

Numerical Simulation of Three Dimensional Detonation Waves Dynamics in Highly Unstable Mode.

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1 Introduction

The gaseous detonation wave propagating through mixture gas is basically unstable. This unstable detonation structure is separated from weakly unstable to highly unstable mode owing to composition of mixture. In weakly unstable mode, structure of detonation wave is very regular, smooth and is shown the uniform cell size with regular period in the smoked-record. However, in highly unstable mode, instead of stable and regular movement, there has tendency of extremely irregular and wrinkled wave front and cell shape. J. M. Austin et al.[1] used chemical composition from weakly to highly unstable mode to observe and research the distinct difference between weakly and highly unstable mode. 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 becomes 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. Deledicque et 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 fixed grid systems. Regardless of many studies done previously there are quite a many unknowns still unresolved and need a systematic investigation. Especially, there have not been many studies on detailed 3-D numerical analysis is of highly unstable detonation wave front so far. This is due to calculation time of large number of grids and performance of computers. This study is to find out basic characteristics of the detonation wave front using 3-D numerical simulation and comparison with 2-D case.

2 Numerical Approach

The phenomena are modeled by full conservation equations in three-dimensional coordinates. Euler equations and a conservation equation of reaction progress variable are summarized in the conservative vector formulation as follows. 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. Austine et al. [1]

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial G}{\partial z} = H$$

$$Q = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ e \\ \rho Z_f \end{bmatrix}, \quad E = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ (e+p)u \\ \rho u Z_f \end{bmatrix}, \quad F = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vw \\ (e+p)v \\ \rho v Z_f \end{bmatrix}, \quad G = \begin{bmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ (e+p)w \\ \rho w Z_f \end{bmatrix}, \quad H = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \dot{\omega} \end{bmatrix}$$

The fluid dynamics equations were discrete using finite volume cell-vertex method and numerical flux in cell boundaries was calculated by 3rd order accuracy MUSCL-type TVD Scheme using Roe's approximate Riemann solver. And the time integration is used 4th order accurate classical Runge-Kutta scheme. MPI standard library was used to perform parallelization by domain decomposition. The incoming boundary condition was used with C-J detonation speed. Periodic boundary is used at the wall conditions. The exit boundary condition was used base on the characteristic boundary condition using C-J condition as a far-field condition. Physical values of grid system and parameters used in the simulation are summarized in table 1 and table 2.

Table 1: Summary of computational grids

Grid system	Minimum spacing	Domain size
2-D		
506×402	$\Delta x = \Delta y = 0.0025$	5.13×1.0
200,000 cells, uniform 401×402 + 3.85% stretching 105×402		
3-D		
506×402×402	$\Delta x = \Delta y = \Delta z = 0.0025$	5.13×1.0
81,700,000 cells, uniform 401×402×402+ 3.85% stretching 105×402×402		

Table 2: Computational cases adopted from Austin et al. (2005)

Weakly unstable detonation	
$\theta = 5.2$	$2\text{H}_2 + \text{O}_2 + 12\text{Ar}$
$\gamma_U = 1.602$	$\gamma_B = 1.288$
Highly unstable detonation	
$\theta = 12.7$	$\text{C}_3\text{H}_8 + 5\text{O}_2 + 9\text{N}_2$
$\gamma_U = 1.336$	$\gamma_B = 1.161$

[†] Austin et al. (2005)

3 Result and Discussion

Figure 1 show the 3-D structures of the detonation wave stabilized in the uniform grid for different pre-exponential factor, k after certain time has passed. 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 was large and distribution gradient of initial values was large, wave front show irregular and wrinkled results.

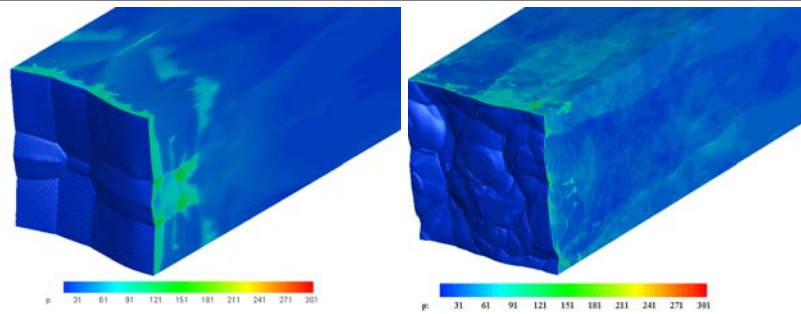


Figure 1. Pressure distribution, $k=10^5$ (left at time=35.48), $k=4 \times 10^5$ (right at time=39.76)

These features are more distinct in Fig. 2. Both results show length of induction length between shock wave and combustion region much longer than reaction region which is the feature of highly unstable region. Also unreacted pocket where reaction hasn't taken place can be seen clearly between combustion reaction regions. Similar to 2-D studies, results of low reaction constants show longer reaction length between front shock wave and combustion region.

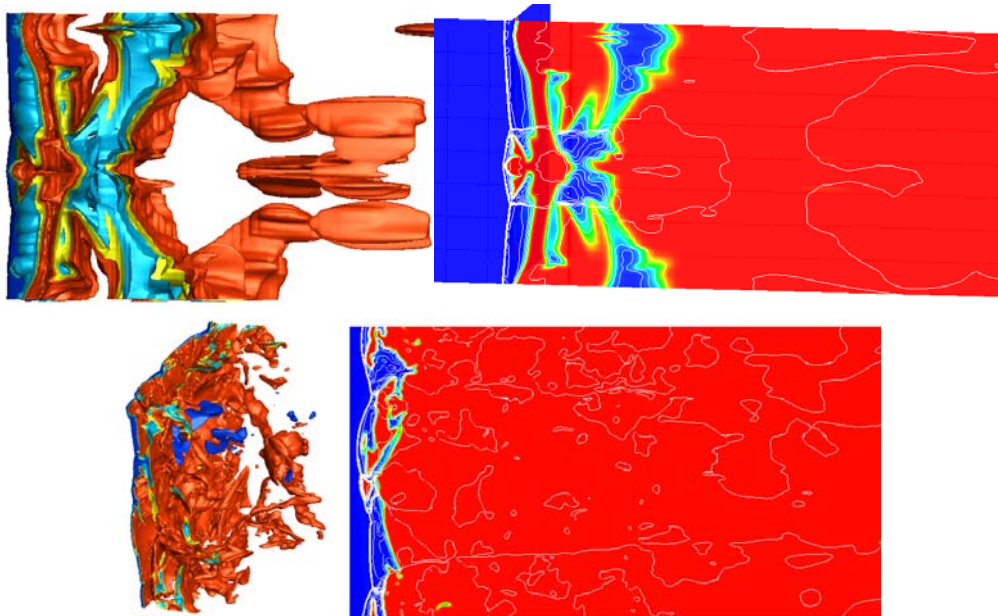


Figure 2. Pressure and reaction progress variable (left) and cross-sectional structure (right) at $k=10^5$ (top) and $k=4 \times 10^5$ (bottom).

Blue color represents the pressure in the front and within the combustion region of 3-D iso-surface in Figure 2(left). Other colors represent reaction progress variable Z_f . Reaction progresses occur in longer area when low reaction constant. When reaction constant k is increased, combustion takes place rapidly in the short region.

Figure 3 and Fig. 4 show pressure and combustion reaction progress rate in 2-D and 3-D, respectively. 2-D figures show difference along the changed time, and 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 results of 2-D weakly unstable & 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 areas having periodic boundary conditions, etc. But more studies through analysis should be performed to understand such results.

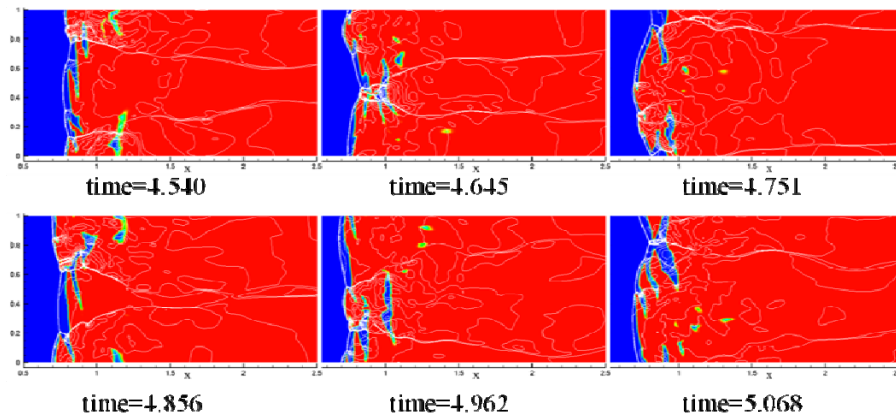


Figure 3. 2D pressure and Z_f contours for $k=4 \times 10^5$.

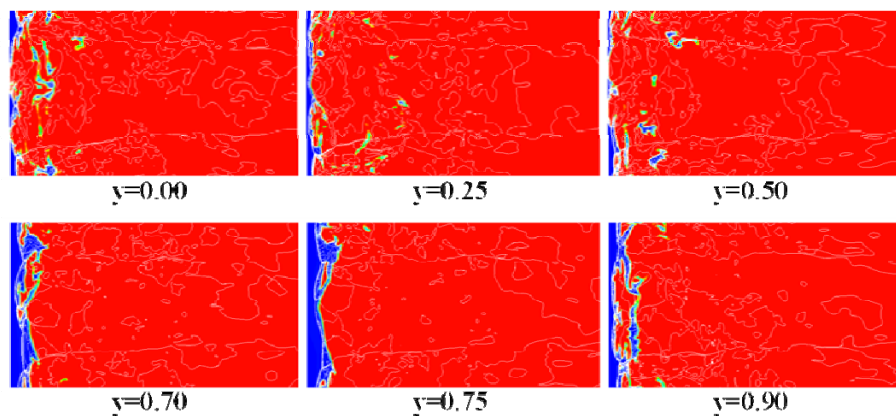


Figure 4. 3D pressure and Z_f contours for $k=4 \times 10^5$ at time $t=39.76$.

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. Left and center figures are results of weakly unstable mode. Left figure is comparison of results which have different constant reaction speed k and initial shape. When having equal reaction speed constant, result shows same analysis outcome. But, when calculating with same initial condition but different reaction speed constant, graphs show distinct difference. Initial peak value is the maximum peak value when $k=1,000$, and peak pressure decreases overall. 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 $f_{\text{maxpeak}} \approx 2.928$, frequency interval between peak values is $\Delta f_{\text{peak}} = 5.856$. And, at $k=1,500$ maximum peak frequency is $f_{\text{maxpeak}} \approx 8.6$, frequency interval between peak values is $\Delta f_{\text{peak}} = 4.2$. Peaks in both results are shown as separated pulse form with steady interval.

However in highly unstable region, both $k=10^5$ and $k=4 \times 10^5$ show irregular interval between peaks and unsystematic nose. Overall strength increases as reaction constant increases. At $k=10^5$ where maximum peak value appears, $f_{\text{peak}} = 3.25$, and at $k=4 \times 10^5$, $f_{\text{peak}} = 3.67$. As reaction speed grows the amplitude of maximum peak value rose, overall strength has larger value in equivalent frequency region.

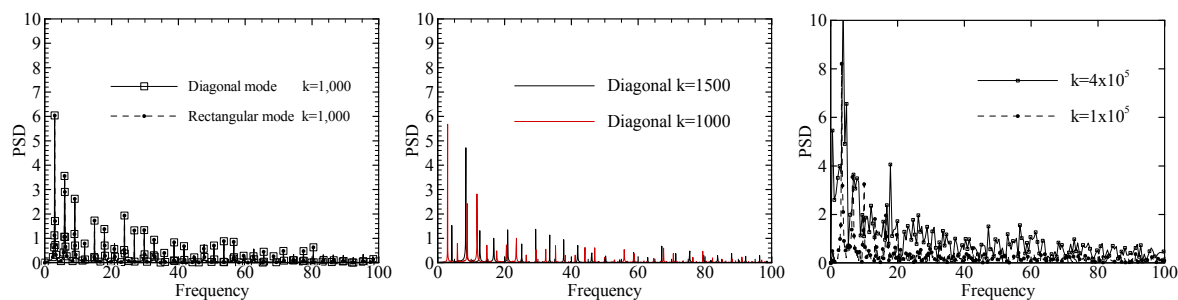


Figure 5. Amplitude of the oscillation mode as function of pre-exponential k . Weakly unstable results (left and middle) and highly unstable result (right).

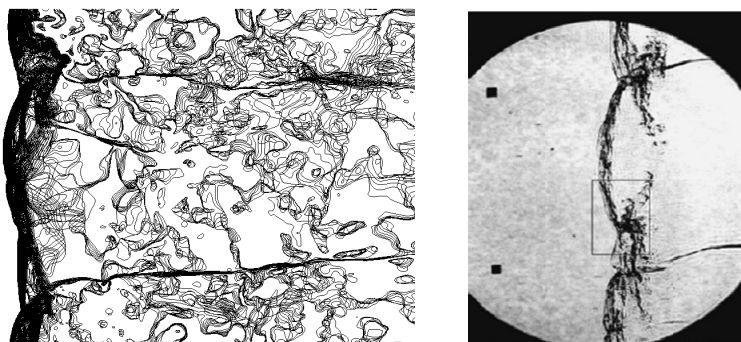


Figure 6. The pressure contour line is overlaid from $y=0.7$ to $y=0.75$ (left) and schlieren image by J.M Austin¹ in $C_2H_4-3O_2-8N_2$, $P_1=20kPa$ in the narrow channel (right).

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

Numerical analysis field of detonation phenomena has been progressed well thanks to improvement of computer performance, more effective and accurate mathematical model as well as algorithms for numerical analysis. Through this advancement various physical facts of various fields were described, and numerous questions were solved using numerical analysis method for last several decades. However, a lot of problems in detonation field are yet 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 & 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 area was done, and schlieren image and overlaid image of 3-D analysis results were compared to discuss irregularity due to interference of 3-D wave front.

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