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Theoretical Notes on the Mathematical Modelling of Gaseous Detonations Using Boltzmann Equation

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Abstract: In this study, we present some theoretical notes on the use of the Boltzmann equation in computing detonation of combustible gases. The scarceness of relevant study, as well as the sensitivity of the topic, were the major motivations behind the intention to present these notes for publication. A timeline of the detonation phenomenon and its physical comprehension was drawn to justify the unsuitability of the continuum hypothesis of describing gaseous detonations. Then, the theory behind the Boltzmann equation and DSMC is elaborated. Finally, a discussion of the available study on the topic is introduced and concluded.

Key words: Gaseous detonation, Boltmann equation, DSMC, Knudsen number, molecular physics, physical chemistry, computational methods, CFD

INTRODUCTION

This study 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 article theoretically 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 detonation phenomenon in future hypersonic propulsion systems through pulse detonation engines (Saqr *et al*., 2010) and in power generation systems (Wahid *et al*., 2008a, b, 2009). Another important motivation to use a molecular level methodology in simulating gaseous detonations is the lack of comprehensive 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 (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 (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 (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 10^3 to 10^8 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 10^{10} W cm^{-2} of its detonation front. Two square meters detonation wave gives energy more than the total electric generating capacity of the United States in 2006, which was 1.075×10^{12} W.

This enormous energy conversion rate has motivated researchers since the early days of the twentieth century

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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 study, 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.

The ZND theory was named after Zildovich in 1914-1987, von Neumann in 1903-1957 and Döring in 1911-2006, who were conducting their research independently in the 1940s. They based their study on the inviscid equations of Euler hydrodynamics. This theory was the first to divide the detonation structure into a leading shock front followed by a chemical reaction zone. Zel'dovich (1940) investigated the effects of including the heat and momentum losses on the detonation structure. This investigation aimed to rise above the assumptions of the CJ theory. His study showed that at some critical values of the loss terms, it was possible to explain the onset of detonation as the velocity is much less than the equilibrium CJ value. In the same time, von Neumann managed to demonstrate the pathological detonations which have velocities higher than the CJ velocity. A year later, Döring studied the thermodynamic states within the detonation zone. The ZND theory of detonation gave the most firm explanation of the propagation mechanism in this furious form of combustion. It proposes that in detonation, energy transfers by mass flow in strong compression wave, on the contrary of deflagration, where the important energy transfer depends on conduction. The detonation front-a shock wave is propagating with a supersonic speed into the combustible medium causing its temperature to rise sharply. The sharp temperature rise occurs due to the adiabatic compression effect of the shock wave. Chemical reactions are being triggered simultaneously due to the explosive nature of the combustible medium. Then, these chemical reactions supports the propagation of the shock wave further into the medium (Fickett and Davis, 1979).

One of the main significant contributions of the ZND theory is the presentation of a thickness for the detonation front. This was achieved by series of the Hugoniot curves representing the successive fractions of a reaction in detonation. Later on, several researches have been conducted to evaluate the value of such thickness under different conditions. Typically, this thickness equals two to three mean-free-paths, which in return represent the characteristic length scale of the detonation (O'Connor *et al*., 2006).

As a result, the Kn (Knudsen number) for detonations ranges between 0.3 to 0.5. This would take the detonation problem far beyond the limits of continuum fluid mechanics, since that Kn limit for Euler and Navier-Stokes equations is zero and 0.05, respectively (Long, 1991). For this reason, in order to study the thermodynamic changes in the transition region of the detonation front, it is necessary to use a governing equation that is valid for Kn values greater than 0.05, which is able to model the macroscopic momentum and heat fluxes within the detonation front. Boltzmann equation is the only equation capable of achieving this goal since it is valid for all values of Kn because of its molecular nature. Here, will be discuss the physics and advantages of using Boltzmann equation in detonation problems as well as highlighting the DSMC (Direct Simulation Monte Carlo) method to solve the Boltzmann equation.

THE BOLTZMANN EQUATION AND DSMC

Whenever Boltzmann equation is mentioned for gas dynamics problems, DSMC (Direct Simulation Monte Carlo) method must come into consideration. Fundamentally speaking, both the Boltzmann equation and DSMC are based on the kinetic theory of gases. Classical texts explained this theory by giving the example of a billiards table, where each ball represents a molecule of the gas and the cushions represent the container (Jeans, 1925). Just the same as this mechanical illustration, the kinetic theory assumes that all molecules have the same size and are spherically identical. All molecules are constantly in motion, translating and colliding with each others and with the cushions of a billiard table (or the walls of a gas container). The kinetic theory describes the macroscopic behavior of the system in respect to the microscopic motion of its molecules. Temperature, for example, represent the intensity of random motion of the molecules, while pressure represents the molecular force

exerted on the container surfaces (i.e., collision of the balls on the cushions.). It is vital in this sense to comprehend this example and concepts in order to understand the physics behind the Boltzmann equation and the DSMC method.

Microscopic interactions are accountable for all the phenomena that occur in a gas flow. They govern the variation in properties across the fluid flow and also govern the transfer of heat across surfaces as well as the generation of forces on these surfaces. These variations in fluid properties are often formulated in terms of statistical distributions, which are also used to formulate the surface boundary condition. The Boltzmann equation arises from the attempt to equate the variations in fluid properties to the behavior of the microscopic interactions that generate these variations (Agbormbai, 2002; Azwadi and Tanahashi, 2006, 2007).

The theory to connect between kinetic theory and fluid dynamics was commenced by Hilbert (1912), Zeytounian (2002), Azwadi and Tanahashi (2008) and Azwadi *et al*. (2010). The famous mathematician Hilbert indicated how to approximately solve the Boltzmann equation for the kinetic theory of gases in 1912. In the same year, Chapman and Enskog, independently devised approximate solution of the Boltzmann equation valid for dense gases. Enskog followed a method that generalizing Hilbert idea. His method was adopted by Chapman and Cowling (1952) and Azwadi and Irwan (2010) and became known as the Chapman-Enskog method.

In Bird (1963), expanded the Monte Carlo method into gas dynamics and the method came to be known as Direct Simulation Monte Carlo, or DSMC. The fundamental approach of this un-deterministic simulation method is to take statistical samples as the basis for predicting the physical behavior of the fluid. In details, the DSMC method discretises the collision and convection terms of the Boltzmann equation by calculating them separately within a time interval that is small compared to the mean time between two collisions. Within this small time interval, molecular interactions are decoupled from molecular motions and within a discretised flow field molecules are moved, searched for and allowed to collide. Associated colliding molecules are sampled from near adjacents within the discrete cells. Molecules that are determined to have crossed a surface boundary are made to undergo gas-surface interactions, whereas those that cross out of the flow field are abandoned Upstream, new molecules constantly enter the flow field (Sone, 2007; Cercignani, 2000; Agbormbai, 2002).

The use of DSMC method with detonation problems started very recently in 2000 (Long and Anderson, 2000). The standard DSMC algorithm consists of 5 steps, required for the simulation of gaseous detonations. Before the simulation starts, initialization of the cells and molecules must be taken over. A cell is a three dimensional computational domain in physical space that will initially contain some random fraction of the total number of molecules specified for the simulation. Normally, each cell has dimensions smaller than the mean-free-path. The time-step size should be a small fraction of the mean collision time between two molecules. After the initialization of the cells, molecules are randomly introduced into the domain (i.e., cell) and the following four uncoupled steps are repeated for every time step:

- Allow the molecules to move according to the time-step and their velocity, while applying the boundary conditions
- Organize the molecules into cells based on their new positions relative to their local cell
- Allow random collision between selected molecules
- Provide the molecules with the opportunity (i.e., time) for chemical reaction and/or redistribution of energy
- After specified number of time steps, sample the microscopic properties in each cell. Macroscopic flow properties are calculated after a specified number of microscopic samples have been collected (O'Connor *et al*., 2006)

One major obstacle in developing codes using DSMC for gaseous detonations is the computational power demand. Cell size would have to be infinitesimal in order to be less than the mean free path. This implies that in order to investigate detonation wave in a few millimeters size domain, the DSMC would have to run over hundreds of thousands on cells. Keeping in mind the probabilistic nature of DSMC, this would require lengthy hours to reach a steady detonation, even with monatomic or diatomic gas mixtures.

A REVIEW OF LITERATURE

Research publications studying gaseous detonations using the Boltzmann equation and DSMC are very scarce. A very important research was published in 2002 on the pulse detonation engine. The research investigated two-dimensional nano-scale detonations which are dominated by wall effects (Genovesi and Long, 2002). The researchers, who conducted this study in Pennsylvania State University concluded that there is a relationship between the curvature of the detonation wave and its detonation speed. However, they stated that the existence of higher computational power to be utilized with the DSMC method is the only way to investigate this relationship through multi-dimensional simulation of detonations.

In 2004, a similar problem was simulated using DSMC (Sharma and Long, 2004). The blast impact problem was formulated using an assumption that the impact does not deform the container. The DSMC code was operated on a parallel computing system. In the following year, another research paper was published by the same group in Pennsylvania, U.S. The researchers studied the ultra fast detonations which exceeds the steady-state velocities predicted by the CJ and ZND theories (O'Connor *et al*., 2005). Their results describe a case where the detonation front and the reaction zone overlap, with an unpredictable behavior. However, the results obtained from the DSMC simulation of such unusual detonations have not been verified to this moment.

Two years later, a ground-breaking paper was presented in the Annual Joint Propulsion Conference and Exhibit, U.S. The study analyzed and reported the initial results of bimolecular detonations using DSMC in order to plot the thermodynamic properties across the detonation wave front. This was successfully obtained, while it was impossible using the continuum equations (i.e., Euler and/or Navier-Stokes). The DSMC structure described in this paper was modified in order to comprise more complex chemical reactions (O'Connor *et al*., 2006).

CONCLUSIONS

The Boltzmann equation through DSMC is capable of studying gaseous detonations at levels of detail that can not be reached by continuum approaches. The major challenges in developing the DSMC codes for detonation problems are:

- The computing resources demand: which can be addressed through the implementation of parallel computing facilities and algorithms and object oriented programming approaches
- The inclusion of complex chemical reaction models
- Physical reasoning and fundamental explanation of the results obtained across the detonation wave front, which can not be verified experimentally

REFERENCES

Abel, F.A., 1869. Contributions to the history of explosive agents. Phil. Trans. R. Soc., 159: 489-516.

Agbormbai, A.A., 2002. The Bolztmann equation and DSMC method for rariefied gas dynamics. Proceedings of the 40th AIAA Aerospace Sciences Meeting and Exhibit, January 14-17, Reno, NV., AIAA 2002-0215.

Azwadi, C.S.N. and T. Tanahashi, 2006. Simplified thermal lattice Boltzmann in incompressible limit. Int. J. Modern Phys. B., 20: 2437-2449.

Azwadi, C.S.N. and T. Tanahashi, 2007. Three-dimensional thermal lattice Boltzmann simulation of natural convection in a cubic cavity. Int. J. Mod. Phys. B., 21: 87-96.

Azwadi, C.S.N. and T. Tanahashi, 2008. Simplified finite difference thermal lattice Boltzmann method. Int. J. Modern Phys. B., 22: 3865-3876.

Azwadi, C.S.N. and M.A.M. Irwan, 2010. Macro and mesoscale simulations of free convective heat transfer in a cavity at various aspect ratios. J. Applied Sci., 10: 203-208.

Azwadi, C.S.N., M.M.Y. Fairus and S. Samion, 2010. Virtual study of natural convection heat transfer in an inclined square cavity. J. Applied Sci., 10: 331-336.

Bacon, F. and G. Rees, 2000. The Instauratio Magna. Oxford University Press, Oxford, pp: 295.

Becker, R., 1922. Impact waves and detonations. Z. Phys., 8: 321-362.

Berthelot, M. and P. Vieille, 1883. L'oude explosive. Ann. Chim. Phys., 28: 289-289.

Bird, G.A., 1963. Approach to translational equilibrium in a rigid sphere gas. Phys. Fluids, 6: 1518-1519.

Cercignani, C., 2000. Rarefied Gas Dynamics. Cambridge University Press, Cambridge, pp: 117-124.

Chapman, D.L., 1899. On the rate of explosion in gases. Philos. Mag., 47: 90-104.

Dixon, H.B., 1893. The rate of explosion in gases. Phil. Trans. R. Soc. Lond. A, 184: 97-188.

Fickett, W. and W.C. Davis, 1979. Detonation: Theory and Experiment. Dover Publications, Mineola, New York.

Genovesi, D.J. and L.N. Long, 2002. A java-based direct monte carlo simulation of a nano-scale pulse detonation engine. Proceedings of the 23rd Rarefied Gas Dynamics Conference, (RGDC'02), Whistler, BC, Canada, pp: 1-8.

Hilbert, D., 1912. Justification of the kinetic gas theory. Math. Ann., 72: 562-577.

Jeans, S.J., 1925. The Dynamical Theory of Gases. Dover Publications, New York, pp: 1-66.

Long, L.N., 1991. Navier-stokes and monte carlo results for hypersonic flows. AIAA J., 29: 200-207.

Long, L.N. and J.B. Anderson, 2000. The simulation of detonations using a Monte Carlo method. Proceedings of the 22nd International Symposium on Rarefied Gas Dynamics, July 9-14, Sydney, Australia, pp: 653-657.

O'Connor, P.D., L.N. Long and J.B. Anderson, 2005. Direct simulation of ultrafast detonations in mixtures. AIP Conf. Proc., 762: 517-522.

O'Connor, P.D., L.N. Long and J.B. Anderson, 2006. The direct simulation of detonations. Proceedings of the 42nd AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit, July 9-12, Sacramento, CA., pp: 1-11.

Saqr, K.M., A. Faiz, H. Kassem, M.M. Sies and M.A. Wahid, 2010. Transient Characteristics of C3H8/O2 turbulent mixing in a hypersonic pulse detonation engine. Proceedings of the 9th WSEAS International Conference on Applications of Computer Engineering, Malaysia.

Sharma, A. and L.N. Long, 2004. Numerical simulation of the blast impact problem using the Direct Simulation Monte Carlo (DSMC) method. J. Comput. Phys., 200: 211-237.

Sone, Y., 2007. Molecular Gas Dynamics. 1st Edn., Birkhauser, Boston.

Wahid, M.A. and M.H. Ujir and B. Azwan, 2008a. Effect of inlet section on pulse combustor performance. J. Teknos-2K, 8: 9-14.

Wahid, M.A., H.M. Ujir and M.M. Sies, 2008b. Impulse measurement of pulse combustion tube using accelerometer. Proceedings of the 9th Asia-Pacific International Symposium on Combustion and Energy Utilization, (APISCEU'08), Beijing, China, pp: 1-6.

Wahid, M.A., H. Ujir, K.M. Saqr and M.M. Sies, 2009. Experimental study of confined biogas pulse detonation combustion. Proceedings of the 2nd International Meeting on Advances in Thermo-Fluids, Indonesia.

Zel'dovich, Y.B., 1940. On the theory of the propagation of detonation in gaseous systems. Zh. Eksp. Teor. Fiz., 10: 542-568.

Zeytounian, R.K., 2002. Theory and Applications of Nonviscous Fluid Flows. Springer, Berlin, Heidelberg, pp: 11-20.