Numerical Study of a Highly Unstable Detonation with Viscosity and Turbulent Effects

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1 Instruction

In the last decade years, there have been many numerical simulations conducted [1-9] to comprehend the unstable detonations. In early works, Taki and Fujiwara[1] and Oran et al.[2] have studied the triple-shock behavior of gaseous phases detonation using simple chemical models. Oran et al.[3] have demonstrated unstable detonations in a low-pressure H2-O2-Ar mixture using a detailed chemical reaction mechanism. In their numerical works, much detailed information of the cellular structure that include the formation of unreacted gas pockets, collision of triple points, and evolution of the transverse waves. Lee[10] has appealed that the instability of detonations can be a source of turbulence. Bourlioux et al.[11] have reproduced the transition to two-dimensional turbulence in the wake of unstable detonations by varying the heat release, activation energy, and overdriven. In their simulations, the strong turbulence contributes to the irregularity of the cellular pattern. Singh et al.[5] consider the viscous effect by comparing solutions obtained from the Euler and Navier-Stokes equations. They conclude that physical diffusion is important for high grid resolution when the numerical diffusion becomes negligible, and that cellular structures from the Euler-equation simulation depend on the grid resolutions. Nikolic et al.[7] utilized much larger domain in their simulation to study the effect of channel width on detonation cell size. The grid resolution effect was carefully examined by Sharpe [8] with a one-step Arrhenius chemical model. More recently, Hu et al.[9] studied the cellular structure of detonation waves using a detailed chemical kinetics model.

The present work revisits those issues raised previously, such as the viscous effect by comparing solutions obtained from the Euler and Navier-Stokes equations with different numerical methodologies. The analysis treats the full conservation equations in two-dimensional coordinates with variable formulation and single-step Arrhenius reaction model. The fluid dynamics equations are solved by 5th order MUSCL-type TVD scheme [12-13] and 4th order accurate classical Runge-Kutta time integration scheme. Furthermore, MILES is implemented to comprehend turbulent phenomenon in unstable detonation. Roe's flux difference splitting scheme for numerical flux is applied MILES where the inherent dissipation of the numerical algorithm is taken as model of the sub-grid scale stresses. The numerical method have a roll of built-in LES filter that naturally accounts for the effect of the turbulence phenomena on scales too small to be resolved by grid Boris et al.[14]. A series of numerical studies are carried out applying different numerical methodologies to the highly unstable detonation phenomena by high energy release and activation energy.

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2 Numerical Approach

The governing equations are the Euler equations for inviscid flow, Navier-Stokes equations for viscid flow and filtered Navier-Stokes equations for Large Eddy Simulation.

$$\frac{\partial \mathbf{Q}}{\partial t}+\frac{\partial \mathbf{F}}{\partial x}+\frac{\partial \mathbf{G}}{\partial y}=\frac{\partial \mathbf{F_v}}{\partial x}+\frac{\partial \mathbf{G_v}}{\partial y}+\mathbf{S}$$

$$\mathbf{Q}\equiv\begin{bmatrix}\bar{\rho}\\ \bar{\rho}\tilde{u}\\ \bar{\rho}\tilde{v}\\ \tilde{e}\\ \bar{\rho}\tilde{Z}\end{bmatrix},\ \mathbf{F}\equiv\begin{bmatrix}\bar{\rho}\tilde{u}\\ \bar{\rho}\tilde{u}^2+\bar{p}\\ \bar{\rho}\tilde{u}\tilde{v}\\ (\tilde{e}+\bar{p})\tilde{u}\\ \bar{\rho}\tilde{u}\tilde{Z}\end{bmatrix},\ \mathbf{G}\equiv\begin{bmatrix}\bar{\rho}\tilde{v}\\ \bar{\rho}\tilde{u}\tilde{v}\\ \bar{\rho}\tilde{v}^2+\bar{p}\\ (\tilde{e}+\bar{p})\tilde{v}\\ \bar{\rho}\tilde{v}\tilde{Z}\end{bmatrix},\ \mathbf{F_v}\equiv\begin{bmatrix}0\\ \tau_{xx}\\ \tau_{xy}\\ (f_v)_4\\ \dfrac{\bar{\rho}\nu_t}{Sc_t}\dfrac{\partial\tilde{Z}}{\partial x}\end{bmatrix},\ \mathbf{G_v}\equiv\begin{bmatrix}0\\ \tau_{yx}\\ \tau_{yy}\\ (g_v)_4\\ \dfrac{\bar{\rho}\nu_t}{Sc_t}\dfrac{\partial\tilde{Z}}{\partial y}\end{bmatrix},\ \mathbf{S}\equiv\begin{bmatrix}0\\ 0\\ 0\\ 0\\ \bar{\dot{\omega}}\end{bmatrix}$$

One-step Arrhenius reaction model with variable specific heat ratio formulation is used to simulate the various regimes of detonation phenomena without the complexity of dealing detaile chemical mechanisms. The thermo-chemical parameters were selected from Austine et al. [15]. The incoming boundary condition was used with C-J detonation speed. The wall is assumed be slip wall and adiabatic. The exit boundary condition was used base on the characteristic boundary condition using C-J condition as a far-field condition. More details could be found in the literature.[16]

3 Result and Discussion

Natures of a gaseous detonation are widely comprehended by experiments from Austine et al. [15] and computational simulations from lots researchers. Before carrying out high order computational simulation, third order MUSCL TVD are performed for understanding detonation phenomena. Fig. 1 shows instantaneous flow fields of a highly and weakly detonation. Keystone region and triple points are shown well in Fig. 1 (left) and unreacted gas pockets are observed.

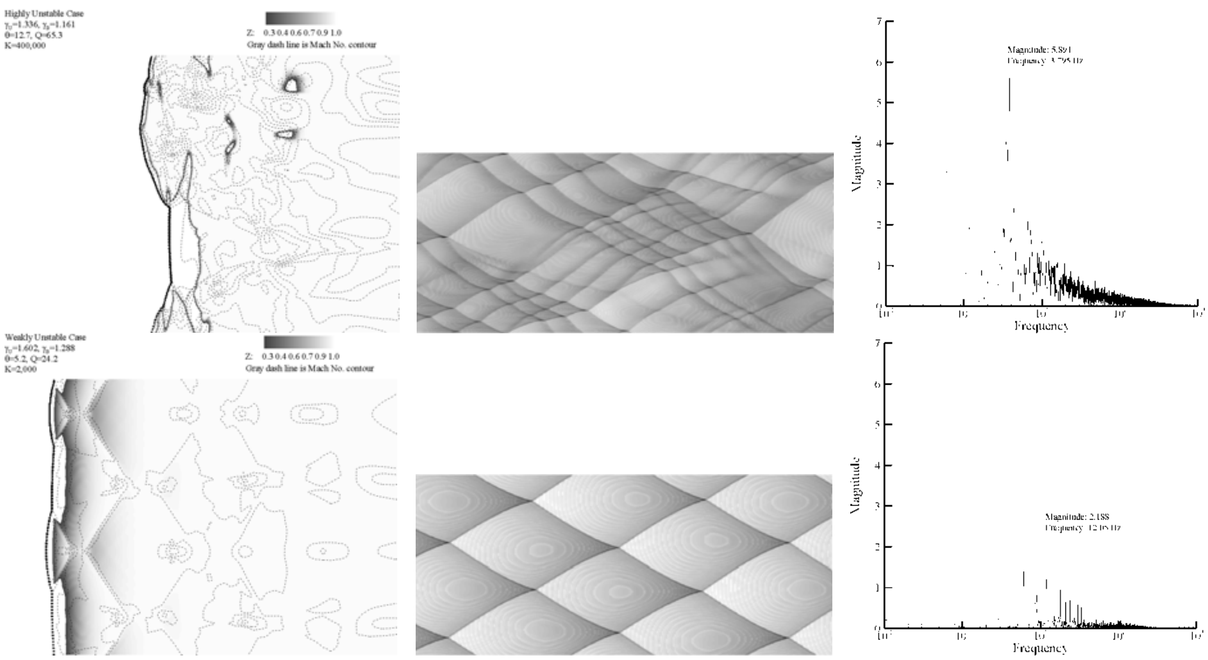

Figure 1. Progress variable, Z, distribution with cutoff color band 0.25 below and Gray dash line is Mach No. contour. Upper: Highly unstable detonation, Bottom: Weakly unstable detonation. Left: Snap Shot, Middle: Smoked-foil records, Right: FFT

There are different pre-exponential factors. Highly and weakly are K=400,000 and 2,000 respectively in Fig. 1. Irregular pattern is shown in Fig. 1 upper) smoked-foil of highly unstable detonation. Highly unstable detonation pattern has lots small cells into a larger cell. It is difficult to measure cell size and count cell size. Distinctively, two cells pattern is shown in Fig. 1 bottom) weakly unstable detonation. In Fig. 1 right), highly unstable case has wide range of frequency from FFT (Fast Fourier Transform) result which is computed with measurement pressure along center line. Contrast, weakly unstable case with less pre-exponential factor shows that none dimensional primary frequency is 12.05 Hz, second is 6 Hz and third is 9 Hz in Fig. 1 right). From both FFT analyses, we are able to predict that smoke-foil pattern would have regularly or irregularly recoded on foil.
All cases show irregular nature of highly unstable detonation. All simulations have the same initial condition and boundary. But there are different smoked-foil records in Fig. 1 middle). These results also the nature of highly unstable detonation phenomena which are not countable the cell size. These irregular fashions are leaded by high activation energy.

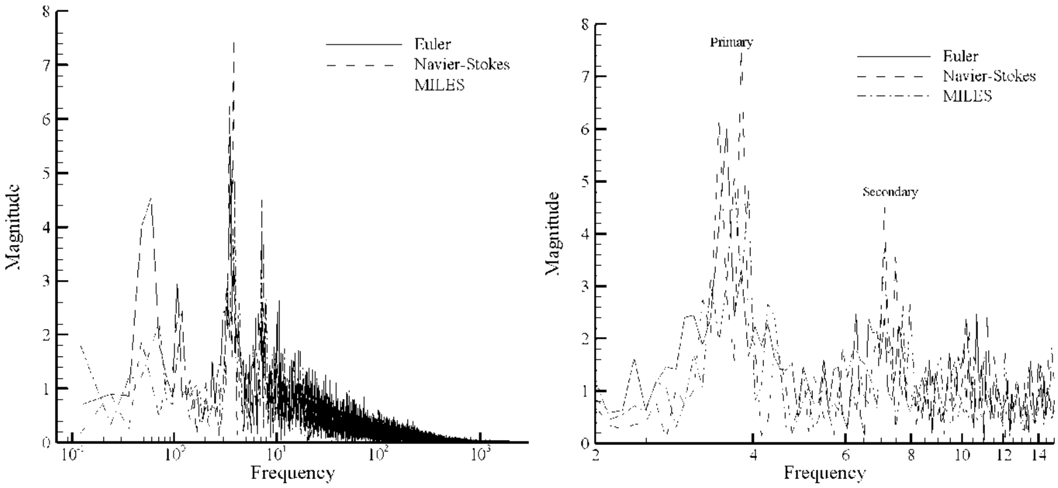

Figure 2. Magnitude-Frequency plot; Left: Roe’s FDS scheme, Right: Detailed view of frequency range from 2~15 Hz

All methodologies show similar trend of frequency, the primary frequency is 3.5 ~ 3.8 Hz with 5.0 ~ 7.5 of magnitude in Fig. 2 left). The roll of primary frequency makes up formation of big cell and small cells of over 20 Hz are frequently occurred within big cell. Different frequency is shown among methodologies in detailed view Fig. 2 right). For primary frequency, Euler is 3.558 Hz, Navier-Stokes is 3.795 Hz and MILES is 3.676 Hz. These different frequencies seem to be viscous effect in the methodologies.

4 Conclusion

Present study examines the Monotone Integrated Large Eddy Simulation (MILES) on highly unstable detonation wave cell structure simulation. Inviscid/viscous fluid dynamics equations and one-step Arrhenius reaction model are solved simultaneously by temporally 4th-order classical Runge-Kutta method and 5th-order MUSCL TVD scheme based on Roe’s approximation FDS for calculating numerical fluxes. A series of numerical studies are carried out based on Favre-filtered Navier-Stokes equation including deliberate formulations of heat transfer and viscosity term with high activation energy and on fine grid system. The computational results are investigated by comparing the results from inviscid Euler equations, Reynolds Averaged Navier-Stokes (RANS) equations, and Monotone Integrated Large Eddy Simulations (MILES). All approaches are capable of capturing the highly unstable detonation wave, but shows distinctive differences in FFT analysis of highly unstable detonation. Primary frequencies and magnitudes are a little bit difference in all methodologies in which viscosity models are different.

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