Modeling of high velocity flows with chemical reactions

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Abstract. - The numerical algorithm for the decision of non-stationary two-dimensional problems of dynamics of compressible multi phase media is developed on the base of the method of particles in cells. With the purpose of elimination of non-physical fluctuations of the numerical decision inherent in methods of this type, there are offered method of integration of the equation of mass conservation and procedure of determination of pressure in nodes of numerical grid. On the base of algorithm some examples of modeling were executed: propagation of gas detonation with cellular structure in tube, explosion in a planet interiors and bubble detonation.

Key words: - modeling, two-phase media, compressible flows, particle, detonation, explosion

1 Introduction.

A Harlow method of particles in cells described in [1], was an ancestor of group of methods, in which continuous medium is represented as Lagrangian particles moving on motionless in space Eulerian grid. Such approach has a number of advantages in comparison with pure Lagrangian or pure Eulerian mode of flow description. In particular, within the framework of the method flows with large deformations accompanied by a number of contact and free surfaces. All-round research of properties of the method of particles in cells, description of its advantages and lacks are made in [2, 3].

Method GAP (grid and particles) [4] also belongs to group of methods of particles in cells. Its distinctive feature is that in number of parameters describing a particle, besides its mass and coordinates, an internal energy of particle, its volume and velocity are included. It has allowed carrying out integration of system of the equations of gas dynamics for Lagrangian particle, using Eulerian a grid for storage of space average meanings of density, internal energy and pressure.

Some lacks are inherent in these methods. In particular, not physical fluctuations occur because of the mode of density computations. The method of large particle [5] is a further development of Harlow method, when the flow into a numerical cell corresponds to a singular particle with its subsequent deformation and variations of parameter values. The method allows getting a qualitative picture of the processes. Then the method of individual particles [6] appears which deals with multy phase high velocity flows. The basic idea of the method is that the system of the equations in partial derivatives, describing the compressible flow, is numerically integrated for each particle. For the determination of the values of space derivatives in particles the rectangular Eulerian grid is used, in which the meanings of components of tension tensor and velocity vector from the nodes of irregular Lagrangian grid are interpolated. The nodes of irregular Lagrangian are the centers of particles. After calculation of spatial derivatives in nodes of Eulerian grid, their interpolation in particles is carried out. These derivatives are used for computation of new values of particle parameters - its coordinates, velocity, density and internal energy.

The present paper is devoted to modification of the method of individual particles for the problems with chemical reactions.

2 **Problem Formulation**

1. In a numerical field according to the initial data the bodies are placed which are broken into separate particles. Each particle represents individual volume (that is a volume, consisting from the same molecules of medium) and is also characterized by the following parameters: M - mass, z and r - coordinates of its centre, u and v - velocity components of the centre in directions z and r accordingly, ρ - density, E - specific internal energy, p - pressure.

For each particle the system of gas dynamics equations is integrated.

The basic equations are based on laws of conservation of mass, pulse and energy for two-dimensional non-stationary flow of the compressible medium without taking into account effects of dissipation:

$$\frac{d\rho}{dt} + \rho \left(\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r} + S \frac{v}{r} \right) = 0,$$

$$\rho \frac{du}{dt} + \frac{\partial p}{\partial z} = Q_z,$$

$$\rho \frac{dv}{dt} + \frac{\partial p}{\partial r} = Q_r,$$

$$\frac{dE}{dt} + \frac{p}{\rho} \left(\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r} + S \frac{v}{r} \right) = 0,$$

$$\frac{dY}{dt} = W_Y, \quad \frac{d\mu}{dt} = W_\mu.$$
(1)

Here S = 0 for plane and S = 1 for axial symmetry (z is axis of symmetry) respectively, *t*- time, μ - mean molecular mass of gas, *Y* - the period of the induction, at the beginning of the induction zone Y = 1 and at the end Y = 0; μ is the mean molecular mass of gas; W_{μ} and W_{Y} - velocities of change of μ and *Y*, respectively; Q_{z} , Q_{r} - components of the vector of outward mass forces.

The propagation of shock and detonation waves through chemically active gas was modeled in the paper. Therefore for the description of possible chemical reactions the two-stage model of chemical kinetics was used [7], when chemical reactions occur at the point of the flow after a chemical ignition delay time t_{ig} , counted after the passage of a leading shock wave front.

If
$$1 > Y > 0$$
, then
 $W_Y = -\frac{1}{t_{ig}}, W_\mu = 0,$
 $E = \frac{1}{\gamma_0 - 1} \frac{p}{\rho} + E_{\mathcal{A}} \left(\frac{1}{\mu_0} - \frac{1}{\mu_{\min}} \right),$ (2)

After the expiration of the delay Y = 0, then $W_Y = 0$, (3)

and W_{μ} is defined according to the model:

$$W_{\mu}(T,\mu,\rho) = 4K_{+}\rho^{2}\frac{1}{\mu}\left(1-\frac{\mu}{\mu_{\max}}\right)^{2} - A_{2}T^{3/2}\rho\left(1-\exp\left(-\frac{\theta}{T}\right)\right)^{3/2}\exp\left(-\frac{E_{\pi}}{RT}\right)\left(\frac{\mu}{\mu_{\min}}-1\right)^{4/2}$$
(4)

Here μ_{max} - molecular mass of gas in a recombined state, T - temperature of gas, R - a universal gas constant, θ is the effective temperature of excitation of oscillatory degrees of freedom; K_+ , A_2 - constants. For internal energy of gas the caloric equation of state is valid:

$$E(T,\mu) = E_{\mathcal{A}} \left(\frac{1}{\mu} - \frac{1}{\mu_{\min}} \right) + \left(\frac{3}{4} \left(\frac{\mu}{\mu_a} + 1 \right) + \frac{3}{2} \left(\frac{\mu}{\mu_a} - 1 \right) \frac{\theta/T}{\exp(\theta/T) - 1} \right) \frac{RT}{\mu}$$
(5)

Where μ_a is molecular mass of gas in an atomic state.

The system of basic equations becomes is completed by the thermal equation of a state of ideal gas:

$$\frac{p}{\rho} = \frac{RT}{\mu} \ (6)$$

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3 Problem Solution

The process of calculation of spatial derivative meanings in particles for system (1) - (6), is separated into three stages (further description of a method we shall conduct for a uniform grid with square cells).

First stage is interpolation "particles - grid". The interpolation can be made by various ways, for example by "weighing" by areas S_N^{ij} (fig. 1)

$$A_{ij} = \frac{\sum_{N} A_N S_N^{ij}}{\sum_{N} S_N^{ij}},$$

Where the indexes *i*, *j* concern to numerical cell node (*i*; *j*), index *N* - to a particle with number *N*, $A = (\rho, u, v, Y, \mu)$. The summation is made on all particles located in four cells, for which unit (*i*, *j*) is common. In fig. 1 crosses and circles are the centers of particles of two classes. The dotted line shows splitting of a cell into the areas, proportional to which the interpolation of parameters in nodes of a cell (containing the centre of a particle) is carried out. The interpolation can be made in another way as well, supplying higher order of accuracy.

In parallel with interpolation "particles - grid" each particle in nodes of Eulerian grid leaves the information on number of substance, to which it belongs. From fig. 2 it is clear, how such marking of nodes is carried out. Here dotted line designates contact border between two bodies and their common free surface. At the second stage the statement of **boundary conditions on Eulerian grid** (described in detail later in the paper) is carried out.

The third stage is interpolation "grid - particle". In nodes of Eulerian grid, necessary for integration of system (1) - (7), spatial derivatives are calculated by that or other mode. The good results are achieved if approximation of spatial derivative in internal nodes is executed by the central differences. For example derivative on coordinate z is:

$$\left(\frac{\partial A}{\partial z}\right)_{ij} = \frac{A_{i+1,j} - A_{i-1,j}}{2h}$$

In boundary nodes the unilateral differences are used, except for derivative of pressure in nodes on contact border, in which differences are central. The values of derivative in particles are determined by interpolation from nodes of a grid:

$$\left(\frac{\partial A}{\partial z}\right)_{N} = \sum_{ij} \left(\frac{\partial A}{\partial z}\right)_{ij} \frac{S_{N}^{ij}}{\sum_{ij} S_{N}^{ij}}, \quad \sum_{ij} S_{N}^{ij} = h^{2}.$$
(7)

The summation is spent on nodes of a cell, in which there is a centre of a particle. Here $\left(\frac{\partial A}{\partial z}\right)_N$ is

derivative value in particles, $\left(\frac{\partial A}{\partial z}\right)_{ij}$ are derivative

values in grid nodes, h is a step of a grid.

The received in such a way meanings of spatial derivative in a particle are used for calculation of the next time step by following finite difference scheme:

$$U_{N}^{k+1} = \overline{U}_{N}^{k} - \frac{\Delta t}{\rho_{N}^{k}} \left(\frac{\partial \overline{p}}{\partial z} \right)_{N}^{k},$$

$$V_{N}^{k+1} = \overline{V}_{N}^{k} - \frac{\Delta t}{\rho_{N}^{k}} \left(\frac{\partial \overline{p}}{\partial r} \right)_{N}^{k},$$

$$z_{N}^{k+1} = z_{N}^{k} + U_{N}^{k+1} \Delta t, \qquad r_{N}^{k+1} = r_{N}^{k} + V_{N}^{k+1} \Delta t, \qquad (8)$$

$$\rho_{N}^{k+1} = \frac{\rho_{N}^{k}}{1 + \left(div \overrightarrow{V} \right)_{N}^{k} \Delta t},$$

$$E_{N}^{k+1} = \overline{E}_{N}^{k} - \frac{\overline{\rho}_{N}^{k}}{\rho_{N}^{k}} \left(div \overrightarrow{V} \right)_{N}^{k} \Delta t.$$

The following designations are accepted here:

$$\left(div\vec{V}\right)_{N}^{k} = \left(\frac{\partial U}{\partial z}\right)_{N}^{k} + \left(\frac{\partial V}{\partial r}\right)_{N}^{k} + S\left(\frac{V}{r}\right)_{N}^{k},$$

where k is number of a time step, Δt is step of integration on time, p represents the sum of hydrostatic pressure and linear artificial viscosity.

We shall note that at the calculation of the component of particle velocity U_N^{k+1} and V_N^{k+1} , in the right hand part of the appropriate formulas there are not old meanings of velocity but intermediate values U_N^k and V_N^k , obtained from meanings of grid velocities by interpolation in a particle under the formula similar to (7). From a condition of conservation of full energy of a particle, the value of its specific internal energy in this case is corrected:

$$\bar{E}_{N}^{k} = E_{N}^{k} + \frac{\left(U_{N}^{k}\right)^{2} + \left(V_{N}^{k}\right)^{2} - \left(\bar{U}_{N}^{k}\right)^{2} - \left(\bar{V}_{N}^{k}\right)^{2}}{2}.$$

Full energy and pulse of system of particles do not change thus

Such procedure of "smoothing" of velocity of a particle is expedient for applying through 5-10 steps on time to increase of the decision monotony. The smoothing on each step results in increase of a shock wave spreading on 2-3 cells. At calculation of a step

on time without smoothing, the values U_N^k, V_N^k and

(determined in a particle) are used in scheme (8)

instead of intermediate values U_N^{k} , V_N^{k} and E_N^{k} .

The scheme (8) is not conservative, has the first order of approximation on time and on space. The stability of one-dimensional variant of the scheme for the equation of state $p = p(\rho)$ is investigated in linear approximation for two cases of arrangement of particles. The conditions of stability look as follows:

a) The particles are located in nodes of a grid at $B \leq 2$: $k \leq B$,

at
$$B > 2$$
: $k \le \frac{4}{B + \sqrt{B^2 - 4}}$;

δ) The particles are located at the centers of cells at $B \leq 2,3$: $k \leq B$,

at
$$B > 2,3$$
: $k \le \frac{8}{1,26(B \cdot 0,94 + \sqrt{B^2 \cdot 0,89 - 4})};$

Here B is a factor of linear artificial viscosity q, determined by ratio

$$q = -B \cdot C_N^k \cdot \rho_N^k \cdot h \left(div \bar{V} \right)_N^k, k = c \cdot \Delta t / h \qquad \text{is}$$

Courant number, C - velocity of a sound. It is visible, that the introduction of artificial viscosity in the scheme is necessary condition of its stability.

As a test variant, one-dimensional problem of disintegration of arbitrary break in ideal gas was solved. Misbalance of full energy in the decision does not exceed value of 1 percent. The shock wave is smeared on 6-8 cells, contact break - on one cell.

During the procedure of computation there can be a situation, when between two next particles there will be two (or more) emptier cells. It can take place, for example, in a zone of expansion or in a zone of strong deformations. Such particles cease "to feel" each other, since (according to situation, described above) the region of influence of each particle is limited to a cell, in which its centre at the fixed instant is located. This effect is characteristic for methods such as particles in cells. The simple way of its elimination is accommodation of large number of particles at the initial instant in region with prospective break of continuity. However this mode is too tiresome and insufficiently reliable since it is impossible to foresee always the areas with strong change of form or with the large expansion. It seems more rational to use the method of local elimination of areas of continuity infringement.

For observation of local infringements of continuity, the vector of the form is included in number of parameters describing a particle. In plane case the particle represents rectangular parallelepiped of length equal to 1; in case of axial symmetry it represents a torus. The cross section of parallelepiped or torus by a plane (z, r) has the rectangular form. Lengthening and turn of the rectangular are set by components of a vector of the form. Knowing them, it is possible to determine orientation of a particle in a computational field. So, lengths of a particle sides a and b are connected with components of a vector of the form L_k and L_r by ratios:

$$a = \sqrt{L_z^2 + L_r^2}, \qquad b = \frac{M}{d \cdot \rho \cdot a},$$

where parameter d has dimension of length, it is equal to 1 for plane and $2\pi r_N$ - for axial symmetry (r_N -r is a coordinate of a particle. The angle of a particle turn with respect to z axis is $\varphi = arctg(L_r/L_z)$.

The changing of components of a vector of the form is determined ratios:

$$\frac{\partial L_z}{\partial t} = \frac{\partial u}{\partial r} L_r + \frac{\partial u}{\partial z} L_z,$$
$$\frac{\partial L_r}{\partial t} = \frac{\partial v}{\partial r} L_r + \frac{\partial v}{\partial z} L_z$$

During a particle motion in a flow field without changing its rectangular form, it may:

1) to be extended and to turn in a zone of deformations.

2) to be increased in the sizes, practically not being extended (for example, in a rarefaction wave).

In both cases there can be a break of continuity: in case 1 - in a direction of lengthening of a particle, in case 2 - in a direction of orientation of its sides. It is natural to introduce virtual particles into consideration ("virtual" - because the parameters of these particles are not stored in memory of the computer), that is to consider, that the basic particle consists of two (in case1) or from four (in case 2) particles. The masses of such virtual particles are equal and its sum is a sum of the basic particle. Other their parameters coincide, except for coordinates. Thus, the interpolation on grid nodes is conducted now from not one, but two (in case 1) or from four (in case 2) centers of virtual particles. The degree of continuity infringement is characterized by undimensional parameter η . The particle is

replaced with two virtual at $a > \eta \cdot h$, $b < \eta \cdot h$ and four at $b > \eta \cdot h$, where *a* is long side and *b* is short one of the basic particle. In majority of practical computations the value of parameter η is accepted equal to 1,2. With its increase the quality of observation of continuity infringements is worsened, with reduction - the time of computation grows because of occurrence of the large number of virtual particles.

In case when the particle was extended more than twice or volume of a virtual particle became equal to one of Eulerian cell, it is useful to make «partition» of a particle. As a result of such operation all virtual particles become urgent, that is in memory of the computer the necessary quantity of cells is allocated.

For example, the problem of impact of aluminum body with a rigid was solved. The size of body is 5x5mm, and the velocity is 1 mm / μ s. The results of calculations show that in case of neglect of the form of particles the breaks of continuity appear with course of time owing to deformation, and the decision ceases to describe a real physical situation. The account of the form with introduction of virtual particles and their partition excludes such opportunity.

For correct statement of boundary conditions of sliding and rebound on contact borders, and also on a free surface, at calculations of flows with not spherical tension tensor, it is necessary to know orientation of borders in space. In our method for this purpose the following procedure is used. The individual normal vector, specifying orientation of border, is determined for each node of Eulerian grid containing markers of two substances (node on contact border), and also for nodes, near to which "vacuum"nodes" are located (ones on free border). In the first case the normal vector is equal to the normalized sum of individual vectors focused from considered node in a direction of eight nearest nodes, which contain one marker of any bodies.

In the second case the addition of vectors focused on nearest vacuum nodes is similarly made. Let's note, that node belonging simultaneously to free and contact borders, is considered as node on free border.

Sometimes in calculations there is a situation, when among nodes nearest to one on contact border, there is no internal one (marked only by one marker). The normal vector in such node is determined with the help of interpolation from the nodes (next to it) belonging to contact border. The normal for the node D. V. Voronin

containing markers of three and more substances is there as well.

And, at last, with the purpose of increasing of accuracy of definition of borders orientation the averaging of normal in the next boundary nodes separately for nodes on contact and on free borders is spent. The usual condition of tension vector equality to zero is put on free border. For described gas dynamical variant of a method it means, that in nodes belonging to free border, the pressure is necessary equal to zero.

Sliding of materials along contact borders is provided as follows. At definition of spatial derivative, velocities in a particle in nodes of contact border recalculated so that their component (normal to border) remains without changes, and tangential one becomes equal to appropriate component of a particle velocity:

$$\bar{U}_{ij} = U_{ij}N_z^2 + U_NN_r^2 + (V_{ij} - V_N)N_zN_r,$$

$$\bar{V}_{ij} = V_NN_z^2 + V_{ij}N_r^2 + (U_{ij} - U_N)N_zN_r.$$

Here U_{ij} , V_{ij} are components of velocity in node

with index *i*, *j*, belonging to contact border, U_{ij} , V_{ij} are appropriate recalculated values, N_z , N_r are the components of an individual normal vector in node (*i*; *j*), calculated on the described above algorithm, U_N , V_N are the components of velocity in a particle with number *N*.

At excess by dragging out tension in node on contact border of some critical value p^* , appropriate node is announced as one belonging to free border. The value of its pressure is necessary equal to zero, and velocity is equal to one of a particle, considered at the same instant. It achieved an opportunity of division of materials along contact border. The choice of p^* is arbitrary enough. As a rule, the good results turn out at value p^* two order of magnitude smaller on absolute size than characteristic tensions arising in a flow field.

4 Numerical decisions of some problems

Consider some applications of the method for the solution of physical problems.

1. Let's consider the problem of initiation of gas detonation in tube with generation of cellular structure of detonation wave (DW).

The research area represents the plane channel with the closed left end and open right one. Width of the channel (diameter) L_0 is variable. Length of the channel is supposed to be sufficient for an establishment of self-supported mode of a detonation wave. Thin flat or semispherical layer of explosive substance settles at the closed end of the tube. The other part of the tube is filled with gas mix $2H_2 + O_2$. The explosion of the layer at instant t = 0 generates a shock wave (SW), propagating within the area. The walls of the channel are assumed to be rigid. The simulations have been executed within the framework of model of non-stationary two-dimensional flow of ideal compressible medium. The main equations of motion are based on the conservation laws of mass, pulse and energy without taking into account the dissipation effects (1)-(6). Some details could be found in [8]. Energy release in the reaction zone of DW was described according to two-stage model of chemical kinetics, using the equation for mean molecular mass of gas mix. The problem was solved numerically.

In fig. 3 the pressure maps for $2H_2+O_2$ gas mix are submitted at t > 0. More dark tones correspond here to higher meanings of pressure p in the range from 0.8 bar up to 40 bar. $L_0=100$ mm, initial radius of the initiator is 5mm, the energy of initiation $E^* = 435$ J/m, initial pressure $p_0 = 0.8$ bar. The area 1 is gas before SW, area 2 is the induction zone behind SW, where no chemical reaction occur, body 3 is the zone of chemical reactions, body 4 is a gaseous products of initiating explosive, continuous line 5 is a front of a flame. At first stages the flame lags behind SW, and length of the induction zone grows, achieving the maximal size 48mm in the middle of the channel by instant $t = 58 \ \mu s$. The velocity of leading SW thus passes through a minimum value. For this meaning of energy of initiation the simulations show attenuation of a detonation in boundless area. The presence of walls changes a situation: the gas is ignited in Mach waves reflected from them and powerful transverse waves of detonation appear (cadres 3-8 in the figure). The last ones collide, generating the area with high values of pressure and temperature (body 6 in cardes 8.9). Overdriven wave of a detonation (macrowave) occurs in the middle of the channel as a result of collision (cadre 10). For the subsequent intervals all stages of process repeat. At instant $t = 58 \ \mu s$ the velocity of a shock wave in the middle of the channel is less than 1.5 km/s, and at $t = 120 \ \mu s$ exceeds 3.5 km/s. Thus, a pulsing mode of detonation is temporarily established in the channel. With course of time the intensity of such cross waves decreases, and after 4 - 7 pulsations the detonation structure is transformed to a usual mode with auto oscillatory

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transformed to a usual mode with auto oscillatory micro-cells of detonation. The irregular cross structure of microwaves always occurs (more precisely, becomes visible) on the macrowave, as soon as pressure values in a vicinity of flame front decreases down to meanings, less than 30 bar (for example, area 8 on the cadre 9).

When cross macrowaves move from walls, the areas of not reacted gas are involved in the burned down gas (spots 7 in cadres 5-9), where they slowly burn, penetrating deep in area 3 and disappearing by instant t = 115 µs. The existence of such spots is shown experimentally. The size of spots found out in that experiment and caused by transverse waves (microwave), is comparable with the one of a detonation wave cell. The spots submitted in fig. 3 appear owing to geometry of an initiating charge and are formed by powerful cross macrowaves, and the size of spots exceeds length of a detonation cell. In fig. 3 (cadre 8), for example, one of spot achieves 6 mm of length. The computations show, that they occur in the following cases: (1) for the curved front of a flame interacting with a transeverse wave, (2) at the wall, when reflection of a shock wave occurs, (3) after collision of transverse waves. In the latter case they arise, if the waves are not too intensive (that is for microwaves). According to cadres 5-9 in fig. 3 the longitudinal velocity of a flow at the spots can be negative in laboratory system of coordinates because of waves collision (gas velocity in spots generated by cross microwaves remain positive, that becomes cleare due to their displacement in the figure). The number of fluctuations of the pulsing mode of detonation increases with reduction of the cross size of the channel L_0 , and their amplitude decreases as well. If L_0 is comparable with the size of a detonation cell, the mode becomes self supported without pulsations with parameters appropriate to a detonation with cellular structure. As a whole, at a variation of L_0 the map of wave interactions and formations of not reacted gas spots are similar. The formation of detonation structures with several powerful fluctuations at energies of initiation close to critical, growth of the wave velocity up to values much exceeding stationary value D_{CJ} , subsequent deep failures of the velocity and then exit to selfsupported mode is experimentally confirmed.

At $E^* = 400$ J/m there is also a pulsing detonation mode, the minimal velocity at the centre of the channel achieves 1100 m/s, the front of ignition lags behind SW, but after several fluctuations there is an attenuation of the wave. The critical value of energy $E^*min = 420$ J/m. With the further reduction of E^* the ignition of gas at the walls of the channel stops. The maps of the process at $E^* = 380$ J/m shows that that for the same instants, as in fig. 3, there is no ignition of a mix at walls of the channel yet. When the mix ignites, the formed transverse waves are too weak to excite a detonation. The variation of the diameter of the channel L_0 and radius of initiating charge r have shown, that the values of the critical energy of initiation at $L_0 > 9b$ and r > b is well correspond to the formula (within 6 % range) under condition of instant of initiating allocation of energy charge:

$$E^*_{\min} = a_v p_0 \left(\frac{150}{\sigma_0 \xi} b\right)^2, \quad \xi = 1 \div 2, a_v \sim 1. \text{ Here } \sigma_0$$

degree of compression in leading SW, *b* - longitudinal size of a detonation cell.

2. Next interesting problem is one of bubble detonations.

Let's consider the following physical problem. There is a horizontally located tube having diameter L₀ and filled with water. In the center of the tube on its axis of symmetry a bubble having diameter d₀ with a gas mix $2H_2+O_2$, is situated. The system liquid / gas is in a condition of dynamical balance at temperature $T_0=300$ K and initial pressure in a liquid $p_0=1$ bar. The acoustic complex, consisting of a wave of compression (its length L_1 , amplitude P=115 bar) and the following wave of rarefaction of the same length and amplitude, begins to move from the left closed end of the tube to the right one at instant $t_0=0$. The pressure profile in the complex has sine wave character. Such initial pulse is created by the electromagnetic generator of shock waves. At some instant the acoustic complex passes through the bubble vicinity, the flow leaves a equilibrium state, and there is a complicated current with deformation of interface border and formation of secondary waves.

Theoretical research is carried out within the framework of model non-stationary two-dimensional motion of ideal compressible media in case of axial symmetry. The current in a liquid (water) was described by laws of conservation of mass, pulse and the ratios, specifying shock adiabatic curve of water. Current in gas was modeled on the basis of laws of conservation of mass, pulse and energy supplied with the equation of state of ideal gas. Chemical reactions in a gas phase were described by two-stage model of chemical kinetics when at achievement of some minimal temperature in a particle readout of a chemical ignition delay began, the subsequent energy release was determined by the kinetic equation for average molecular mass of gas. Interface borders were considered as contact surfaces where a condition of a continuity of normal to a surface component of a flow velocity vector and a continuity of normal component of tension tensor were satisfied in view of effects of a superficial tension on interface border. Completely the mathematical model of flow motion is formulated in paper [9].

The numerical simulations of the problem have shown, that a single bubble dynamics essentially varies depending on initial parameters of the flow. At d₀ less than critical value, the bubble is quickly compressed in a falling wave of compression till the sizes of one particle in a numerical cell without appreciable distortion of the form (quasi-spherical collapse). At increase of d_0 , a cumulative water jet is formed on the left bubble wall, directed inside the bubble; it reaches opposite wall of the bubble, the latter one gets the toroidal form with subsequent collapse. At the further growth of d_0 the cumulative jet stops inside the bubble, subsequent unloading comes in a falling rarefaction wave at the left bubble wall, so the gas bubble arises on the left wall, directed towards to the wave of rarefaction. Then the jet fragmentation occurs, generating ob micro bubbles with significantly smaller (the order of magnitude) size, than the initial bubble. The last two cases we shall name as jet deformation of a bubble. As calculations confirm, a transitive zone between different scripts of a bubble deformation is very narrow. In fig. 4 the calculated changes of a bubble dynamics is submitted depending on values of initial flow parameters. The curve 1 in fig. 1 divides areas with spherical and non-spherical deformations of a bubble in an initial stage after passage of a compression wave, the curve 2 separates the area appropriate to a bubble collapse in a falling wave, from the area of its deformation without the collapse. Thus, area I corresponds to quasi-spherical collapse, II - to spherical deformation without a collapse, III - to jet deformation of a bubble without a collapse, IV - to jet deformation with the subsequent collapse.

If the acoustic complex passes through the group of nearby located bubbles their mutual influence generates more complicated wave structure and facilitates the occurrence of jet deformation. In fig. 5 the field of pressure in a vicinity of originally spherical bubbles (their initial diameter $d_0 = 800$ microns, the channel diameter $L_0 = 4$ mm) is submitted. More dark of tone in figure corresponds to waves of compression, light ones- to waves of rarefaction. In the top figure (t=9,2 us) it is visible, that the first bubble from the left side is deformed with formation of gas get, the second one- with formation of cumulative water jet inside the bubble, the third is compressed and gets a plate form, the fourth is punched by the cumulative jet and has the toroidal form. At the subsequent instant (the bottom figure, *t*=12,0 us) the first bubble is fragmented, micro bubbles are appears: at the second bubble a gas jet arises; the third keeps its form; the fourth bubble is in a condition of a collapse and is not distinct in the figure. In course of time the distance between the bubbles enlarges.

Thus, in a bubble cluster a jet deformation of bubbles and their crushing takes place. If for explosion of a spherical bubble (taking place at initial pressure of 1 bar), reduction of its diameter more than in 3 times is necessary, at jet deformation the ignition begins in jets or nearby micro bubbles at more great values of average bubble diameter. Therefore the explosion of a single bubble is possible in a weak acoustic wave and even in the single waves of rarefaction providing jet deformation of a bubble.

Micro explosions of not spherical bubbles may result in propagation of a of self-supported detonation wave sliding along a bubble chain. In fig. 6 a bubble detonation wave velocity is shown depending on initial volumetric concentration of a gas phase in a mix β_0 . A shaped curve in the figure is the data of experiment, continuous curve are the results of calculations. It is visible, that the model describes adequately enough the parameters of a detonation in bubble media.

3. Consider of the method application to problems of cosmogony.

The group of explosive hypotheses explains an origin of some celestial bodies by a nuclear explosion inside Proto-planets which fragments became germs of celestial bodies with unusual characteristics and abnormal chemical composition. According to some data, near a planet core there may appear an active layer, consisting of particles of dioxides and carbides of uranium, wheighed in liquid iron. Possible collision of large asteroid with a planet may result in nuclear explosion in a planet interiors. Modeling of the

consequences of such an explosion was executed. Full statement of the problem is made in [10]. Some results are represented in fig. 7. Here body 1 is a planet core, 2 is a stony shell, 3 is asteroid, 4 is a products of a nuclear explosion (plasma), 5 - dusty plum, 6 vacuum. The system of basic equations was solved numerically inside each body for the case of particle self-gravitation. The boundaries between bodies are time-dependant contact discontinuity surfaces, where conditions of pressure equality on both sides and continuity of velocity vector component (normal to boundary) are valid. In the figure we can see the generation of cumulative jet at nuclear explosion near to a planetary core due to gravitation forces. Depending on explosion energy it may penetrate in interplanet space or remain inside a planet. Anyway the jet promotes planet partial fragmentation with generation of planet fragments with unusial characteristics. The value of the energy of explosion here is equal to $3 \cdot 10^{21}$ MJ. The instant *t*=0 meets here the moment of the impact of the planet with the asteroid also. The profiles of velocity *u* along *r*-axis (Fig.7b, z=17500km) and z-axis (Fig7c, r=0) at the moment t=1327s show, that the flow velocity in the jet is much higher than in other regions of the planet. It achieves 7km/s. It is not enough for the emission of substance from the core into the interplanetary space. By instant t=2302s the velocity u in the jet falls up to zero, and it begins to be involved back in the core. Nevertheless, here again the products of the nuclear explosion break off the shell of the planet, and part of its substance comes off the planet, that it is visible in Fig.7.

5 Conclusion

In summary we list some specific features of the described method. Its basic difference from the scheme of a method GAP [4] consists in a way of integration of the equation of mass conservation and procedure of definition of pressure in nodes of Eulerian grid. Offered method of computation besides elimination of the decision strong fluctuations results in the following consequences:

1). The problem of pressure calculation in the socalled "mixed" cells [1, 3] is removed, that is in cells of Eulerian grid, in which there are particles of various substances. In the described method the pressure is calculated in a particle, and then it is interpolated on a grid. 2). The computation is possible to do with one particle on a cell.

3). For calculation of the next step on time, only the information on particles is necessary, since after interpolation "grid - particle " grid information is possible to wipe out. This property of algorithm allows rather simply solving a problem of memory.

Useful property of algorithm is that he easily allows parallel numerical modeling.

References.

[1] Harlow F.H. The numerical method of particles in cells for problems of hydrodynamics, *Computational methods in hydrodynamics*, Moscow, Mir, 1967, pp. 316-342.

[2] Ianenko N.N., Anuchina N.N., Petrenko E.E., Shokin U.I. On the methods of calculations of account of gas dynamics problems with the large deformations, *Numerical methods of continua mechanics*, 1970, Vol. 1, No 1, pp. 40-62.

[3] Anuchina N.N. On the methods of compressible flow computations with large deformations, *Numerical methods of continua mechanics*, 1970, Vol.1, No 4, pp. 3-64.

[4] Marder B.M. A PIC-TIPE fluid codes, *Mathem. of comput.*, 1975, Vol. 29, No 130, pp.434-446.

[5] Belotserkovsky O.M., Davydov U.M. *Method* of large particles in gas dynamics, Moscow, Nauka, 1984.

[6] Agureikin V.A., Kriukov B.P. Method of individual particles for computation of flows of multi component media with great deformations, *Numerical methods of continua mechanic*, 1986, Vol. 17, No 1, pp. 17 - 31.

[7] Nikolaev J.A., Zak D.V. The coordination of models of chemical reactions with the second beginning of thermodynamics, *Physics of Combustion and Explosion*, 1988, Vol. 24, No 4, pp. 87 - 90.

[8] Voronin D.V. On the initiation of gas detonation in a smooth tube. *Nauchnyi vestnik NGTU*, 2009, No 4, pp. 79-88.

[9] 3. Voronin D.V. On the excitation of detonation in a liquid with chemically active gas bubbles. *J.Chemical physics*. 2005, Vol. 24, No 9, pp. 51-58.

[10] Voronin D.V. Modeling of planet partial fragmentation under explosion. *Doklady Academii* nauk VS of Russian Federation, 2009, No1, pp. 19-29.



Fig. 1. Interpolation "particles - grid".



Fig. 2. Marking of grid nodes.



Fig. 3. Initiation of detonation in a tube



Fig. 4. Bubble dynamics dependence on values of initial flow parameters.



Fig. 5. Pressure maps in a vicinity of originally spherical bubbles.



Fig. 6. Bubble detonation wave velocity dependence on initial volumetric concentration of a gas phase.



Fig. 7. Dynamics of formation of the cumulative jet in interiors of the planet and its influence on the process of the fragmentation.