HADMÉRNÖK

VII. Évfolyam 2. szám - 2012. június

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HISTORY OF THE BASIC MODELS OF SHOCK AND DETONATION WAVES

Absztrakt/Abstract

A lökéshullám és az azt előidéző detonációs hullám leírásához három alapvető fontosságú modell ismerete elengedhetetlen. Ezek a gázok állapotváltozóinak ugrásszerű változását okozó lökéshullámok irreverzibilis módon lezajló adiabatikus terjedését leíró Rankine-Hugoniot (RH) modell, valamint az ezen alapuló, a robbanóanyagban letrejövő detonációs hullám terjedését megadó Chapman-Joguet (CJ) modell és annak Zeldovich, Neuman és Döring (ZND) által kiegészített változata. A cikkben ezen alapvető elméletek fejlődését tekintjük át.

To describe the detonation process and the resulting shock wave, above all, the importance of three major theories are to be emphasised. These are the Rankine-Hugoniot jump conditions, modelling the propagation of a one-dimensional shock wave; the Chapman-Joguet model for detonation waves in high explosives and its extension by Zeldovich, von Neuman and Döring, the so called ZND detonation model. In this paper we review the development of these basic ideas behind detonation and shock waves.

Kulcsszavak/Keywords: *robbanás, lökéshullám, Chapman-Jouget model ~ detonation, shock wave, Chapman-Jouget model*

INTRODUCTION

Consider a small perturbation in a gas as a pure sinusoidal function of time. This signal propagates through the material. The frequency of the oscillations does not affect the propagation velocity, called the speed of sound in the gas, until (called linear region) it approaches the collision frequency between the molecules of the gas (under normal circumstances approximately 10^8 Hz). Consequently, any sound wave satisfying this latter condition may be constructed by multiple superimposed trigonometric functions, that is, the Fourier decomposition can be applied for the amplitude of the disturbance, *A*:

$$A(t) = \sum_i \left[a_i \cdot sin\left(\frac{2\pi i}{T}t\right) + b_i \cdot cos\left(\frac{2\pi i}{T}t\right)\right]$$

As the amplitude of a sound wave is increased, that is, the energy cannot be dissipated from the source by sound waves, as rapidly as it is deposited. The result is the compression of the gas surrounding the source to the point that the resultant compressive heating increases the local sound speed. If the dissipation of the energy caused by the expansion of the gas within the compressive wave does not reduce the sound speed of the front of the wave to that of the ambient gas, the energy accumulates at the front and a shockwave results.

In general, therefore, a mechanical shock wave is a disturbance propagating in a medium, which can be solid, fluid, gas or even plasma. Contrary to normal acoustic waves, shock waves are characterised by an abrupt and nearly discontinuous change in the state variables (pressure, density and temperature) of the material at the wave front. In our case most shock waves are caused by rapid exothermic chemical reactions of high explosives, this process is known as detonation. A *detonation* wave is essentially a shock wave through a highly combustible or chemically unstable medium. The chemical reaction of the medium occurs following the shock wave, and the chemical energy of the reaction drives the wave forward.

Distinction must be made between the most important terminologies of the above mentioned exothermic chemical reactions. *Combustion* is the term used to describe any oxidation reactions. When the explosive material decomposes at a rate below the speed of sound in the material, no shock wave occurs, and the combustion process is known as *deflagration*. In this case, it is driven by the liberated reaction heat surplus and the reaction products flow towards the opposite direction to that of the decomposition. On the other hand, if the reaction rate, described by the detonation velocity, is higher than the speed of sound in the material, consequently producing a high intensity shock wave, the combustion process is called *detonation*. Contrary to the previous one, the reaction products flow in the direction of the decomposition, and the process is driven by the abrupt changes in the state variables, i.e., the energy is transmitted by the work of compression rather than by heat conduction.

It is also important to emphasise that not only explosions can produce shock waves. In fact, many of them are encountered in our everyday life. These are, for example, the clapping of our hands, the snapping of belts and whip-cracking (the acceleration o its tip to supersonic velocity) to mention a few. A bit more technical occurrences impose some practical limitations. For instance, the forward velocity of a helicopter is limited because the forward moving blade tip cannot exceed the speed of sound in air. If it does, a shock wave forms and causes serious vibration of the blades. High speed trains travelling through tunnels create shock waves which may cause damage to structures near the exit of the tunnel. Finally the most common technical occurrence is the so called sonic boom, caused by supersonic aircrafts reaching the speed of sound. It can readily be seen, that shock waves are possible to be handled separate from detonation theory, and, as it started to develop around a century before scientists managed to describe the mechanism of detonation, we also follow this approach in the subsequent sections.

SHOCK WAVE

History

From a historical point of view, the first period of the evolution of modern shock wave physics started from the birth of supersonic aeroballistics, when an English mathematician and military engineer *Benjamin Robins* started to quantitatively determine the velocity of a moving bullet using a ballistic pendulum in 1746 [3]. During his experiments he managed measure spherical projectiles travelling at velocities of up to about 500 m/s, $M \approx 1.5$ at 20°C, and concluded that aerodynamic drag increases significantly when approaching the speed of sound.

In 1759 *Leonhard Euler*, the famous Swiss mathematician reported in a letter to Lagrange, that contrary to sound waves of infinitesimal amplitude, the velocity of sounds of finite amplitude depends on the disturbance amplitude. However, he incorrectly assumed that the velocity diminishes with increasing amplitude.

Although, this was the time of basic observations and initial experiments, the lack of mathematical apparatus and sufficient thermodynamic foundations still prevented scientists to understand shock phenomena until the paper of *Henri Hugoniot* in 1887 [8].

From this aspect, the importance of *Gaspard Monge* is unquestionable. Not only had his works on solutions to first order partial differential equations established the foundations for the method of characteristics in 1773 [4], but he also participated in creating one of the most prestigious education centres in the world at that time, the Ecole Polytechnique of Paris, from where scientist like Lagrange, Poisson, Fourier, Duhamel, Cauchy, Carnot, Biot, Fresnel, Hugoniot, Navier, Saint-Venant, Sturm, Liouville and Poincaré graduated, to list but a few. This school and the rival English scientific community created the foundations in the 19th century enabling the development of modern shock wave theory.

In 1808 the paper by *Poisson* [5], based on his lecture on the theory of sound delivered the previous year, presented the exact solution of the one dimensional wave propagation. Later in 1823 he also managed to formulate the isentropic gas law for sound waves of infinitesimal amplitudes. This is regarded as the foundation for shock wave theory and theoretical nonlinear acoustics.

Riemann also made a significant contribution to shock wave theory in 1860 in his paper [6] on the theory of waves of finite amplitude , in which using Monge's method of characteristics he showed that the original disturbance splits into two opposite waves, the rarefaction wave and the condensation wave (a shock wave). While the former grows thicker, the latter grows thinner, and the gas passed over by the shock wave will be compressed and heated while that passed over by the rarefaction will be expanded and cooled. However, using the static adiaba, he erroneously assumed that the entropy (the measure of disorder in a system) remains unchanged through the shock wave. This, based on the second law of thermodynamics, implies a reversible process, whereas the shock wave propagation is irreversible.

Rankine was the first to recognize in 1969 [7], and later, individually by *Hugoinot*, in 1887 [8], [9], that the shock wave is irreversible. The theory formulated by them is still the basic model of shock wave propagation.

The Rankine-Hugoniot jump condition

Consider a shock wave front propagating with velocity U in one dimension in an ideal gas under adiabatic conditions with negligible body forces. The picture below depicts a possible set-up in a long tube with constant cross section, where indices 1 and 2 refer to the state before and after the shock wave front respectively. The initial stage is shown above; the subsequent one, after Δt time, is shown below. The variables are: the density (ρ), the specific internal energy (e), the pressure (p) and the velocity (u).

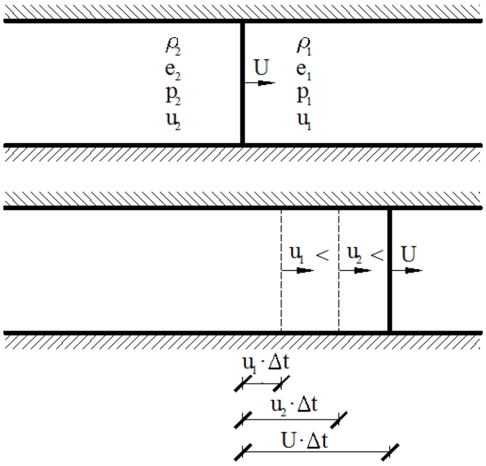

Figure 1. Shock wave propagation in one dimension

The shock wave front is assumed to be infinitesimal and the functions of state variables are not continuous there. An abrupt change occurs, hence the name: jump condition. It is worth noting, that in the 18th century the idea of a function describing nature not being continuous was a source of general philosophic debate, like that between Euler and d'Alambert over the solution of a vibrating string. This issue traces its roots back to the ancient Rome, as the famous saying by Lucretius Caro (98 BC – 55 BC), a Roman Epicurean poet, says: "Natura non facit saltus", that is, Nature does not make jumps. The resolution can be made with a short reasoning on nonlinearity. While, up to the elastic limit, the speed of sound in a material is constant, beyond that, it increases with increasing pressure. Consequently, the wave front is getting more and more narrow, until it consists only of a thin surface.

Using only the three conservation equations and the state equation of the gas, it is possible to form the model:

The mass conservation states that mass is not produced or annulled:

$$\rho_2 \cdot (U - u_2) = \rho_1 \cdot (U - u_1).$$

The momentum conservation yields from Newton's second law:

$$p_2 - p_1 = \rho_1 \cdot (u_2 - u_1) \cdot (U - u_1).$$

The energy conservation:

$$e_2 - e_1 = \frac{p_2 \cdot u_2 - p_1 \cdot u_1}{\rho_1 \cdot (U - u_1)} - \frac{1}{2}(u_2^2 - u_1^2)$$

The state equation relates the energy to the pressure and the density, or any other two state variables. Here we only give the formula for an ideal gas, where γ is the ratio of the specific heats of the gas measured under constant pressure (izobar) measured in constant volume (izochor):

$$p = (\gamma - 1) \cdot \rho \cdot e$$

DETONATION

The phenomenon of detonation was first observed individually by two groups of French scientists: *Mallard* and *Le Chatelier* [12], and *Berthelot* and *Vieille* [13], both in 1883. During their detailed investigations on one dimensional flame propagation in tubes, they concluded, that the detonation wave differs from all other types of flame propagation. During flame propagation, the transmission from layer to layer is governed by thermal conductivity and diffusion exchange between the combustion zone and the unreacted gas by molecular thermal motion, consequently the propagation must be slower than the sound speed in the media; whereas, according to the experiments, the detonation front travels with a constant supersonic velocity particular to each gas mixture: this velocity is independent of the tube properties, provided that the diameter exceeds a certain limiting value for each mixture composition. Mallard and Le Chatelier explained this with compression being the principal mechanism for combustion propagation.

Chapman-Jouguet detonation theory

Detonation theory based on the theory of shock waves was originally proposed by the Russian physicist *Michelson* [14], who published it in 1893. Within six years it was independently developed by *Chapman* in 1899 [15], and valuable contribution was also made by *Jouguet* in 1905 [16], [17], [18]. Since Michelson's publications were unknown outside Russia, the it came to be known as the Chapman-Jouguet (CJ) theory, where the detonation wave is represented as a shock wave with energy release inside the wave front. Basically it means an additional energy source in the RH model. Another important assumption, agreeing with the experiments, that the detonation wave velocity is constant and well defined for each material. Furthermore, based on considerations about the rarefaction and the compression waves, they assumed it to be equals to the local sound speed. This thermodynamic analysis of the phenomenon and the generalization of the shock wave theory was the major breakthrough in the progress of detonation theory.

In essence, the CJ theory deals only with energetic characteristics of detonation waves. Hence, the theory does not take into account chemical reaction kinetics; it is also called the "Zero-reaction zone" model. Since the theory had not taken into account the finite zone of chemical reaction nor any perturbations originating behind the zone not reaching the front of the self-sustained detonation wave, it failed to give any interpretation of detonation failure diameter d_f first documented by *Rosing* and *Chariton* in 1940 [19] (the smallest diameter of explosive charge at which propagation of a steady detonation is still possible without any outside influence). It also failed to interpret so-called spinning detonations, which were discovered by *Campbell* and *Woodhead* in 1926 [20]. As detonation is a multidimensional phenomenon, CJ theory is unable to describe it fully. Therefore, for a long time, spinning detonation was considered as a separate and distinct phenomenon.

Zeldovich-Neumann-Döring detonation theory

A physical model of a detonation wave with finite chemical reaction zone was developed independently by *Zeldovich* in 1940 [21], *Neumann* in 1942 [22] and *Döring* in 1943 [23], hence the acronym: ZND theory. It is also based on the Euler equations of hydrodynamics, i.e. the inviscid flow equations, in which transport effects and dissipation processes apart from the chemical reaction are neglected. The flow is still one-dimensional, the shock is also treated as a discontinuity, but now the reaction, is detached from there and assumed to be triggered by the shock, therefore having a finite rate. It takes place in the reaction zone of finite length, bounded by the shock front on one side, and the CJ plane on the other. As a result, the CJ hypothesis still holds, consequently, in this model, the well described detonation velocity is independent of the form of the reaction rate law.

Acknowledgement

TÁMOP-4.2.1.B-11/2/KMR-2011-0001 „The project was realised through the assistance of the European Union, with the co-financing of the European Social Fund."

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