Reynolds Number Effects on the Structure and Stability of Highly Unstable Detonation Wave

Deok-Rae Cho, Kiha Kang, Jae-Ryul Shin, Jeong-Yeol Choi

Pusan National University

Busan, Korea

1 Instruction

There have been many numerical simulations conducted to comprehend the unstable detonations. Shephered emphasized recently the role of turbulence on gaseous detonation [1] and summarized the up-to-date studies on this issue. 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 has been studied by Oran et al.[2] Lee et al. has appealed that the instability of detonations can be a source of turbulence.[3] Bourlioux et al. have reproduced the transition to two-dimensional turbulence in the wake of unstable detonations and found that the strong turbulence contributes to the irregularity of the cellular pattern.[4] Powers showed the viscous effect by comparing solutions obtained from the Euler and Navier-Stokes equations.[5] 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. The grid resolution effect was carefully examined by Sharpe [6] with a one-step Arrhenius chemical model. Radulescu et al. have considered this issue in some detail.[7]. Regardless of many studies done previously, there are quite a many unknowns still un resolved and needs a systematic investigation. One of the issues is the numerical modeling of the highly unstable detonation. As a preliminary step toward, the effect of Reynolds number and grid resolution is investigated by a series of numerical studies. Simulations are carried out for wide range of Reynolds number using coarse and fine grid system. The role of diffusion and the effect of grid resolution on the detonation structures and stabilities are clearly understood from these simulations.

2 Numerical Approach

The phenomena is modeled by full conservation equations in two-dimensional coordinates. Navier-Stokes equations and a conservation equation of reaction progress variable is 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 without the complexity of handling detailed chemistry. The thermo-chemical parameters were selected from Austine et al. [8]. Viscosity is assumed as a function of temperature and Prandtl number and Schimdt number are assumed 1.0 for the calculation of thermal and mass diffusions.

Correspondence to: aerochoi@pusan.ac.kr

$$\frac{\partial \mathbf{Q}}{\partial t}+\frac{\partial \mathbf{F}}{\partial x}+\frac{\partial \mathbf{G}}{\partial y}=\frac{\partial \mathbf{F}_\mathrm{v}}{\partial x}+\frac{\partial \mathbf{G}_\mathrm{v}}{\partial y}+\mathbf{S}$$

$$\mathbf{Q}=\begin{bmatrix}\rho\\ \rho u\\ \rho v\\ e\\ \rho Z\end{bmatrix},\ \mathbf{F}=\begin{bmatrix}\rho u\\ \rho u^2+p\\ \rho uv\\ \left(e+p\right)u\\ \rho uZ\end{bmatrix},\ \mathbf{G}=\begin{bmatrix}\rho v\\ \rho uv\\ \rho v^2+p\\ \left(e+p\right)v\\ \rho vZ\end{bmatrix},\ \mathbf{F}_\mathrm{v}=\begin{bmatrix}0\\ \tau_{xx}\\ \tau_{xy}\\ f_v\\ \dfrac{\mu}{Sc}\dfrac{\partial Z}{\partial x}\end{bmatrix},\ \mathbf{G}_\mathrm{v}=\begin{bmatrix}0\\ \tau_{yx}\\ \tau_{yy}\\ g_v\\ \dfrac{\mu}{Sc}\dfrac{\partial Z}{\partial y}\end{bmatrix},\ \mathbf{S}\equiv\begin{bmatrix}0\\ 0\\ 0\\ 0\\ \dot{\omega}\end{bmatrix}$$

The fluid dynamics equations are solved by 5th order MUSCL-type TVD scheme and 4th order accurate classical Runge-Kutta time integration scheme. Furthermore, MILES is implemented to comprehend turbulent phenomenon in unstable detonation. The incoming boundary condition was used with C-J detonation speed. Periodic boundary is used at the lower and upper surfaces. The exit boundary condition was used base on the characteristic boundary condition using C-J condition as a far-field condition. Computation grid is plotted in Fig. 1 where uniform grid is used in the focus region ($0.5 \le x \le 1.5$) while stretched grid used for inflow and exit boundaries. The channel height is considered as 1.0. Inclined distribution of analytic ZND solution is used as initial condition. More details of numerical modeling are addressed in Ref. [8].

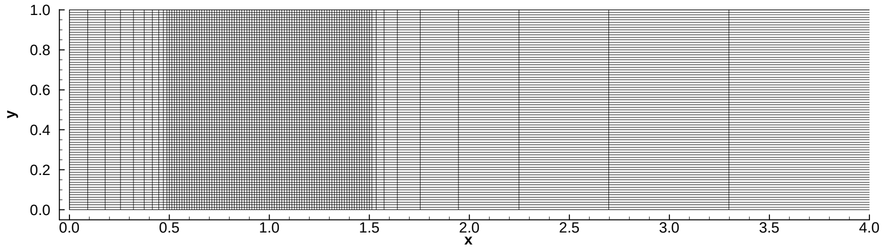
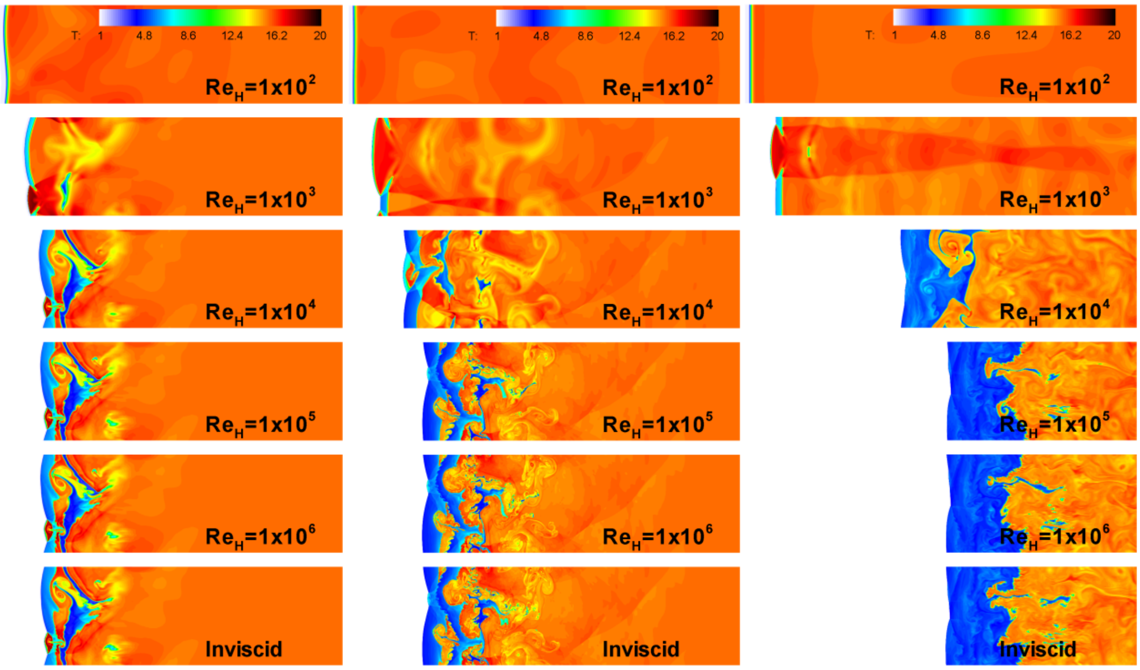


Figure 1. Coarse computational grid. Every fifth point is plotted in each direction.

3 Result and Discussion

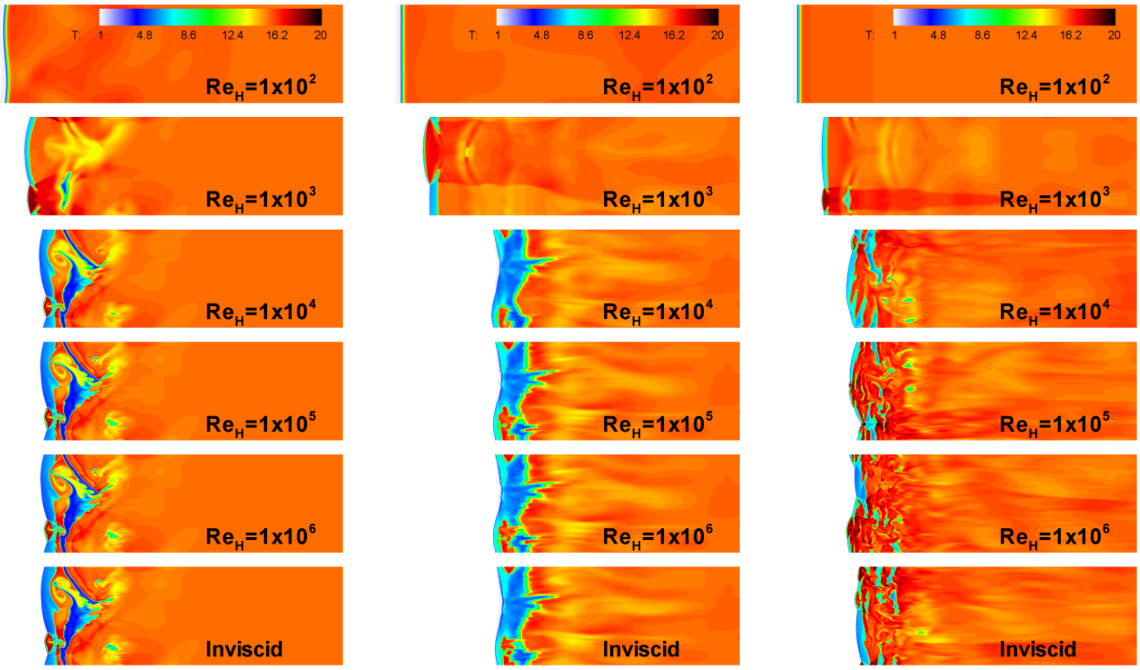
Numerical study is carried out for fine and coarse grid systems for Reynolds numbers, ranging from 10^2 to infinity where inviscid assumption applies. Figure 2 is the temperature contours at several instances. It is found that the results of the case $Re_H=1x10^2$ is quickly stabilize to the normal ZND solution. Chemical induction zone and reaction zone thickness seem to be much thinner than the initial ZND solution with inviscid assumption. It is considered that diffusion process has primary responsibility, similarly to the premixed flame structure in low speed flows. In case of $Re_H=1x10^3$, very periodic detonation structure is obtained at this high activation energy condition. It is clear that viscous terms damps out the source of small instabilities and stabilized the detonation. Since the diffusion effect is 1/10 of the previous case, detonation structure seems to be thicker than the former case. For the case where $Re_H \ge 1x10^4$, highly unstable nature of reaction zone structure is observed. Higher Re_H has more fine details, difference are not found with naked eye for $Re_H \ge 1x10^5$ at least for early instances. For $Re_H \ge 1x10^5$, the shock and reaction begins to decouple and never returns back. Finally the detonation blow out of the computational domain.

In case of coarse grid, the solution develops similarly to the fine grid cases. However little difference is found after the cases of $Re_H=1x10^4$. A great difference between the fine and coarse grid is that the stabilized solution of highly unstable detonation is attained with coarse grid due to higher numerical damping. Differently from fine grid cases, as shown at t=0.686, coupling of shock and reaction occurs when the shock and reaction zone blows back to the stretched grid region where numerical damping is greater in flow direction. Finally sustained highly unstable detonation is obtained regardless of Re_H. It is considered that the numerical damping increase the mixing and combustion leading to the completion of combustion. Therefore it is recommended to introduce some sort of mathematical models to account for the physical process of turbulence mixing and combustion in the highly unstable detonation structures.



(a) t=0.227 (b) t= 0.455 (c) t=0.682

Figure 2. Instantaneous temperature distributions from fine (2,001×1,001) grid simulations.



(a) t=0.257 (b) t= 0.686 (c) t=6.004

Figure 3. Instantaneous temperature distributions from coarse (501×401) grid simulations.

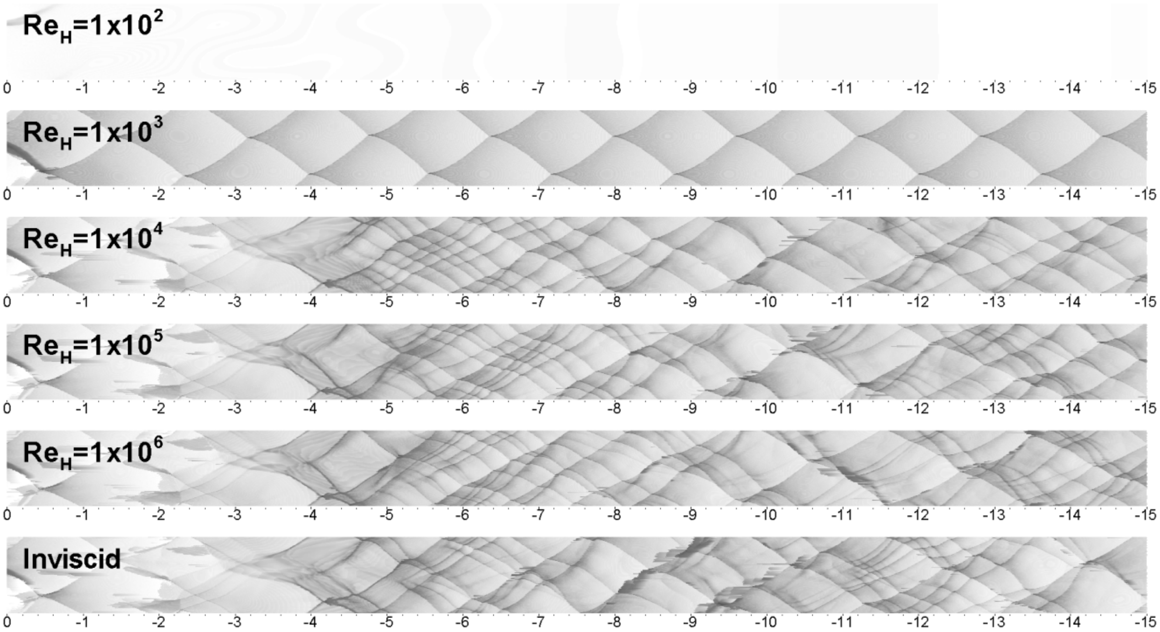


Figure 4. Maximum pressure traces from coarse (501×401) grid simulations.

References

[1] Shepherd JE. (2009) Detonation in Gases. Proc. Combust. Inst. 32:83.

[2] Oran ES, Weber JW, Stefaniw EI, Lefebvre MH, Anderson JD. (1998). A Numerical Study of a Two-Dimensional H_2-O_2-Ar Detonation Using a Detailed Chemical Reaction Model. Combustion and Flame. 113:147.

[3] Lee HI, Stewart DS. (1990). Calculation of linear detonation instability. I. One-dimensional instability of plane detonation. Journal of Fluid Mechanics. 216:103.

[4] Bourlioux A, Majda AJ. (1995). Theoretical and Numerical Structure of Unstable Detonations. Philosophical Transactions. Physical Sciences and Engineering. 350(1692):29.

[5] Powers JM. (2006). Review of Multiscale Modeling of Detonation. J. Prop. Power 22:1217.

[6] Sharpe GJ. (2001). Transverse Waves in Numerical Simulations of Cellular Detonations. Journal of Fluid Mechanics. 447:31.

[7] Radulescu MI, Sharpe GJ, Law CK, Lee JHS. (2007). The Hydrodynamic Structure of Unstable Cellular Detonations. J. Fluid Mech. 580 :31.

[8] Choi JY, Ma F, Yang V. (2008). Some Numerical Issues on Simulation of Detonation Cell Structures, Comb. Expl. Shock Waves 44(5): 560.

[9] Austin JM. (2003). The Role of Instability in Gaseous Detonation. Ph.D. Dissertation, California Institute of Technology, Pasadena, CA.