 300 cells per hrl. The existence of secondary triple points and vortical structure, which give rise to the appearance of irregular structure, are observed in this figure. The details of the structure are reported by Mahmoudi and Mazaheri [2]. A is a primary and Band C are secondary triple points. A jet flow, which is produced by the mechanism of RM instability, is clearly

detected at lower boundary. Figure 1b shows the structure of detonation for the same mixture and grid resolution which is provided by solving the Navier-Stokes equations. It is seen that the results obtained by solving the Euler and the Navier-Stokes equations are qualitatively similar. However, some smallscale vortices along the shear layer which are produced by KH instability are suppressed in Fig. 1b (Region surrounded by black line in Fig. 1a. In addition, the compression waves that are produced due to the ignition of un-reacted gas inside the jet flow are disappeared in Fig. 1b. Moreover, the flow circulation inside the large vortical structure associated to shear layer (Fig. 1a) are eliminated in Fig. 1b. Furthermore, the size of vortical structure close to the upper wall is reduced due to the diffusion effect. Due to the low flow circulation inside the vortical region in Fig. 1b, the un-reacted gas along the primary shear layer cannot be consumed; as a result, the shear layer lengthens to the upper wall. Figure 1c shows the contour of density that is obtained by solving the Navier-Stokes equations when the diffusion coefficients are modified by a factor of 4.5. It is observed that the diffusion uniforms the flow field and reduces the gradient of the field variables behind the shock front. In addition, the smallscale vortices produced by KH instability are smeared out due to the diffusion. It is also clear that the incident wave is changed to a normal shock wave. The diffusion also reduces the size of the jet flow and leads to the disappearance of secondary triple point B. Figs. 1a and 1b also show that, the repeated interactions of primary transverse wave with shear layers (e.g. shear layer pertinent to triple point B and the shear layer inside the jet flow) causes localized explosions inside the unburned gas pockets which are shown by E in Fig. 1b. Such explosions cannot be observed in Fig. 1c. This is because as the diffusion increases the size of the jet flow decreases and the shear layers are highly damped. Hence, the interaction of the transverse wave and shear layers cannot occur and consequently the localized explosions do not emerge in Fig. 1c. This leads us to the conclusion that as the diffusion increases, the role of transverse waves in detonation structure decreases.





Figure 1. Contour of density for mixture with E=20, Q=50, $\gamma=1.2$ and N=300 cells/hrl. Γ , is the amplification factor of diffusion coefficients.



Figure 2. Contour of reaction progress variable for mixture with E=20, Q=50, γ =1.2 and N=300 cells/hrl. Γ , is the amplification factor of diffusion coefficients, solid white line indicates the shock position.

Figures 2a to 2c show the contour of reaction progress variable for the same problem. Fig. 2b depicts that, due to the less circulation inside the large vortex close to the upper wall, the un-reacted gas pocket extends to the upper boundary. Moreover, the small scale vortices (produced by KH instability) along the large vortex (produced by RM instability) are vanished in Fig. 2b. Therefore, it may be concluded that diffusion reduces the mixing rate of hot and cold gases along the shear layers and pocket boundaries and decreases the burning rate of the unburned gas pockets. However, comparison of regions which are shown by black color (i.e. U) in Fig. 2a and Fig. 2b, shows that the thickness of shear layer is decreased in Fig. 2b. The diffusion of heat and mass, from hot neighboring gases to the gases engulfs by the shear layer, consumes the un-reacted gases, and reduces the thickness of shear layer. Shown in Fig. 2c is the reaction progress variable obtained by solving the Navier-Stokes equations when the diffusion coefficients are amplified by factors of 4.5. Figure 2c shows that as the jet flow suppressed, due to the diffusion effect, the reaction zone length behind the incident wave (AN) increases and a large un-reacted gas pocket forms behind the incident wave.

5 Effect of grid resolution in irregular structure

Figure 3 shows the contour of density for the same mixture, with resolution of 50 cells per hrl. Figure 3a corresponds to the solution of Euler equations, while Fig. 3b shows the structure obtained by solving the Navier-Stokes equations (the diffusion coefficients are increased by a factor of 2.5). It is seen that the structures obtained by solving the Euler equations and Navier-Stokes equations, with 50 cells per hrl, are similar. In fact, in low grid resolution, the numerical diffusion is dominated the physical diffusion, hence the solutions of Euler and Navier-Stokes equations are very similar.



Figure 3. Contour of density for mixture with E=20, Q=50, γ =1.2 and N=50 cells/hrl. Γ is the amplification factor of diffusion coefficients.

Generally speaking, as it is observed, even in high-resolution simulation the results obtained by solving the Euler and the N.S equations are qualitatively the same, where the secondary triple points and hydrodynamic instabilities are observed in the structure. Now the question arises is that "why the structure obtained by solving the Euler and N.S are qualitatively the same?" Numerical study of Mahmoudi and Mazaheri [2] and experimental investigation of Radulescu et al. [4] both indicate that in highly unstable detonations the RM instability (interaction of shock with density gradient) is the main mechanism for the generation of turbulent structure behind the front. Previous investigations in the context of exploring Richtmyer-Meshkov (RM) instability (e.g., Li et al. [12]) indicated that the effect of viscosity on the features of the RM instability is negligible. Since the RM instability is the dominant mechanism for the appearance of turbulent structure behind the shock front, hence, the structures of detonation obtained by solving the Euler and the Navier-Stokes equations are qualitatively similar. However, it is found that, due to the diffusive phenomena, the effect of small-scale vortices produced by KH instabilities are suppressed, and even vanished somewhere along the shear layers. Hence, to find realistic solution of detonation structure, the diffusive terms should be considered by solving Navier-Stokes equations in numerical simulation of gaseous detonations.

6 Detonation with regular structure

The detonation structure for a mixture with low activation energy (i.e., E=10) that is obtained by solving both the Euler and the Navier-Stokes equations is shown in Fig. 4. Figure 4b is produced by solving the Navier-Stokes equations, where the diffusion coefficients are modified by a factor of 4.5. Triple point A, Mach stem (M), incident wave (I) and the transverse waves are observed in Figs. 4. Besides, interaction of the roll-up structure along the shear layer with the Mach stem causes the genesis of weak kink k. kk is a distinct kink that separates the main segment of the transverse wave from the extending part of it. Figure 4a shows that the detonation structure in such mixture is regular, where no secondary triple point and noticeable un-reacted gas pockets observed behind the front. Very little evidence of turbulence can be observed behind the front, along the detached shear layer.



Figure 4. Contour of density for mixture with E=10, Q=50, γ =1.2 and N=300 cells/hrl.

Detached shear layer is a shear layer, which has been isolated from the front during the collision of a triple point with the upper wall at previous cell cycle. Comparison between Fig.4a and 4b, reveals that, even though the diffusion coefficients are amplified by 4.5, however, the solution of the Euler and the N.S are still very the same in regular structure detonations. Because in such stable detonations, the shock ignites almost all the gases that have passed through it. Hence, very little evidence of turbulence and very small partially unburned gas pocket appears behind the front.



Figure 5. Contour of density for mixture with E=10, Q=50, γ =1.2 and N=50 cells/hrl.

The gradients of field variables (e.g. density gradient) are not emergent and a uniform and smooth flow field is observed behind the front. Consequently, the hydrodynamic instabilities have no important role in such detonations. It was observed in previous sections that the major effect of diffusion occurs at shear layers and un-burned pocket boundaries where it suppresses the small-scale vortices. Thus, in regular structure, the effect of hydrodynamic instabilities is negligible. Hence, diffusion has no crucial role in such detonations. Figure 5 illustrates the detonation structure for the

mixture with low activation energy that is obtained with resolution of 50 cells per hrl. Comparison of Fig. 5a with 4a indicates that the kink points, kk and k, the main section of transverse wave, and the detached shear layer cannot be captured with low-resolution simulation. However, the main feature of detonation structure (i.e., triple point, incident wave and Mach stem) are seen in Fig. 5a. Figures 5b is produced by solving the N.S equations where the diffusion coefficients are amplified by a factor of 4.5. It is observed that there is no difference between the solution of Euler equations and Navier-Stokes equations in low activation energy mixtures and low grid resolution.

7 Concluding remarks

Two-dimensional reactive Navier-Stokes equations with single step Arrhenius kinetics are solved in the present work to clarify the role of diffusive phenomena in detonation structure. It was found that, in irregular structure detonation, the physical diffusion is important at high resolution, where the numerical diffusion becomes negligible. Hence, for detonations with irregular structure, to capture and resolve accurate detonation wave structure, one needs to solve full reactive Navier-Stokes equations. In addition, in high activation energy mixtures, the diffusion suppresses the jet flowbehind the incident wave, leads to the formation of large un-reacted gas pocket behind the incident wave, where the secondary triple points are disappeared. In addition, some small-scale vortices along the shear layer, which are produced by KH instability, are smeared out due to the diffusion. In contrast to the results obtained for irregular structure detonations, comparison of detonation wave solutions obtained by solving the Euler and Navier-Stokes equations reveals that, due to the absence of hydrodynamic instabilities, the diffusion has no role in detonations with regular structure.

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