Numerical Simulation of Detonation behind Slit-Plate

Fumiya Togashi¹, Rainald Löhner¹, Nobuyuki Tsuboi², Tetsuro Obara³, Jayan Sentanuhady³, and Shigeharu Ohyagi³

> ¹College of Science, George Mason University 4400 University Dr., Fairfax, VA 22030, USA

²Institute of Space and Astronautical Science, Japan Aerospace Exploration Agency Yoshinodai 3-1-1, 229-8510, Japan
³Graduate School of Science and Engineering, Saitama University Shimo-Okubo 255, 338-8570, Japan

Abstract

2-D simulation to investigate the phenomena of the detonation wave in a tube with the slit-plate was conducted. During the propagation in a tube with the slit-plate, the detonation wave might be quenched and reinitiate behind the slit-plate. The computed results will be compared with the experimental data in the final presentation.

1 Introduction

Recently, detonation has been applied to the next generation engines such as Pulse Detonation Engine (PDE) and Supersonic Combustion Ram Jet engine (SCRAM Jet) [1, 2]. On the other hand, a detonation of the type considered here can also be applied to some fuel-air explosives. In order to understand the nature and structure of a detonation under these various situations, more analysis of a detonation under various circumstances is required. Especially, the development of proper numerical analysis tools is necessary to enhance understanding and reduce cost and risk. Numerical simulation of these flow fields is not an easy task because the computation includes complicated combustion kinetics, diffusion processes, and huge energy releases into the field and requires much more nodal points compared to inert compressible flow computations. However, due to the recent progress in both computational methods and available computer facilities, the computation with detailed reaction models has been possible, though it is limited to smaller spatial domains [3-9].

To observe the phenomena in detail, 2-D computation was very important under current computational resources. The purpose of this study is to simulate the detonation wave propagating through the slit-plate with a fine enough to capture cell structures of the detonation waves and to study the phenomina behind the slit-plate and the quench/reignition of detonation waves.

2 Flow Solver

In this study, the Petersen & Hanson model (PH model) is used for chemical kinetics that consists of 9 species (H₂, O₂, H, O, OH, HO₂, H₂O₂, H₂O, and N₂) and 18 elementary reactions. The data for the chemical reaction was taken from the paper of Petersen & Hanson [10].

The chemical reaction model described above was implemented into FEFLO, a general-purpose CFD code based on the following general principles:

- Use of unstructured grids (automatic grid generation and mesh refinement);

- Finite element discretization of space;
- Separate flow modules for compressible and incompressible flows;
- ALE formulation for body fitted moving grids;
- Embedded formulation for complex/dirty geometries;
- Edge-based data structures for speed;
- Optimal data structures for different supercomputer architectures;
- Bottom-up coding from the subroutine level to assure an open-ended, expandable architecture.

The code has a long history of relevant applications [11-16]. Over the last three years, FEFLO has been ported to both shared memory [17-18] and distributed memory [13, 19, and 20] machines.

3 Computational Domain and Result

The computation modeled a detonation propagating in a stoichiometric H_2 -O₂ gas, diluted with N₂. The mole concentration ratio of the $H_2/O_2/N_2$ gas mixture was 2:1:3.76, initial pressure is 1 atm, and temperature is 300K. At first, the 1-D detonation wave was initiated and let it propagate until it reached CJ velocity. Then the 1-D computed result was placed on a 2-D grid with a sheet of unburned gas mixture behind the detonation front and also let it propagate until it formed the cell structures [21]. Finally the 2-D detonation results were interpolated to the computational grid with a slit-plate. Figure 1 shows the computational domain with computational mesh. The width of tube and slit is 2mm and 0.2mm respectively. The computational mesh size is 5µm average and the number of tetra elements are 1.2 million.



Figure 1. Computational domain and computational mesh.

Figure 2 shows the computed pressure contours at each time. The required CPU time was about 40 hours by SGI ALTIX using 16 CPU processors. The detonation wave propagated and hit the slit-plate as shown in Fig.2(a) and (b). In Fig.2(c), the detonation wave entered the slit and reflected on the wall of the slit-plate. In Fig. 2(d), Curved shock waves were formed behind the slit-plate due to the affect of the expansion wave generated on the corner of slit-exit. The reaction surface couldn't pass through the slit-plate and only shock waves propagate behind the slit-plate. Therefore the shock and the reaction front are decoupled. The high pressure and high temperature point was generated due to the interference of generated two shock waves in Fig.2 (d) and (e), however, the re-initiation of the detonation wave couldn't be observed in this computation as shown in Fig.2 (e)-(i). One of the reasons for the detonation initiation failure might be that the slit width is too narrow for the cell structure of the detonation wave to pass through the slit plate. From some experiments, the detonation re-initiation is only observed under the condition that at least one detonation cell have to pass through the slit plate. To investigate this initiation failure and to observe the re-initiation of the detonation, the larger scale computational domain is required.





Figure 2. Computed pressure contoures at each time.

4 Conclusion

2-D computation of the detonation propagation in a tube with the slit-plate was conducted. In this computation, the detonation initiation behind the slit-plate was not observed.

21st ICDERS – July 23-27, 2007 - Poitiers

In the final presentation, the simulation with a larger scale computational domain will be conducted. The computed results will be qualitatively compared with the experimental results.

References

- Kailasanath, K., "Review of Propulsion Applications of detonation waves," AIAA J. vol. 38, No. 9, 2000, pp. 1698-1708
- [2] Henry, J. R., and Anderson, G. Y., "Design Considerations for the Air Flame Integrated Scramjet," NASA TM X2895, 1973
- [3] E. S. Oran, T. R. Young, and J. P. Boris, "Weak and Strong Ignition. I. Numerical Simulations of Shock Tube Experiments," *Combustion and Flame*, vol. 48, 1982, pp. 135-148
- [4] E. S. Oran, J. W. Weber, Jr., E. I. Stefaniw, M. H. Lefebvre, and J. D. Anderson, Jr., "A Numerical Study of a Two-Dimensional H₂-O₂-Ar Detonation Using a Detailed Chemical Reaction Model," *Combustion and Flame*, vol. 113, 1998, pp. 147-163
- [5] G. J. Wilson and R. W. MacCormack, "Modeling Supersonic Combustion Using a Fully Implicit Numerical Method," AIAA J., vol. 30, No. 4, Apr. 1992
- [6] N. Tsuboi, S. Katoh, and K. Hayashi, "Three-dimensional Numerical Simulation for Hydrogen/Air Detonation: Rectangular and Diagonal Structures," Proceedings of the Combustion Institute, vol. 29, 2002, pp. 2783-2788
- [7] K. Eto, N. Tsuboi, and A. K. Hayashi, "Numerical Study on Three-Dimensional C-J Detonation Waves: Detailed Propagating Mechanism and Existence of OH Radical," Proceedings of the Combustion Institute 30, The Combustion Institute, Vol. 30, pp.1907-1913,2005.
- [8] N. Tsuboi, K. Eto, A.K. Hayashi, "Three-Dimensional Numerical Simulation of H2/Air Detonation in a Circular Tube: Structure of Spinning Mode," 20th International Colloquium on the Dynamics of Explosions and Reactive Systems, No.71, Montreal, Canada, July, 2005.
- [9] A. K. Hayashi, K. Eto, N. Tsuboi, "Numerical Simulation of Spin Detonation in Square Tube," 20th International Colloquium on the Dynamics of Explosions and Reactive Systems, No.85, Montreal, Canada, July, 2005.
- [10] E. L. Petersen, R. K. Hanson, "Reduced Kinetics Mechanisms for Ram Accelerator Combustion," *Journal of Propulsion and Power*, vol. 15, No.4, July-August 1999, pp. 591-600
- [11] J. D. Baum and R. Löhner, "Numerical Simulation of Shock Interaction with a Modern Main Battle field Tank," AIAA-91-1666, 1991
- [12] J. D. Baum, H. Luo and R. Löhner, "Numerical Simulation of a Blast Inside a Boeing 747," AIAA-93-3091, 1993
- [13] R. Ramamurti and R. Löhner, "Simulation of Flow Past Complex Geometries Using a Parallel Implicit Incompressible Flow Solver," pp. 1049, 1050 in *Proc.11th AIAA CFD Conf.*, Orlando, FL, July, 1993
- [14] J. D. Baum, H. Luo and R. Löhner, "Numerical Simulation of Blast in the World Trade Center," AIAA-95-0085, 1995
- [15] J. D. Baum, H. Luo, E. Mestreau, R. Löhner, D. Pelessone, and C. Charman, "A Coupled CFD/CSD Methodology for Modeling Weapon Detonation and Fragmentation," AIAA-99-0794, 1999
- [16] R. Ramamurti, W. Sandberg and R. Löhner, "Simulation of Flow About Flapping Airfoils Using a Finite Element Incompressible Flow Solver," AIAA-99-0652, 1999
- [17] R. Löhner, "Renumbering Strategies for Unstructured-Grid Solvers Operating on Shared-Memory, Cache-Based Parallel Machines," Comp. Meth. Appl. Mech. Eng. 163, 1998, pp. 95-109
- [18] D. Sharov, H. Luo, J. D. Baum and R. Löhner "Implementation of Unstructured Grid GMRES+LU-SGS Method on Shared-Memory, Cache-Based Parallel Computers," AIAA-00-0927, 2000
- [19] R. Löhner and R. Ramamurti, "A Load Balancing Algorithm for Unstructured Grids," Comp. Fluid Dyn. 5, 1995, pp. 39-58
- [20] R. Ramamurti and R. Löhner, "A Parallel Implicit Incompressible Flow Solver Using Unstructured Meshes," *Computers and Fluids* 5, 1996, pp. 119-132
- [21] M. H. Lefebvre, E. S. Oran, K. Kailasanath, and P. J. Van Tigglelen, Combustion & Flame vol. 95, 1993, pp.206-218