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STRUCTURE OF SHOCK WAVES ARISING IN UNDERWATER EXPLOSION

Sergey I. Igolkin, Alexander I. Melker*

Department of Mechanics and Control Processes,

St. Petersburg State Polytechnical University, Polytekhnicheskaya 29, 195251, St. Petersburg, Russia

*e-mail: newton@imop.spbstu.ru

Abstract. In this contribution we report on modeling underwater explosion in the framework of molecular dynamics. Calculations displayed the striking resemblance of the underwater explosions modeled and those of observed in real processes; namely, generation of a shock wave and its expanding; formation of a cavity; disintegrating the shock wave, when reaching a surface, transforming the cavity into a water crater of an arising water volcano. For studying the structure of shock waves, a special technique was developed. It allowed observing the form of a shock wave and estimating its velocity. It was found that the shape of a shock wave is changing with time as if the shock wave disintegrated into two parts.

1. Introduction

Until the present time the study of underwater explosions was a privilege of hydrodynamics, where for description of an incompressible liquid, having continuity and fluidity, as well as viscosity, one uses the continuity equation and the Navier-Stokes equations. However, it is difficult to solve this problem by simply writing a complete system of conservation laws in the form of differential equations and closing defining relations, or by developing unique computer programs and codes [1].

Contrary to this approach, we have used molecular dynamics [2] for studying underwater explosions. The main motive is such: since the accepted methods of studying "a wealth of phenomena which nature is not well understood" seem to be ineffective, it is reasonable trying other methods. It should be noted that molecular dynamics has shown its effectiveness in studies of such phenomena as radiation damage of solids, deformation and fracture of materials, nucleation, evolution and self-organization of biological structures and so on [2]. The problem of modeling underwater explosion using molecular dynamics was carefully argued in [3]. In this contribution we used the approach described in that article.

2. Computational procedure

In classical molecular dynamics [2], the motion of a system of N particles is described with the help of Newton's equations. There are various numerical schemes for solving the classical equations of motion, from the simplest Euler methods to the predictor – corrector scheme of high order accuracy. One of the most common and, at the same time, stable and efficient approach to the time discretization of Newton's equations is the Velocity–Verlet algorithm [4] which was used in the present study as a compromise between speed and accuracy. Integration of the motion equations allows finding the trajectories of particles. If the initial positions and velocities of the particles are given, the evolution of the system in time depends only on the potential, which determines the interaction between the particles. Although there

are a lot of potentials which are used in molecular dynamics calculations [5], we have chosen the Lennard–Jones potential. The reasons are given in [3].

Modeling an explosive. We restricted ourselves to 2D computer simulations. To gain a more penetrating insight into the explosion phenomenon, we excluded explosive debris from further research. For this purpose, we developed a simpler explosive model [3]. A certain number of water particles were placed in a circular area of a given size at a predetermined distance (Fig. 1). Thereafter the particles were subjected to radial compression. As a result of changing the distance between particles, the compressed structure accumulates a large amount of elastic energy. During decompression these particles acquire enormous velocities, producing an explosion.

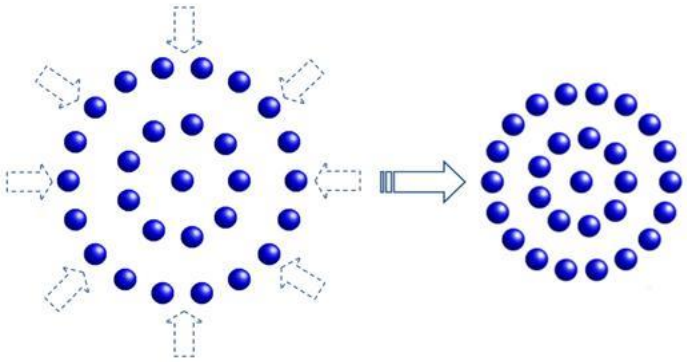

Fig. 1. Model of a self-explosive.

3. Movie

The calculations were done with a system consisting of 27,500 particles. An explosive was inserted into the water after reaching the equilibrium. An example of the temporal evolution of underwater explosion is demonstrated in Fig. 2.

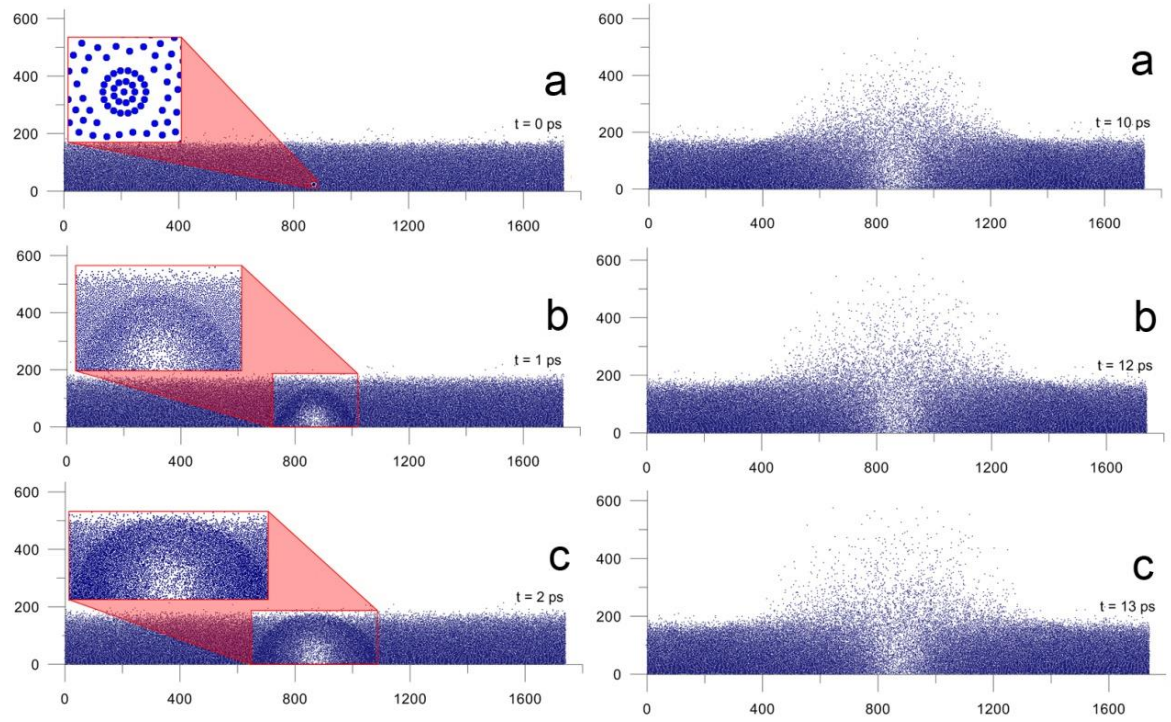

Fig. 2. Time evolution of underwater explosion, t = 0–2 and 10–13. Units are in nm^{-1}.

Figure 2a (left) shows the system before explosion; the zoom area specifies the location and structure of an explosive. Decompression of the explosive creates a shock wave and a cavity (Fig. 2b, left). It should be emphasized that the cavity is not empty and resembles fog (rarefied water). The expanding shock wave produces a dense compression shock in a narrow region (Fig. 2c, left). Thereafter the shock-wave front reaches the free surface. Later the cavity reaches the surface transforming into a water crater (Fig. 2a, right). The following picture resembles a volcanic eruption (Figs. 2b, 2c, right). At first the volcano is very active and then becomes extinct.

4. Studying structure of a shock wave

Up to now there is no complete physical theory describing quantitatively nucleation, development and damping of shock waves. The existing theories have a formal thermodynamical character. The only exception can be found in the book [6] but it contains too many assumptions and became out of date. However, if one wants not only to describe the properties, but understand their nature, one should establish their origin turning to the constituent particles of a system [7]. Unfortunately there are no experimental methods which are able to give such information.

The first step for studying a structure of shock waves with the help of molecular dynamics was done in [8]. However, no description of a special technique developed was given. In this paper we eliminate this drawback. The region in which a shock wave is progressing is divided into three equal circular sectors: 0-30, 30-60, and 60-90 ^{o} (Fig. 3). In its turn, each sector is divided into circular layers of an equal thickness. For each sector, the radial density of particles is calculated with the following formula:

$$\rho_{rad}(t) = \frac{N_{sector}(t)}{L_{sector}} = \frac{6N_{sector}(t)}{\pi R_{sector}}.$$

Here N_{sector} is the number of particles in a sector, L_{sector} is the sector length, and R_{sector} is its radius. The values are taken at definite time intervals. An example of such calculation is represented in Fig. 4 which shows the evolution of shock-wave shape in different sectors (counter-clockwise from x-axis) in an orderly sequence. The wave is moving from left to right.

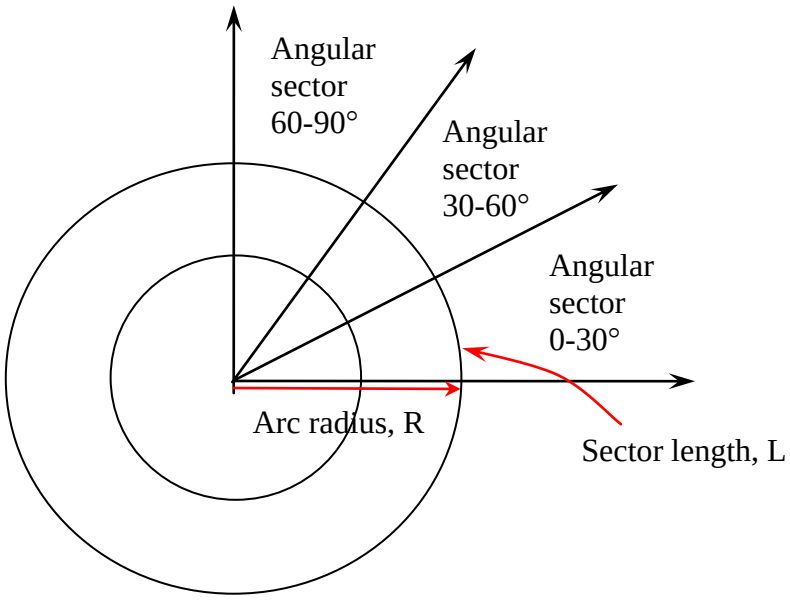

Fig. 3. Fragmentation of a region in which a shock wave is developing.

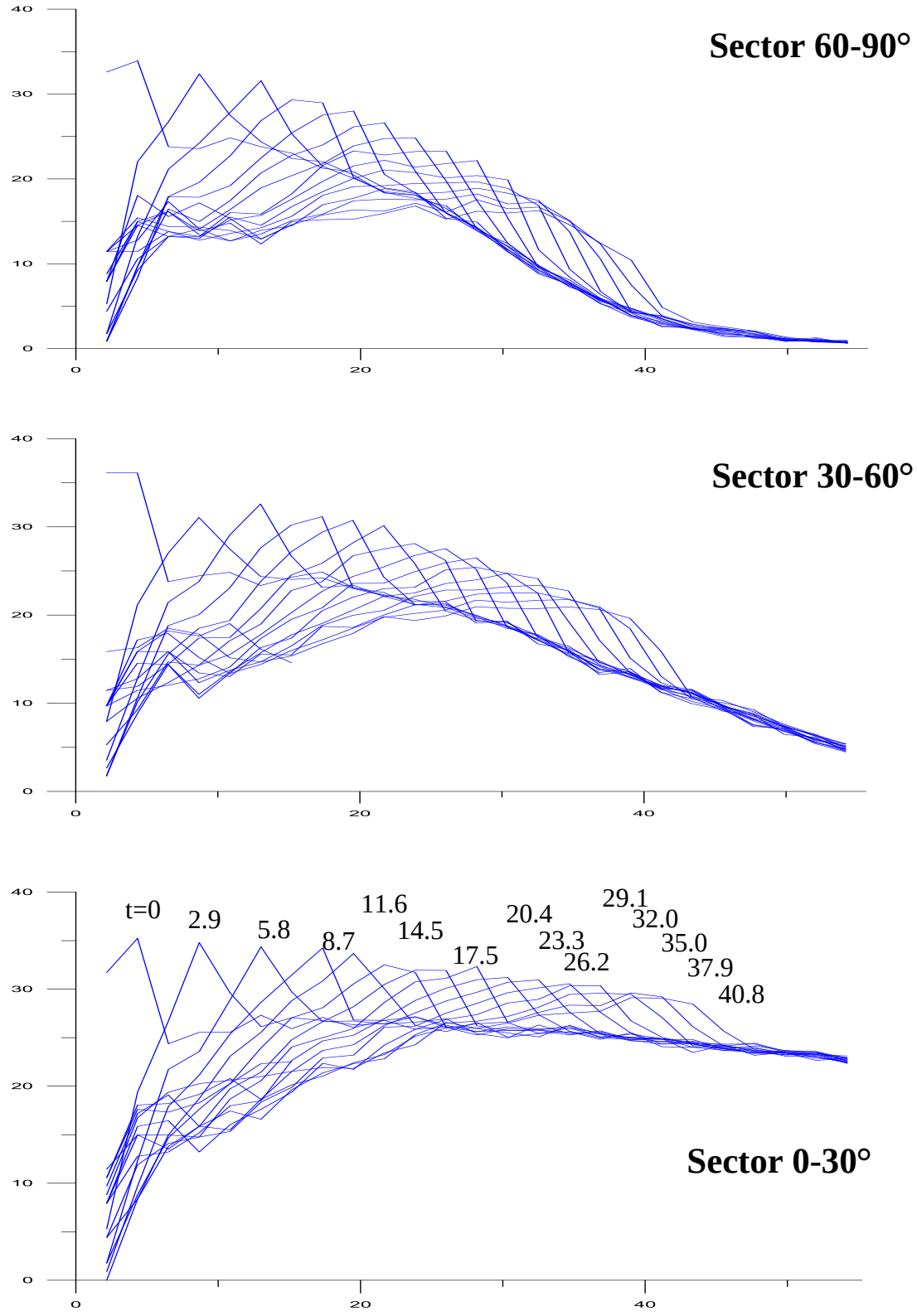

Fig. 4. Time evolution of a shock-wave shape in different sectors; units are in t and nm^{-1}.

One can see that the height of a shock wave decreases with time for all the sectors whereas the width increases. A more careful study of the results shown in Fig. 4 reveals an unexpected phenomenon. The form of a shock wave is asymmetric, and its asymmetry is increasing with

time. The impression is such as if the shock wave disintegrated, at least, into two parts (see Fig. 4, sector 0-30 °, time 37.9 and 40.8, where this process is the most pronounced). It should be emphasized that the disintegration starts from the very beginning of forming the shock wave (Fig. 5).

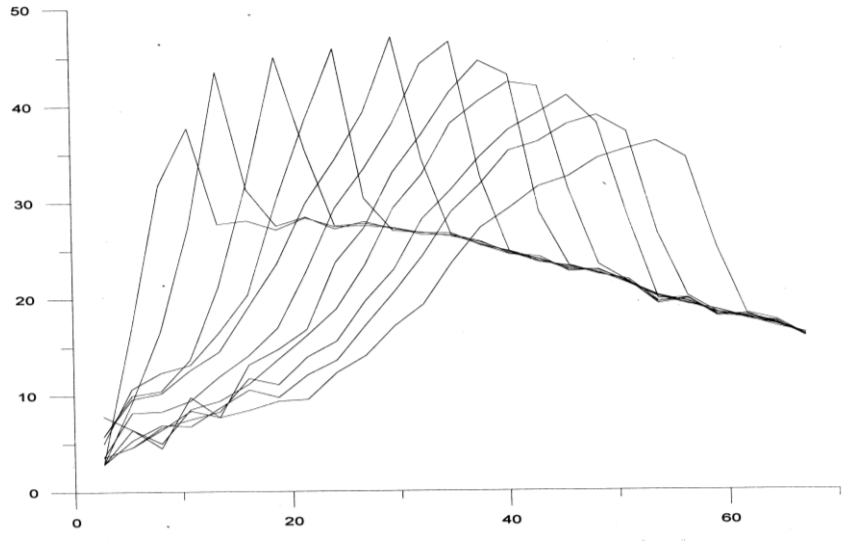

Fig. 5. Time evolution of shock-wave shape, t = 0 – 5. Sector 0-30°, units are in nm^{-1}.

4. Discussion

In the classical books on nonlinear waves [e.g. 9-11] sometimes it is said that the simplest nonlinear equation, which describes the motion of a curve $u = u(x)$ parallel to the $x-$axis,

$$u_t + u u_x = 0$$

has two generalizations; the Burgers equation, a dissipative generalization,

$$u_t + u u_x = \alpha u_{xx},$$

and the Korteweg-de Vries (KdV) equation, a dispersive generalization,

$$u_t + u u_x + \beta u_{xxx} = 0.$$

Here α defines the dynamical viscosity, and β characterizes the dispersion in a system.

It is assumed that the Burgers equation takes place in the systems where diffusion dominates (dissipative systems) whereas the KdV equation occurs in the dispersing medium without energy dissipation. As a rule, in mechanics the structure of shock waves is analyzed on the basis of the Burgers equation. For studying solitary waves which were discovered by John Scott Russell in 1834 as shallow water waves in a narrow channel, one uses the KdV equation. Russell has established some properties of the solitary waves among them the following ones are of interest to our results. They are: velocity constancy of a separated wave and disintegration of a rather large solitary wave into two and more solitary waves; a smaller wave is moving with a lesser velocity.

Molecular dynamics does not know properties of a medium in which a shock wave is propagating beforehand; it knows only the interparticle potential, so it has no prejudice in favor of one or another equation. It seems that our results are better consistent with the KdV equation and its solutions than with the Burgers equation. However, the only solutions of the KdV equation are cnoidal and solitary waves and therefore the KdV equation is unable

ensuring the existence of shock waves [12]. Meanwhile, in real conditions there is always some dissipation, e.g. viscosity in fluids, but the KdV equation does not take it into consideration. Because of the dissipation all the waves will be damping. This situation is considered in the textbook [13]. The author, B.B. Kadomtsev, who is well known for the generalization of the KdV equation for two-dimensional systems (so-called the Kadomtsev-Petviashvili equation, 1970) discussed the consequences of adding a new term into the right part of the KdV equation which takes into consideration viscosity. In this case the equation looks like

$$u_t + u u_x + \beta u_{xxx} = \alpha u_{xx} .$$

This equation was derived by Mei [14] and Johnson [15]. The first considered nonlinear gravity waves in a thin sheet of viscous fluid, the second analyzed a nonlinear equation incorporating damping and dispersion. The equation is known as the Korteweg-de Vries-Burgers equation [12]. The addition of damping makes possible the appearance of solutions in the form of shock waves. In [13] the experimental data illustrating this possibility are given. On this ground we assume that our shock waves may be described with the Korteweg-de Vries-Burgers equation. One can object to this assumption that this equation is a one-dimensional, but the shock waves observed in our computer experiments are two-dimensional. However, the procedure developed for obtaining the structure of shock waves observed, in essence, is reducing a two-dimensional phenomenon to a one-dimensional form. For this reason it is believed that our assumption is reasonable.

5. Conclusion

We have developed a method for studying the structure of shock waves arising in underwater explosions which were observed in molecular dynamics computer experiments. The most striking result of this investigation is that a shock wave disintegrates, at least, into two parts. This phenomenon is analyzed on the basis of the Korteweg-de Vries-Burgers equation.

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