On the use of Boltzmann equation in the mathematical modeling of gaseous detonations

Abstract

This chapter outlines the past and contemporary efforts aim to achieve better understanding of the detonation phenomena in gases. In fact, the majority of these efforts are derived by the persisting demand to understand the detonation wave front, which requires a molecular scope in analyzing the phenomena. In addition, this chapter elucidates the physics of the Boltzmann equation and its connection with DSMC method in the context of non-equilibrium flows. The interest in investigating gaseous detonation come from its tremendous energy conversion rate and the potential of employing the phenomena in future hypersonic propulsion systems through pulse detonation engines. Another important motivation to use a molecular level methodology in simulating gaseous detonations is the lack of understanding of DDT (Deflagration to Detonation Transition). The detonation phenomenon was firstly observed as a "violent chemical reaction" with the discovery and use of explosives in the fifteenth century. In fact, the first explosive known to sustain detonation waves was the gold fulminate; introduced by Oswald Croll in 1608 (Bacon and Rees 2000). However, detonation was not defined and distinguished apart from other forms of combustion until the development of certain diagnostic tools which enabled the measurement of the detonation wave velocity. This was probably done by Abel in 1869 (Abel 1869). The first efforts resulted in defining the range of detonation wave velocity of several gaseous fuels and its dependency factors were revealed by Berthelot and Vieille between 1881 and 1883 (Berthelot and Vieille 1883). By the end of the nineteenth century, detonation as a mode of combustion was clearly distinguished from deflagration based on the propagation velocity. The chemical reaction in detonation waves was reasoned to be initiated by the adiabatic compression in the detonation front (Mallard and Chˆ atelier 1883) and (Dixon 1893).

Detonation can be defined as a shock wave sustained by a chemical reaction. However, to get deeper understanding of the nature and physics of detonation, sophisticated explanation of its mechanism is mandatory to comprehend. The chemical reaction associated with detonation consumes the combustible material about 103 to 108 faster than in other forms of combustion (i.e. deflagration). The meaning of this ultra-high combustion speed can be appreciated if one compared the energy converted through detonation to a well know energy conversion reference. If a detonation process was initiated into a good solid explosive material, energy is converted at a rate of 1010 watts/square centimeters of its detonation front. A 2 meter square detonation waves gives energy more than the total electric generating capacity of the united states in 2006, which was1.075×1012 watts. This enormous energy conversion rate has motivated researchers since the early days of the twentieth century to investigate the various aspects of detonation theory and application. Since the main property distinguishes detonation from other forms of combustion is velocity, researchers fundamentally were interested to calculate it. L. Chapman and E. Jouguet have formulated a theory to predict the velocity of one dimensional detonation waves between 1899 and 1905 (Becker 1922). In their work, Chapman and Jouguet treated the detonation front as a discontinuity plane across which the conservation waves of shock waves apply. In the CJ theory, the velocity of steady detonation is consistent with the conservation conditions. Once the detonation wave is known, and the equation of state of the reaction products is given, the conservation laws determine the final state behind the detonation front. This theory, however, totally disregards the features of detonation structure because of the insinuation of the one dimensional, adiabatic flow assumptions. Basically, it yields the possible solution of the steady one dimensional conservation equations that links the equilibrium states of the upstream reactants and downstream products. In order to know the propagation mechanism of detonation waves, a more detailed and generalized theory had to be introduced.