

## MOLECULAR HYDRODYNAMICS OF DEEP-WATER EXPLOSIONS

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**Abstract.** In this contribution we report on modeling underwater explosion in the framework of molecular dynamics. We have developed a computer program which allows studying the underwater explosion in two dimensional Lennard – Jones liquid. 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. The most striking result of the investigation is that the shape of a shock wave is changing with time as if the shock wave disintegrated into two parts. The phenomenon is analyzed similar to the approach accepted for solitons. An equation for two-dimensional shock waves which generalizes the Korteweg-de Vries equation for a one-dimensional medium is suggested.

### 1. Introduction

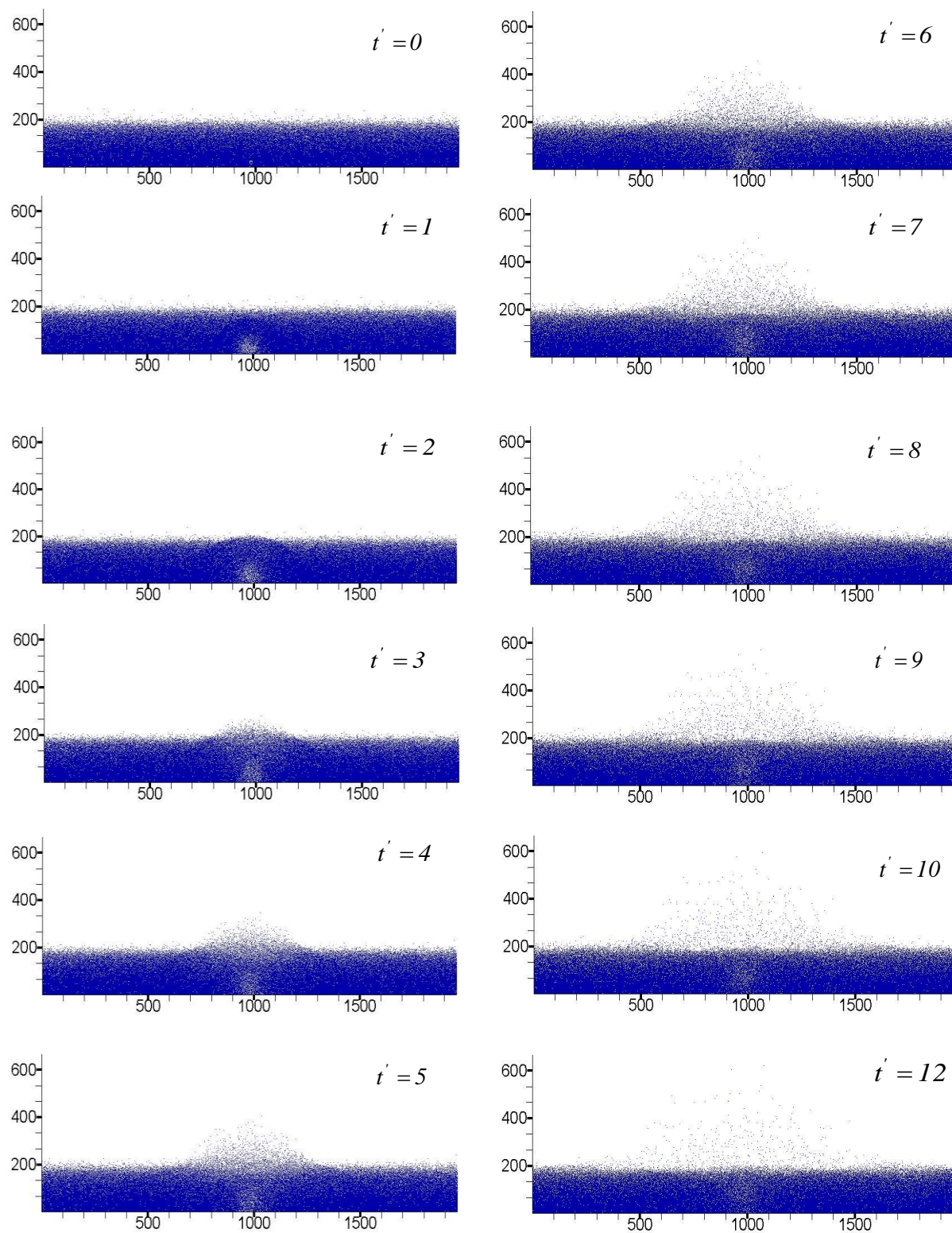
In the previous works [1-3] we described a new approach to studying underwater explosion which is based on molecular dynamics. We have developed a computer program which allows studying the underwater explosion in two dimensional Lennard–Jones liquid. Calculations of dynamical structure of the underwater explosion displayed the striking resemblance of the underwater-explosion evolution obtained and that of observed in real process; 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; its activity and decay.

In [4, 5] the second step was done; a procedure was developed which allowed studying a structure of shock waves observed within the framework of molecular dynamics. In this contribution we used both procedures, one for observing a visual picture of underwater explosions under different conditions, and other for calculating a structure of shock waves arising in deep-water explosions.

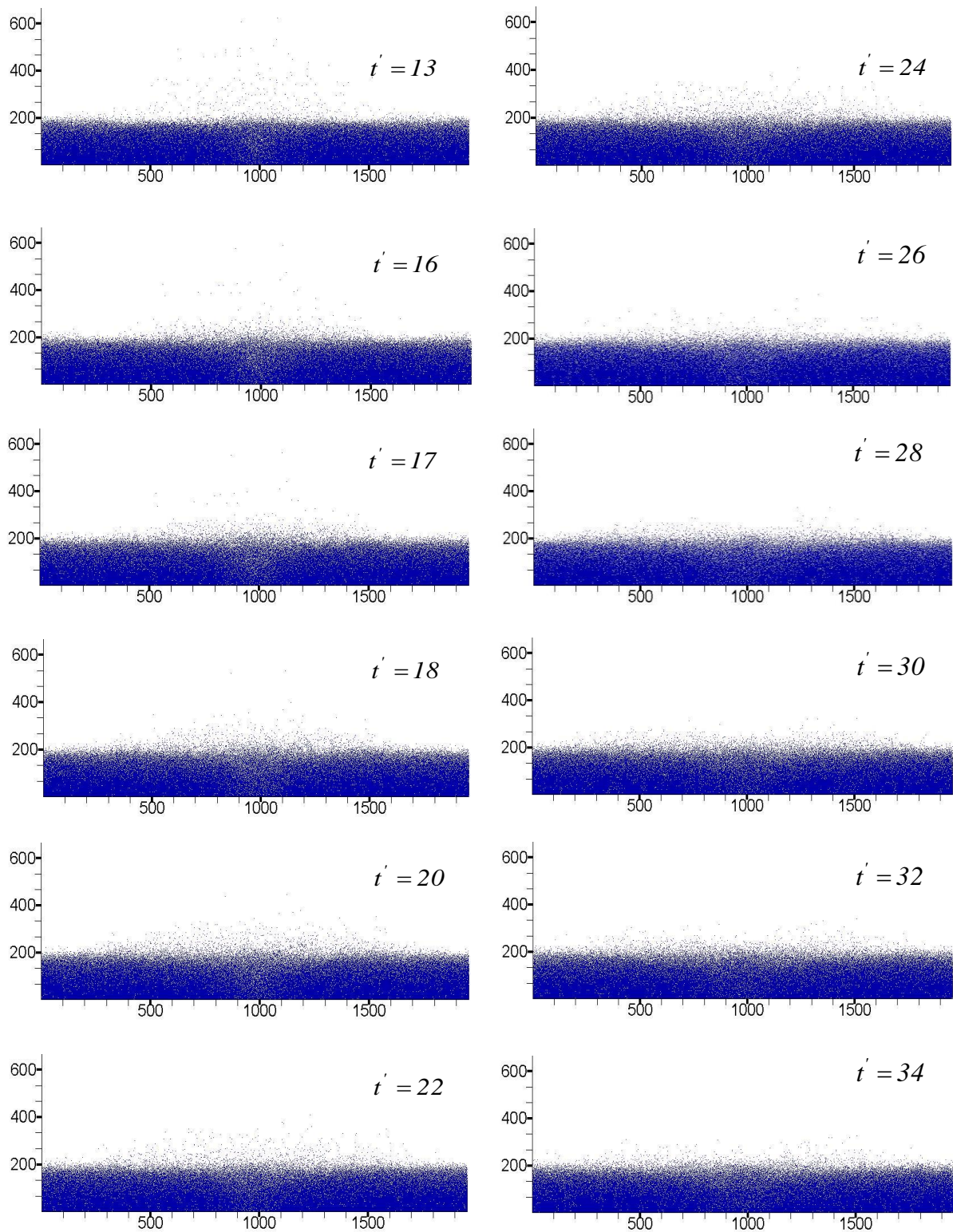
### 2. Deep water explosion

**a) Explosive is the same as in all previous simulations.** The calculations were done with a system consisting of 55,000 particles. An explosive was inserted into the water after reaching the equilibrium. The temporal evolution of underwater explosion is demonstrated in Fig. 1. The calculations were begun at  $t' = 0$  after the state thermodynamic equilibrium was established in the system with an inserted explosive at temperature 300 K. After 4000 time steps, each step being  $t' = 0.00025$ , at  $t' = 1$  one can see the explosion zone which is expanding and reaching a surface. From  $t' = 2$  to  $t' = 10$  water particles emission to atmosphere is observed. Simultaneously at  $t' = 10$  the surface waves are forming which begun moving to both sides from the explosion epicenter. The following collapse of the crater

formed leads to a new emission of particles at  $t' = 10 - 28$ ; the process is accompanied by the appearance of more powerful surface waves at  $t' = 16 - 17$ .

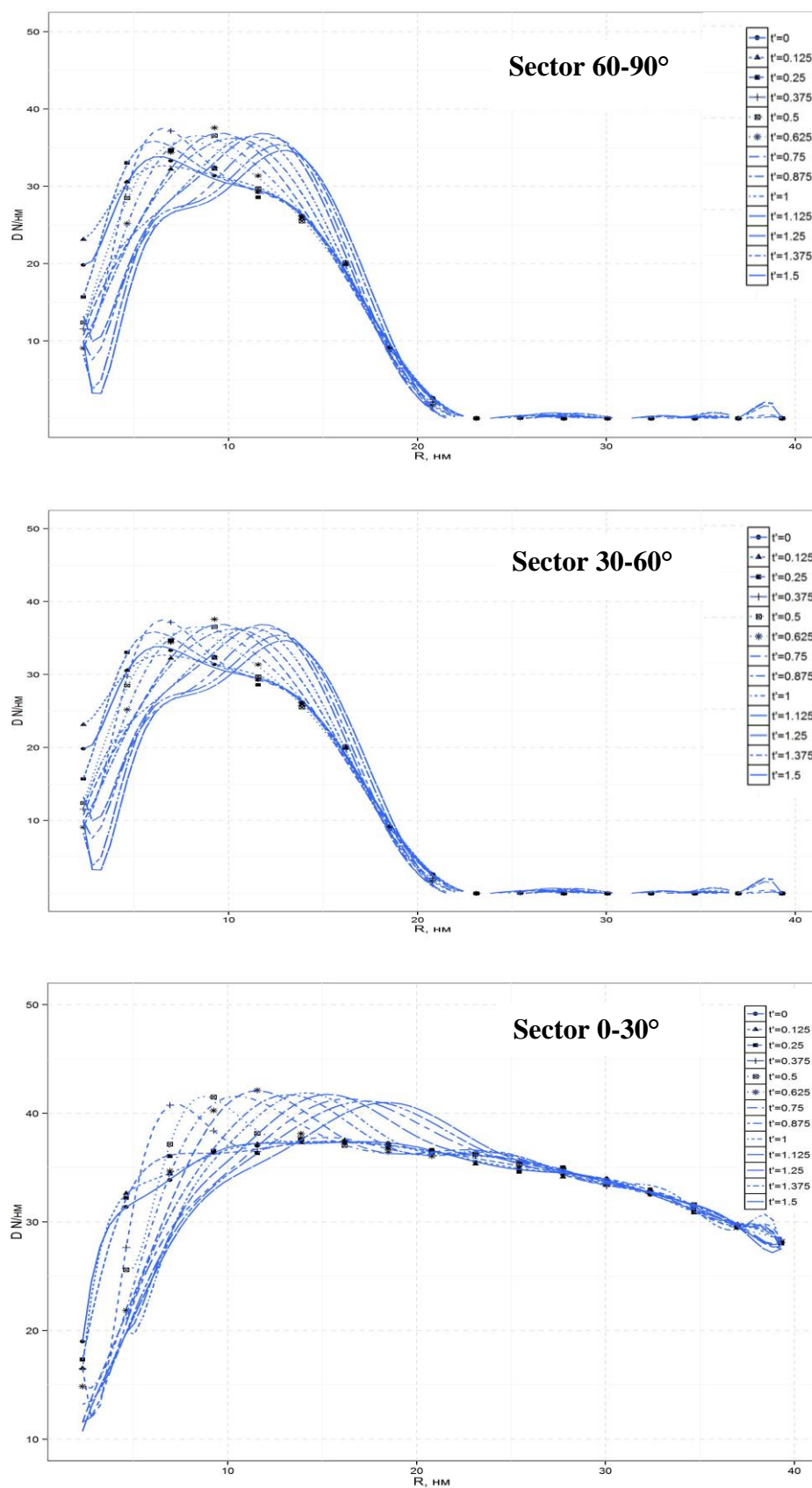


**Fig. 1a.** Time evolution of a deep water explosion.



**Fig. 1b.** Time evolution of a deep water explosion.

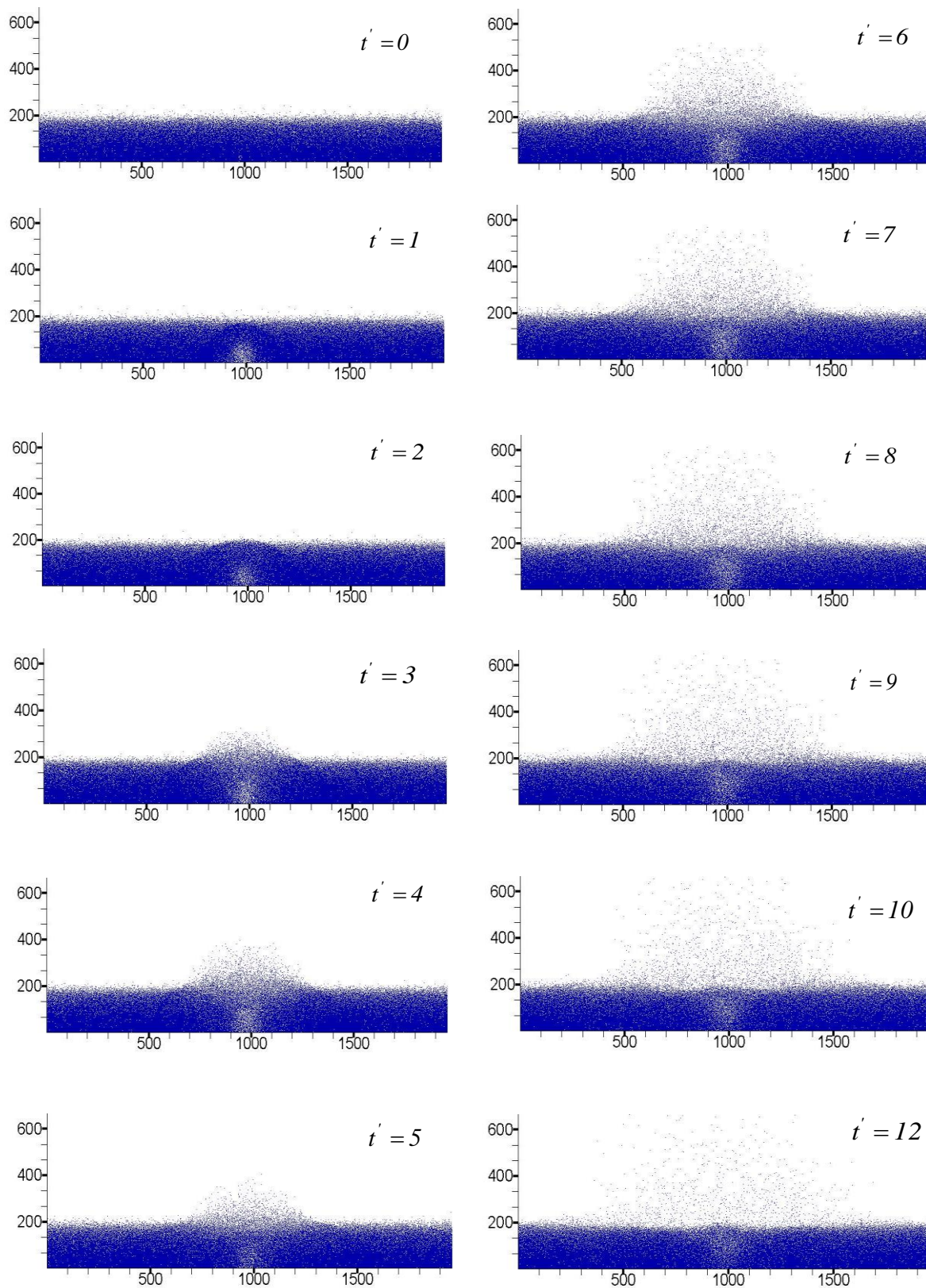
Using the procedure developed in [4, 5], one can calculate the radial density of the shock wave. Fig. 2 shows the evolution of shock-wave shape in different sectors (counter-clockwise from x-axis) in an orderly sequence. The wave is moving from left to right. The temporal dependencies were approximated with polynomials of the seventh degree.



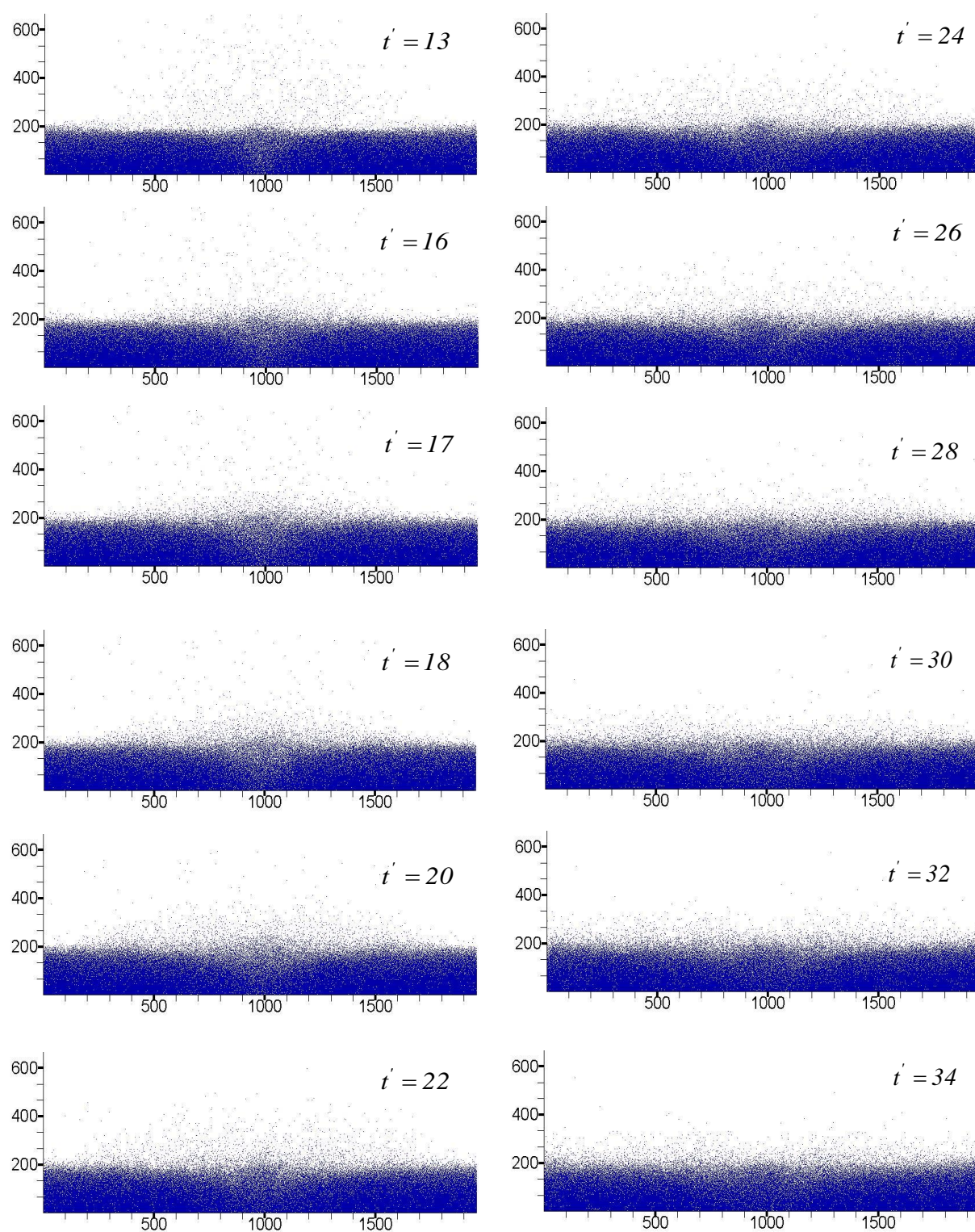
**Fig. 2.** Time evolution of shock-wave shape,  $t' = 0 - 1.5$ .

One can see that 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.

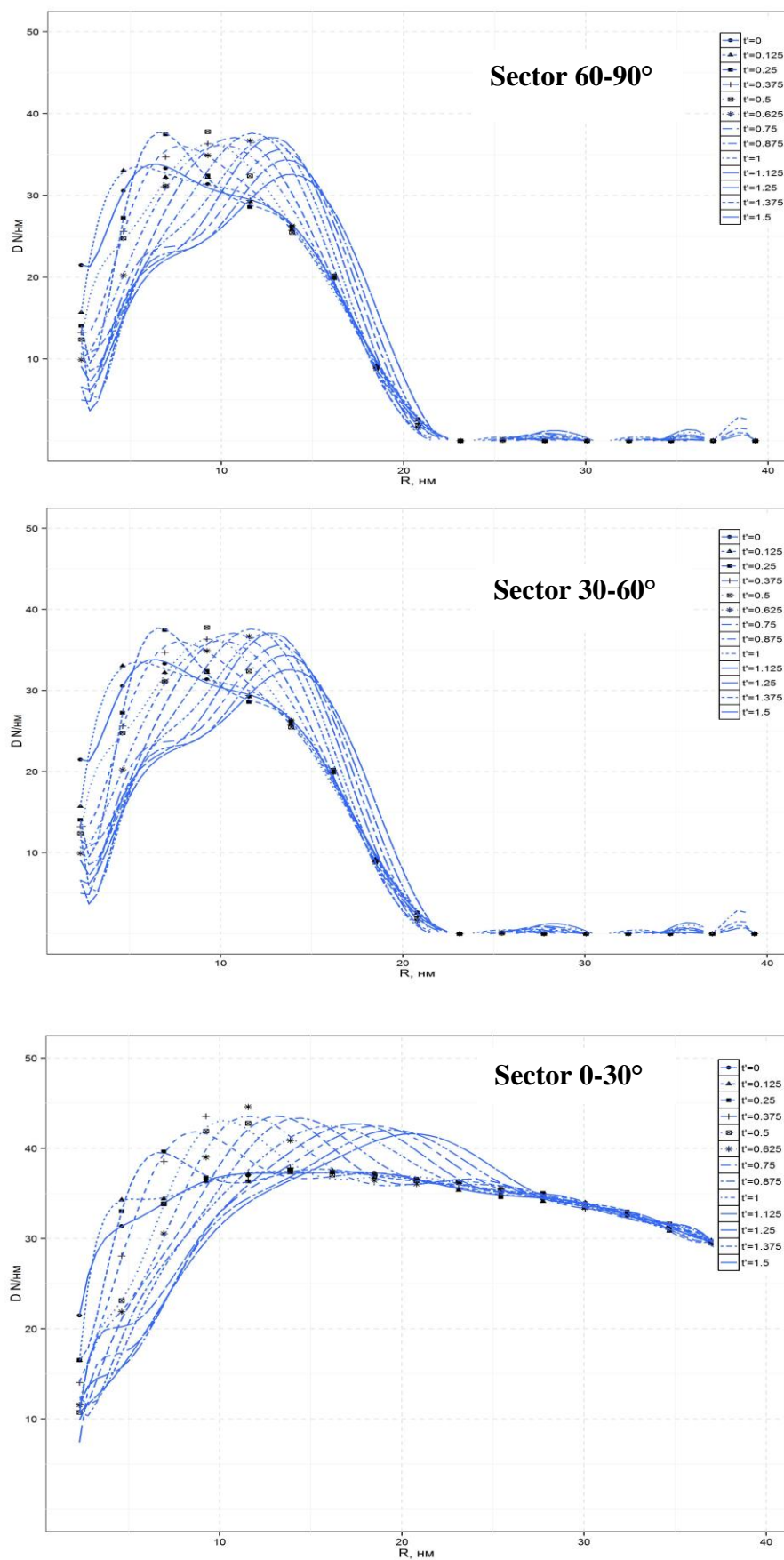
**b) Explosive is doubled.** The temporal evolution of underwater explosion is demonstrated in Fig. 3. The temporal variation of shock wave in different sectors (counter-clockwise from x-axis) is given in Fig. 4. The wave is moving from left to right.



**Fig. 3a.** Time evolution of a deep water explosion.

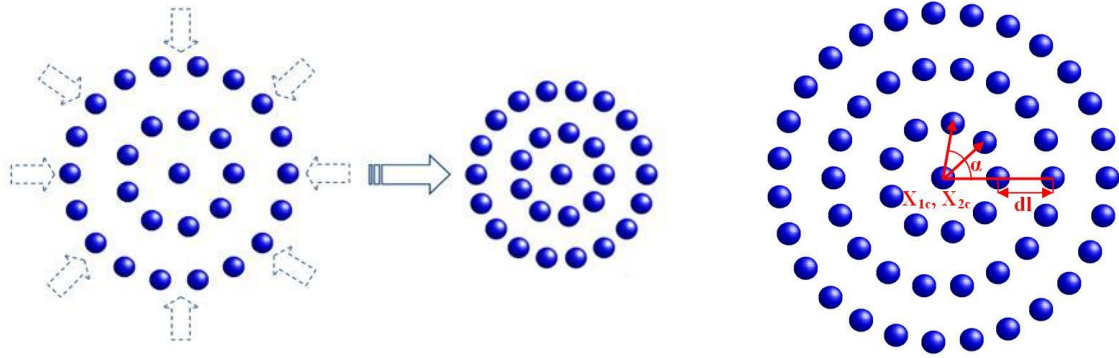


**Fig. 3b.** Time evolution of a deep water explosion.



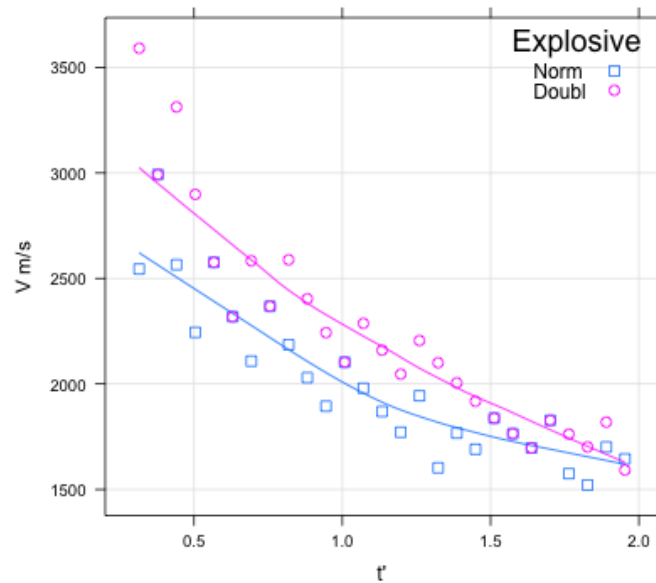
**Fig. 4.** Time evolution of shock-wave shape,  $t' = 0 - 1.5$ .

The arrangement of particles in a standard circular explosive and in a double circular explosive is shown in Fig. 5.



**Fig. 5.** Standard circular explosive (on the left) and double circular explosive (on the right).

The overall picture of explosion resembles that of with a standard explosive, but the intensity of the processes, in particular, water particles emission to atmosphere is larger. The shock wave velocity for standard and doubled explosive is shown in Fig. 6. Time  $t' = 1$  corresponds to real time  $t = 14.145 ps$ . On this interval velocity gradually decrease from 2992 m/s to 1701 m/s for standard explosive and from. 3590 m/s to 1819 m/s for doubled explosive.



**Fig. 6.** Velocity of the shock wave over time ,  $t' = 0 - 2$ .

#### 4. Discussion

**a) Continuum approximation.** In the previous works [4, 5], as well as in the present study, an asymmetric form of a shock wave arising in deep water explosion is discovered. The impression is such as if the shock wave disintegrate, at least, into two parts. It should be emphasized that the disintegration started from the very beginning of forming the shock wave. We have suggested that such waves could be described with the Korteweg-de Vries-Burgers equation [6],

$$u_t + uu_x + \beta u_{xxx} = \alpha u_{xx},$$

which is a combination of the Korteweg-de Vries (KdV) equation

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

and the Burgers equation

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

Here  $\alpha$  defines the dynamical viscosity, and  $\beta$  characterizes the dispersion in a system. It allowed reducing 2D-shock waves observed to 1D-mathematical description. However, no explanation of the disintegration was given. Consider this problem in detail taking as a basis the KdV equation.

**b) Korteweg-de Vries equation at the atomic level. Compression soliton.** Here we will follow the analytical derivation given in [7]. Consider a one-dimensional anharmonic chain of atoms with parameter  $a$ . Denote by  $u_n$  the displacement of atom  $n$  from its equilibrium position. Suppose that only nearest neighbor interact. In this case the potential energy of the chain is

$$U(u_1, u_2, \dots) = \sum_n \varphi(u_n - u_{n-1}),$$

where  $\varphi$  is the energy of one interatomic bond. The corresponding equation of motion can be written as follows

$$M \ddot{u}_n = \varphi'(u_{n+1} - u_n) - \varphi'(u_n - u_{n-1}),$$

where  $M$  is the atomic mass. Denote the change of interatomic bond length as

$$\Delta u_n = u_n - u_{n-1}.$$

Approximate the force of interaction between atoms by the polynomial of second degree

$$\varphi'(\Delta u_n) = \varphi'(0) + \varphi''(0) \Delta u_n + \frac{\varphi'''(0)}{2} (\Delta u_n)^2.$$

Then the equation of motion can be rewritten as

$$M \ddot{u}_n = \varphi''(0) [\Delta u_{n+1} - \Delta u_n] + \frac{\varphi'''(0)}{2} [(\Delta u_{n+1})^2 - (\Delta u_n)^2].$$

Replace the chain by an elastic string, i.e. pass from a discrete argument on the continued coordinate  $x = na$ , restricting ourselves by derivatives of fourth order. For this purpose, expand  $u_{n+1}$ ,  $u_{n-1}$  into series close to  $u_n$ .

Then

$$u_{n+1} = u_n + a u' + \frac{a^2}{2} u'' + \frac{a^3}{3!} u''' + \frac{a^4}{4!} u^{IV}, \quad \Delta u_{n+1} = u_{n+1} - u_n,$$

$$u_{n-1} = u_n - a u' + \frac{a^2}{2} u'' - \frac{a^3}{3!} u''' + \frac{a^4}{4!} u^{IV}, \quad \Delta u_n = u_n - u_{n-1},$$

$$\Delta u_{n+1} + \Delta u_n = u_{n+1} - u_{n-1} = 2a u' + \frac{a^3}{3} u''',$$

$$\Delta u_{n+1} - \Delta u_n = u_{n+1} + u_{n-1} - 2u_n = a^2 u'' + \frac{a^4}{12} u^{IV},$$

$$[\Delta u_{n+1} + \Delta u_n][\Delta u_{n+1} - \Delta u_n] = 2a^3 u' u'',$$

and we obtain the nonlinear equation of motion

$$M \ddot{u} = a^2 \varphi''(0) \left( \frac{a^2}{12} u^{IV} + u'' \right) + a^3 \varphi'''(0) u' u''.$$

Let us seek the solution of the equation in the form of a stationary wave  $u(x, t) = u(x - Vt)$ , which travels with the constant velocity  $V$  and satisfies the wave equation  $\ddot{u} = V^2 u''$ . In this case we obtain the ordinary differential equation

$$\frac{a^4 \varphi''(0)}{12} u^{IV} + [a^2 \varphi''(0) - M V^2] u'' + a^3 \varphi'''(0) u' u'' = 0.$$

Denote

$$u' = \zeta, \quad \frac{a^2 \varphi''(0)}{M} = c^2, \quad -\frac{a^3 \varphi'''(0)}{2 \varphi''(0)} = \gamma,$$

where  $\zeta$  is the dimensionless line density of interatomic bond strain,  $c$  is the sound velocity,  $\gamma$  is Grüneisen constant (*Eduard Grüneisen, 1908*).

Rewrite the equation of motion

$$a^2 \zeta''' + 12 \left( 1 - \frac{V^2}{c^2} \right) \zeta' - 24 \gamma \zeta \zeta' = 0.$$

This is so-called the KdV equation which describes the stationary wave  $\zeta(x, t) = \zeta(x - Vt)$ , which travels with the constant velocity  $V$ . Integrating with respect  $x$ , we obtain

$$a^2 \zeta'' + 12 \left( 1 - \frac{V^2}{c^2} \right) \zeta - 12 \gamma \zeta^2 + f = 0,$$

where  $f$  is a constant. Let us multiply this equation by  $\zeta'$  and integrate once more with respect to  $x$ . Since

$$\int \zeta' \zeta'' dx = \frac{(\zeta')^2}{2}, \quad \int \zeta^n \zeta' dx = \frac{\zeta^{n+1}}{n+1},$$

the equation takes the form

$$\frac{a^2}{2} (\zeta')^2 + 6 \left( 1 - \frac{V^2}{c^2} \right) \zeta^2 - 4 \gamma \zeta^3 + f \zeta = \text{const}$$

or

$$\frac{a^2}{2} (\zeta')^2 + U(\zeta; V) = E.$$

Let us consider the coordinate  $x$  as time, and the dimensionless line density of interatomic bonds strain  $\zeta$  as the dimensionless coordinate of a certain fictitious particle having the mass  $a^2$ , which moves in the field of the effective potential energy

$$U(\zeta; V) = 6 \left( 1 - \frac{V^2}{c^2} \right) \zeta^2 - 4\gamma \zeta^3 + f \zeta.$$

In such notation the last equation expresses the conservation law of the total energy  $E = \text{const}$ ; the velocity  $V$  playing the role of a parameter.

Consider the form of the function  $U(\zeta; V)$ . The constant  $f$  is an external force which displaces the equilibrium position of the fictitious particle. If there is no an external force, we have

$$U(\zeta; V) = 6 \left( 1 - \frac{V^2}{c^2} \right) \zeta^2 - 4\gamma \zeta^3 = A \zeta^2 - B \zeta^3,$$

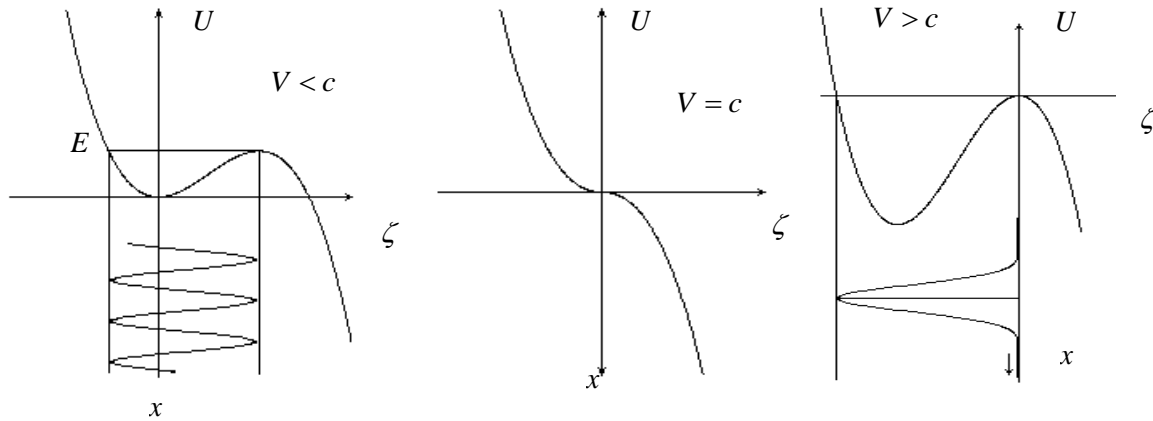
where  $A, B > 0$ . The extremum condition  $U'(\zeta; V) = 0$  gives

$$\zeta \left[ \gamma \zeta - \left( 1 - \frac{V^2}{c^2} \right) \right] = 0.$$

This equation has two roots

$$\zeta_1 = 0, \quad \zeta_2 = \frac{1}{\gamma} \left( 1 - V^2 / c^2 \right),$$

so the potential energy has the following three forms (Fig. 7) depending on the velocity  $V$ . It is equal to zero at  $\zeta = 0$  and  $\zeta_m = \frac{3}{2\gamma} (1 - V^2 / c^2)$ .



**Fig. 7.** Influence of the velocity of a traveling wave on an effective potential energy (above) and the shape of a dimensionless line density of interatomic bonds strain (below).

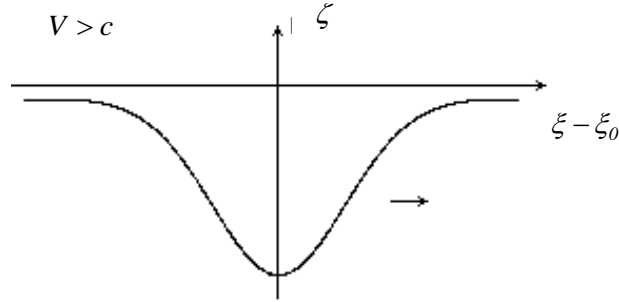
The full analysis of motion for these three cases is given in [7]. We are interested only in the case when  $V > c$ ,  $E = 0$ . In this case one can write the solution in the form [7]

$$\zeta = |\zeta_m| \left[ \text{th}^2 \beta (\xi - \xi_0) - 1 \right] = -|\zeta_m| \text{sch}^2 \beta (\xi - \xi_0).$$

Here  $\beta = \sqrt{3(V/c)^2 - 1}$ ,  $\xi = x/a$ ,  $\xi_0 = Vt/a$ . This solution describes a solitary wave of compression or a compression soliton (Fig. 8).

For convenience of the result interpretation in terms of a continuum, let us pass from the strain  $\zeta$  to the displacement  $u$ . Since  $\zeta = du/dx$ , then integrating with respect  $\xi$ , we obtain

$$\frac{u}{a} = -|\zeta_m| \int \frac{d\xi}{ch^2 \beta(\xi - \xi_0)} = -|\zeta_m| \operatorname{th} \beta(\xi - \xi_0) + \operatorname{const}.$$



**Fig. 8.** Soliton of compression.

This solution in terms of displacement has the form of a shock wave

$$\frac{u}{a} = -|\zeta_m| \operatorname{th} \frac{\beta(x - Vt)}{a} + \operatorname{const},$$

which travels in the positive direction of the  $x$  axis with a constant velocity  $V$ . At point  $x = +\infty$  there is no disturbance, since the wave has no time to come here, therefore  $u = 0$  and

$$\operatorname{const} = |\zeta_m| = u_0 / a.$$

Therefore,

$$u = u_0 \left[ 1 - \operatorname{th} \frac{\beta(x - Vt)}{a} \right] = u_0 \left( 1 - \operatorname{th} \frac{x - Vt}{\Delta} \right),$$

where  $\Delta = a / \beta$  is the width of a shock wave. It should be emphasized that

$$u_0 \Delta^2 = \frac{a^3}{2} = \operatorname{const},$$

i.e. the product of the amplitude of a shock wave by the square of its width is a constant. With decreasing the wave velocity the wave amplitude decreases too, so in the limit  $V \rightarrow c$  the wave smears completely. It is worth noting that the velocity  $V$  is connected with the amplitude  $u_0$  by the expression

$$V^2 = c^2 \left( 1 + \frac{2}{3} \gamma \frac{u_0}{a} \right).$$

Since  $\gamma = -\frac{a^3 \varphi'''(0)}{2 \varphi''(0)}$ , we can assign the physical meaning to spatial dispersion of waves, relating it with the cubic anharmonicity of the potential of interatomic interaction.

For reference it should be remarked that the KdV equation at the atomic level was considered for specific forms of the interatomic potential, namely for the Toda chain [8], although not so elaborately.

**c) Korteweg-de Vries equation and Schrödinger equation.** Here we will follow the approach expounded in [9]. Let the function  $\psi(x, t)$  satisfy the Schrödinger equation

$$i \frac{\partial \psi}{\partial t} = H \psi ,$$

where  $H$  is a Hamilton operator. Quantum mechanics can be formulated also in another way, where the time dependence is transferred from wave functions to operators (Heisenberg representation). If  $L$  is a Hermite operator fitting to some physical quantity, then the time derivative of this operator is defined by the relation

$$\frac{dL}{dt} = \frac{\partial L}{\partial t} + i[H, L],$$

where the commutator  $[H, L] = HL - LH$ . If the operator  $L$  does not depend on time, all its eigenvalues  $\lambda$ , which are defined by the relation

$$L\psi = \lambda \psi ,$$

do not depend on time too.

The condition of conserving the operator  $L$  is  $dL/dt = 0$ . Therefore

$$\frac{dL}{dt} = \frac{\partial L}{\partial t} + i(HL - LH) = 0 .$$

We define the operators  $L$  and  $H$  by

$$L = 6\beta \frac{\partial^2}{\partial x^2} + u \quad iH = 4\beta \frac{\partial^3}{\partial x^3} + \frac{1}{2} \left( u \frac{\partial}{\partial x} + \frac{\partial}{\partial x} u \right) .$$

Considering that  $(uv)' = uv' + u'v$ , i.e.  $\frac{\partial}{\partial x} u = u \frac{\partial}{\partial x} + \frac{\partial}{\partial x} u$ ,

the operator  $H$  may be written in the form

$$iH = 4\beta \frac{\partial^3}{\partial x^3} + u \frac{\partial}{\partial x} + \frac{u_x}{2} .$$

By direct, but rather tedious computation, we obtain

$$\frac{\partial L}{\partial t} = u_t , \quad i(HL - LH) = uu_x + \beta u_{xxx} ,$$

$$\frac{dL}{dt} = u_t + uu_x + \beta u_{xxx} = 0 .$$

Rewrite the equation  $L\psi = \lambda \psi$  in the form

$$-6\beta \frac{\partial^2 \psi}{\partial x^2} + (\lambda - u) \psi = 0 .$$

We may interpret this equation as a one-dimensional stationary Schrödinger equation, where the first term is the kinetic energy,  $\lambda$  is the total energy, and  $u$  is the potential energy. In mathematics this equation is known as the associated eigenvalue equation [8]. For the function  $u(x, 0)$ , which is fast decreasing with  $|x| \rightarrow \infty$ , we have finite number of discrete

negative eigenvalues of  $\lambda$  [10].

As an example, consider the specific initial condition [8]

$$u(x, 0) = -p(p+1) \operatorname{sech}^2 x \quad (p > 0)$$

and follow the time evolution of the solution of the KdV equation. When  $p=1$ , and the amplitude is 2, the wave form does not change with time but it proceeds to the right. This is a soliton or the stable solitary wave which Scott Russell observed and investigated. When  $p=2$ , and the amplitude is 6, the eigenvalues are  $\lambda=0, -1, -4$ . As a result, the initial state decomposes into two solitons, one having the eigenvalues  $\lambda=0, -1$ , and the other having  $\lambda=0, -4$ . All the energy and momentum of the initial state are carried away by these two solitons. When  $p$  is not an integer, we have solitons and some ripples (oscillatory tail). They emerge from the initial state and solitons proceed to the right, while the ripples spread out to the left with diminishing amplitude.

**c) Relation to underwater explosion.** Let us correlate the molecular dynamics computational results concerning the form of shock waves with the analytical description of solitary waves. We see that the form of shock waves observed and their evolution with time resembles those of solitary waves of the KdV equation. However, the KdV equation is one-dimensional, but the shock waves are two-dimensional. Nevertheless, the procedure developed for obtaining the structure of shock waves, in essence, is reducing a two-dimensional phenomenon to a one-dimensional form, so we may act as follows.

Introduce a polar coordinate system with the center in the center of an explosive. We see that the form of a shock wave propagating inside a circular sector is strongly depends on polar angles  $(\theta_1, \theta_2)$ , defining the sector. In principle, it is possible to decrease the magnitude of the sector  $(\theta_2 - \theta_1)$  to an infinitesimal quantity, but it will be connected with huge computational time. However, in this case we may write down the KdV equation for a wave propagating along the direction  $\vec{r}$  in the form

$$u_t + uu_r + \beta u_{rrr} = 0,$$

where coefficient  $\beta$  characterizes dispersion in a system.

In principle, the function  $u$  depends not only on a radius-vector, but also on a polar angle, i.e. we have  $u = u(r, \theta)$ . Besides, the coefficient  $\beta$  is constant only for homogenous continuum. However we see from the pictures showing time evolution of an underwater explosion that one deals with an inhomogeneous medium. This inhomogeneity is of two types; one is connected with initial property of the medium, another is appearing during an explosion. For the sake of simplicity, as well as for conserving remarkable properties of the KdV equation, there are reasons to assume that the function  $u$  does not depend on a polar angle, but the coefficient  $\beta$  is a function of both arguments, i.e.  $\beta = \beta(r, \theta)$ . In this case we may write down the KdV equation for a wave propagating along the direction  $\vec{r}$  in the form

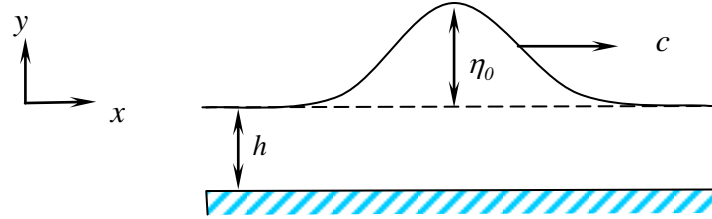
$$u_t + uu_r + \beta(r, \theta)u_{rrr} = 0.$$

Before analyzing the properties of the function  $\beta = \beta(r, \theta)$ , let us discuss the physical meaning of different functions introduced in the preceding sections. It is necessary, because in the majority of books and papers too much attention is given to mathematical transformations and too little attention is focused on physical meaning of functions obtained. As a result, instead of investigating a phenomenon one studies properties of an equation which models this phenomenon. Besides different authors use different designations for ones and the same notions as if they tried to bewilder a reader.

Return to Founding Fathers [8]. Scott-Russell from a horseback observed a solitary wave traveling along a canal without changing its form during a chase of one or two miles. He was so interested that he made an experimental water tank and found an empirical formula for the speed of a solitary wave, of the form shown in Fig. 9:

$$c^2 = g(h + \eta_0).$$

Here  $c$  is the speed of a solitary wave,  $g$  is the free fall acceleration,  $h$  is the depth of the water,  $\eta_0$  is the maximum elevation of the water above the water level.



**Fig. 9.** Solitary wave.

Among many investigations, Korteweg and de Vries discussed the motion of shallow water waves. They arrived at the equation [8]

$$\frac{\partial \eta}{\partial t} + \frac{3}{2} \frac{c_g}{h} \eta \frac{\partial \eta}{\partial x} = \frac{1}{2} c_g h^2 \left( \frac{\sigma}{\rho g h^2} - \frac{1}{3} \right) \frac{\partial^3 \eta}{\partial x^3},$$

where  $\eta$  is the elevation of the water surface,  $c_g = \sqrt{gh}$ ,  $\sigma$  is the surface tension, and  $\rho$  is the density of water.

Writing down the KdV equation in the canonical form

$$u_t + uu_x + \beta u_{xxx} = 0,$$

we reduce the two-dimensional phenomenon to one-dimensional. Since  $\eta(x)$  is proportional to additional mass, we may consider  $u$  of the last equation as a change of the line density of the medium.

Deriving the KdV equation at the atomic level, we have obtained the following equation for a stationary wave

$$a^2 \zeta''' + 12 \left( 1 - \frac{V^2}{c^2} \right) \zeta' - 24 \gamma \zeta \zeta' = 0.$$

where  $\zeta$  is the dimensionless line density of interatomic bond strain.

Since the interatomic bond strain leads either to the increase of an interatomic distance or to its decrease, we may consider strain  $\zeta(x)$  as a dimensionless change of the line density of a medium. We have shown that the Grüneisen constant  $\gamma = -\frac{a^3 \varphi'''(0)}{2 \varphi''(0)}$ . Since  $\beta \sim 1/\gamma$  we can assign the physical meaning to dispersion  $\beta$ , relating it with the cubic anharmonicity of a potential of interatomic interaction.

Now we are able to discuss a possible structure of the function  $\beta(r, \theta)$ . According to the initial form of the KdV equation, it has two parameters which can change depending on experiment conditions, density  $\rho$  and depth  $h$ . In their turn both quantities are connected

with pressure. If a shock wave propagates when  $\theta \sim 0$ , the density and depth almost do not change, and therefore the coefficient  $\beta$  is almost constant, so the shock wave form is also almost constant, at least after some initial stage. This situation is realized for the shock waves propagating in sector  $0-30^\circ$ .

Another limiting value is  $\theta \sim 90^\circ$ . Here the shock wave proceeds from a region of high density and depth to a surface where both quantities are small. According to the initial form of KdV equation  $\beta \sim 1/h$ , and therefore the dispersion is increasing during the motion of a shock to the surface. We may realize this process as an excitation of the system. According to quantum mechanics, any excitation means that an initial state decomposes at least two into states, the higher state having a lesser density. Just the same situation takes place for the shock waves propagating in sectors  $30-60^\circ$  and  $60-90^\circ$ .

## 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 the investigation is that the shape of a shock wave is changing with time as if the shock wave disintegrated into two parts. The phenomenon is analyzed similar to the approach accepted for solitons. The resulting equation for two-dimensional shock waves generalizes the Korteweg-de Vries equation for a one-dimensional medium and in polar coordinates has the form  $u_t + uu_r + \beta(r, \theta)u_{rrr} = 0$ . We assign the physical meaning to dispersion  $\beta$ , relating it with the cubic anharmonicity of a potential of interatomic interaction.

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