Advances in Applied Mathematics and Mechanics
Adv. Appl. Math. Mech., Vol. **6**, No. 6, pp. 718-731

DOI: 10.4208/aamm.2013.m159
December 2014

Numerical Simulation of Deflagration to Detonation Transition in a Straight Duct: Effects of Energy Release and Detonation Stability

Hua-Shu Dou[1,*], Zongmin Hu[2], Boo Cheong Khoo[3] and Zonglin Jiang[2]

[1] *Faculty of Mechanical Engineering and Automation, Zhejiang Sci-Tech University, Hangzhou 310018, China*
[2] *State Key Laboratory of High Temperature Gas Dynamics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100080, China*
[3] *Department of Mechanical Engineering, National University of Singapore, Singapore 119260, Singapore*

Received 18 March 2013; Accepted (in revised version) 19 June 2014

Available online 7 August 2014

Abstract. Numerical simulation based on the Euler equation and one-step reaction model is carried out to investigate the process of deflagration to detonation transition (DDT) occurring in a straight duct. The numerical method used includes a high resolution fifth-order weighted essentially non-oscillatory (WENO) scheme for spatial discretization, coupled with a third order total variation diminishing Runge-Kutta time stepping method. In particular, effect of energy release on the DDT process is studied. The model parameters used are the heat release at $q=50,30,25,20,15,10$ and 5, the specific heat ratio at 1.2, and the activation temperature at $Ti=15$, respectively. For all the cases, the initial energy in the spark is about the same compared to the detonation energy at the Chapman-Jouguet (CJ) state. It is found from the simulation that the DDT occurrence strongly depends on the magnitude of the energy release. The run-up distance of DDT occurrence decreases with the increase of the energy release for $q=50\sim20$, and increases with the increase of the energy release for $q=20\sim5$. This phenomenon is found to be in agreement with the analysis of mathematical stability theory. It is suggested that the factors to strengthen the DDT would make the detonation more stable, and vice versa. Finally, it is concluded from the simulations that the interaction of the shock wave and the flame front is the main reason for leading to DDT.

PACS: 47.40.-x, 47.40.Rs, 47.70.Fw

Key words: Numerical simulation, detonation, DDT, energy release, duct.

*Corresponding author.
Email: huashudou@yahoo.com (H. S. Dou)

1 Introduction

Deflagration to detonation transition (DDT) is one of the ways to produce detonation which starts from low speed combustion and then accelerates and transits to detonation under certain conditions. Alternatively, detonation can also be produced by direct ignition which requires sufficiently high energy input. In most cases, detonation is generated by DDT since only low energy is required and also it is easier to control. The understanding of the DDT process is therefore important for implementation and control of the detonation. In recent years, much interest has been focused on this phenomenon because of the direct potential application in the pulse detonation engines [1, 2]. On the other hand, it is also useful in disaster prevention and loss prediction [3]. Although there are numerous works on the phenomenon of DDT, the mechanism of this process is yet to be fully understood with broad consensus. Therefore, it is deemed that further study is required to clarify the mechanism in the DDT.

It may be reasonable to consider that the main controlling factors in sustained detonation downstream and those in DDT generation are essentially the same. Self-sustained detonation may decay to the deflagration state if the conditions for detonation are not satisfied. On the DDT occurrence, there have been several theoretical, experimental and numerical studies published in the literature [4, 5].

On the theoretical work, Zeldovich et al. [6] proposed the gradient mechanism of reactions for DDT occurrence; they found that there is an appropriate magnitude of temperature gradient for DDT to happen. Lee et al. [7] described the SWACER (Shock wave acceleration coherent energy release) mechanism, in which the shock-flame interaction allows for a large energy release and hence form a concentration gradient in the induction zone; this gradient promotes the occurrence of detonation. These (so called gradient) mechanisms have been used to explain the DDT phenomena for several cases, but it is still not satisfactory for general cases [8]. Next, Brailovsky and Sivashinsky [9] proposed that the wall friction may be a means to enhance DDT. It is shown that the friction resistance causes a gradual precompression and preheating of the unburned gas adjacent to the advancing deflagration. This leads to a localized thermal explosion which may trigger the occurrence of DDT. However, it is also found that detonation can also be formed in unconfined regions in the absence of wall [10]. Jiang et al.'s [11] study showed that detonation can be sustained in a diverging cylindrical detonation via the generation of new transverse waves. In these unconfined detonations, wall friction is not considered. As such, heating associated with wall friction is not the main reason for DDT to occur.

Still, Vasil'ev [12] proposed a criterion for DDT and obtained the critical Mach number. This criterion is independent of the activation energy. Silvestrini et al. [13] suggested some simplified formulas for evaluating the flame speed and DDT run-up distance of flammable mixtures, based on a large quantity of experimental data. Oran and Gamezo [5] summarized the numerical simulations and experimental data and suggested that the interaction of flame and shock wave is the key to the DDT process. The role of turbulence in DDT is to create conditions in nearby unreacted fuel mixtures that lead to