The Study of Turbulence Effects in Highly Unstable Detonation Mode

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1 Introduction

Detonation can be classified form weakly to highly unstable mode depending on the mixture composition. In weakly unstable mode, the structure of detonation wave is very regular, smooth and shows the uniform cell size with regular period in the smoked-record.However, in highly-unstable mode, instead of stable and regular movement, the detonation structures have tendency of extremely irregular and wrinkled wave front and cell shapes. Also by the results of Power Spectrum Density(PSD) using Fast Fourier Transform(FFT), the peak points are shown as separated pulse form with stead interval in weakly-unstable mode, whereas irregular interval peak points and unsystematic noise shapein highly-unstable mode. These seem strengthdifference of turbulence effects. J. M. Austinetal.[1] investigated unstable detonations from weakly to highly unstable modes by using different chemical compositions. J. E. Sheperd[2] discussed the role of turbulence flow in gaseous detonation and summarized the up-to-date studies on this issue. Powers[3] showed 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 become negligible, and that cellular structures from the inviscid simulations depend on the grid resolutions. Sharpes[4] and Redulescue[5] examined carefully the grid resolution effect. Deledicqueet al.[6] described wave front and kinetic characteristics due to activation energy in vicinity of weakly unstable mode in 3-D structure which has periodic boundary conditions. Choi et al.[7] showed that better grid resolution is required to observe cell structure in highly unstable mode compare to weakly unstable mode in numerical analysis of 2-D detonation cell structure using fixing grid systems.Regardless of many studies done previously there are quite a many unknowns still unresolved and need a systematic investigation. Especially, there was little work on the detailed 3-D numerical analysis is of highly unstable detonation wave front so far, presumed being due to heavy computing cost for the fine grid resolution required to capture the unstable detonation characteristics. Present study attempts to simulate the highly unstable detonation wave in three-dimension in comparison with an equivalent two-dimensional case.

2 Numerical Approach

The detonation phenomena are modeled by mass, momentum and energy conservation equations coupled with a conservation equation of a reaction progress variable in three-dimensional coordinates. Single step irreversible Arrhenius reaction model with variable specific heat ratio formulation is used to simulate the highly unstable detonation phenomena with the complexity of handling detailed chemistry. Thermo-chemical parameters used in numerical study were adopted from the J. M. Austineet al.[1] Viscous terms were neglected, thus the model corresponds to the case of infinite Reynolds number. The coupled govering equations are summarized as follows in the conservative vector formulation.

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho \\ \rho u_i \\ \rho e \\ \rho c\end{bmatrix}+\frac{\partial}{\partial x_j}\begin{bmatrix}\rho u_j \\ \rho u_i u_j + p\delta_{ij} \\ (\rho e + p)u_j \\ \rho c u_j\end{bmatrix}=\begin{bmatrix}0 \\ 0 \\ 0 \\ \dot{\omega}\end{bmatrix},\quad i, j=1,2,3$$

$$\dot{\omega} = \rho(1-c)k\exp(-E/RT)$$

The fluid dynamics equations were discretized using finite volume cell-vertex method. Numerical fluxes in cell boundaries were calculated by 3rd order accuracy MUSCL-type TVD scheme using Roe's approximate Riemann solver. Time integration is carried out using standard 4th order accurate Runge-Kutta method. The code was parallelized by domain decomposition technique using MPI standard. The incoming boundary condition was fixed at C-J detonation speed and characteristic boundary condition was used at exit using C-J condition as a far-field condition. Periodic boundary is used at the lower and upper boundaries. Physical values of grid system and parameters used in the simulation are summarized in table 1 and 2. Initial condition over the computational domain is generated using 1-D ZND structures solution with inclined distribution as in initial perturbation.

Table 1: Summary of computational grids

Grid system		Minimum spacing	Domain size
2-D	506×402	Δx=Δy=0.0025	5.13×1.0
	200,000 cells, uniform 401×402 + 3.85% stretching 105×402		
3-D	506×402×402	Δx=Δy=Δz =0.0025	5.13×1.0×1.0
	81,700,000 cells, uniform 401×402×402+ 3.85% stretching 105×402×402		

Table 2: computational cases adopted form Austine et al. (2005)

Weakly unstable detonation	$2H_2+O_2+12Ar$
	$\gamma_U = 1.602, \gamma_B = 1.288$
	$\theta = 5.2, q = 24.2$
Highly unstable detonation	$C_3H_8+5O_2+9N_2$,
	$\gamma_U = 1.336,\ \gamma_B = 1.161$
	$\theta = 12.7, q = 65.3$

3 Results and Discussions.

Figure 1 shows the 3-D structures of the detonation wave stabilized in the uniform gird for different pre-exponential factor, *k*, after certain time has passed in highly-unstable mode. When initial wave front structure is relatively uniform and reaction constant was small, wave front structures showed regular and smooth form. On the other hand, when reaction constant value was larger, wave front structures are shown irregular and wrinkled. These differences are confirmed more clearly in figure 2. Both resultsshow that length of induction length is much longer than reaction regionbetween shock wave and combustion region.Also unreacted pocket where reaction hasn't taken place can be seen clearly inner combustion reaction regions. Similar to 2-D studies, results of low reaction constant show longer reaction length between front shock wave and combustion region. Blue color represents pressure in the front and within the combustion region of 3-D iso-surface in figure 2 (left side). Other colors represent reaction progress variable *c*. Reaction progresses occur at longer areas and the reactive fronts are smoother when reaction constant is lower. When reaction constant *k* is increased, reactive fronts have more curve. So combustion takes place rapidly in the short region. It seem as the result is more stronger turbulence effects.

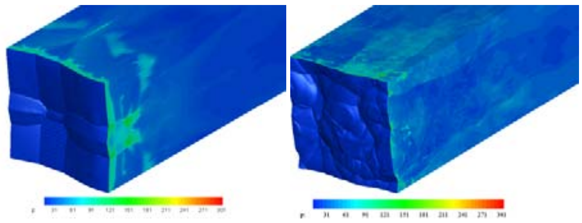

Figure 1. Pressure distribution, left: $k=10^5$ at time 35.48; right: $k=4\times10^5$ at time 39.76

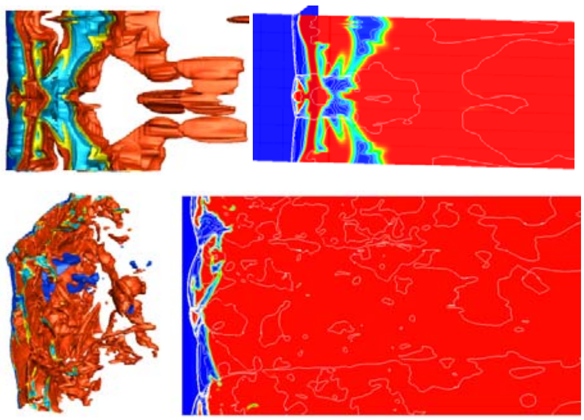

Figure 2. Pressure and reaction progress variable (left) and cross-sectional structure (right),

top: $k=10^5$; bottom: $k=4\times10^5$

Figure 3 and 4 show pressure and combustion reaction progress rate in 2-D and 3-D, respectively. The 2-D figures show difference in process of time, and the results of 3-D show difference of wave front and reaction progress rate of stationary wave in arbitrary time. By the comparing these results, 3-D structures include similar tendency in an instance compared to results of 2-D in time dependence. That is, combined results of 2-D as time passes make up the instant 3-D detonation wave front structure. Interesting thing is when reaction constant was $k=10^5$, combustion is closed by wave front being blown out of exit boundary region before wave front being stabilized. However, in 3-D analysis, the wave front is stably sustained within the grid area. Also, characteristics of wave front stabilization in 3-D result show similar outcome with the results of 2-D weakly and moderately unstable results when k=1,000. This is due to 3-D having one more dimension than 2-D so that combustion reaction occurs in more areas than 2-D, and increase of boundary area having periodic boundary conditions, etc. But more studies through analysis should be performed to understand such results.

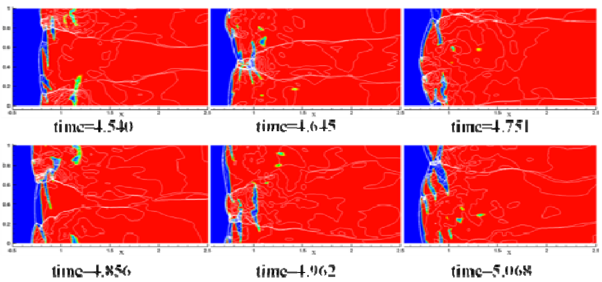

Figure 3. Pressure and reaction progress rate contours for k=4×10^5 at 2-D results.

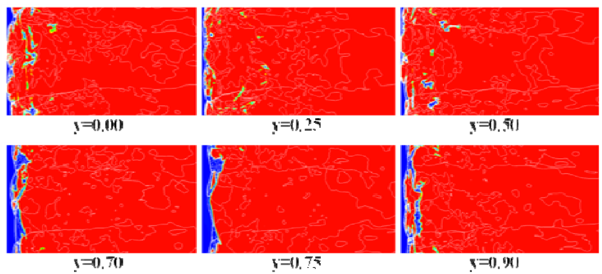

Figure 4. Pressure and reaction progress rate contours for k=4×10^5 in time t=39.76 at 3-D results.

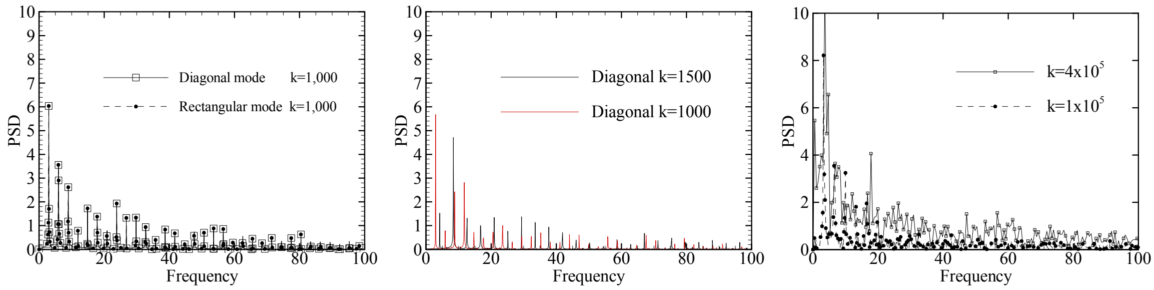

Figure 5. Amplitude of the oscillation mode as function of pre-exponential k. Weakly unstable results (left and middle) and highly unstable result (right)

Figure 5 is the 3-D result of Power Spectrum Density(PSD) using Fast Fourier Transform(FFT) as time variable for the different unstable mode conditions in the region where front shock wave pressure change is stabilized. Top and middle figures are results of weakly unstable mode. The top figure is comparison of results which have different constant reaction speed k and initial shape. When having equal reaction speed constant, the results showsame analysis outcome. But, when calculating with same initial condition but different reaction speed constant, the graphs show distinct differences. Initial peak value is the maximum peak value when k=1,000, and overall peak pressure decreases. When k is increased to 1,500, there is one peak value before the maximum peak. After maximum peak overall peak value decreases when k=1,000. At k=1,000 the maximum peak frequency is $f_{maxpeak}$= 2.928, frequency interval between peak values is Δf_{peak} = 5.856. And, at k=1,500 maximum peak frequency is $f_{maxpeak}$= 8.6, frequency interval between peak values is Δf_{peak} = 4.2. The peaks in both results are shown as separated pulse form with steady interval. These effects are shown that the smoked-foil records are very regular shape and constant size cells. Contrastively, in highly unstable region, both $k=10^5$ and $k=4\times10^5$ show irregular interval peak points and unsystematic noise shape. Overall strength increases as reaction constant increases. The frequency is f_{peak}= 3.67 in the maximum peak value at $k=4\times10^5$, whereas as f_{peak}= 3.25 at $k=10^5$. As reaction speed grows, the amplitude of maximum peak rises and overall strength has larger value in equivalent frequency region. So these effects are shown that the smoked-foil records are very irregular shape and variable size cells. It seems the result of turbulence effects.

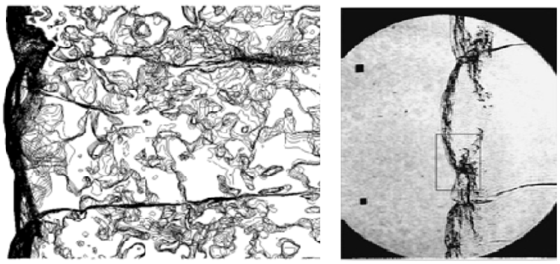

Figure 6. The pressure contour line is overliad from y=0.7 to y=0.75 (left) and schlieren image by J. M. Austin in C_2H_4-$3O_2$-$8N_2$, P_1=20kPa in the narrow channel (right).

Figure 6 is schlieren image (right side) by J. M. Austin et al.[1] and overlaid image of strength of pressure (left side) at arbitrary location by numerical simulation in highly unstable region. The images properly show rough and wrinkle feature of detonation wave front in highly unstable region. In numerical analysis, by combining neighboring cross-section images, characteristics of detonation wave front cab be shown as figure 6. The wave front has irregular form due to the interference of neighboring wave fronts.

Numerical analysis field of detonation phenomena has been progressed well thanks to improvement o computer performance, more effective and accurate mathematical model as swell as development of algorithms for numerical analysis. Through this advancement various physical facts of various fields were described and numerous question were solved using numerical analysis method for last several decades. However, a lot of problems in detonation field are remained to be solved. 3-D numerical study on detonation phenomena has established its foundation for the last decade. Especially numerical studies of detonation phenomena in highly unstable region has very slow advance. This study discussed characteristics of wave front in highly unstable region by 3-D detonation analysis using 3-D Euler equation which applied one-step chemical reaction to minimize numerical effort and time consumption. Additionally, by comparing 2-D and 3-D analysis results, similarity and difference of two results were verified. Also by PSD analysis, understanding of characteristics for different pre-exponential factor k and unstable are was done and Schlieren and overlaid images of 3-D analysis results were compared to discuss irregularity due to interference of 3-D wave front.

References

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