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CONSERVATIVE EULERIAN METHOD FOR NUMERICAL INVESTIGATION OF THE HYDRODYNAMICS OF LIQUIDS WITH A FREE SURFACE

S. E. Samokhvalov

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An effective numerical method is suggested for investigation of the hydrodynamics of liquids with a free surface. The method is a conservative Eulerian method that is useful for investigation of processes with turbulent behavior of the surface of the liquid that are accompanied by generation of waves, splash, spatter, etc. In the present method, apart from hydrodynamic equations, a transfer equation is used to describe transfer of the liquid phase. A method of numerical solution free from grid diffusion is suggested for this equation. It is proved that the conservative Eulerian method is adequate quantitatively for modeling the motions of a liquid with a slight deformation on its surface and adequate qualitatively for complicated motions.

Introduction. Knowledge of the hydrodynamics of a liquid with a free surface is necessary in the solution of many important practical problems such as optimization of the initial filling of molds with melt etc. The processes occurring on the surface are often vigorous, involving formation of splash, spatter, etc. Because of this, it is absolutely impossible to describe these processes analytically, and numerical methods should be used here.

A large number of publications are concerned with liquid flows with a free surface (see survey [1]). Depending on the method used to describe the motion of the liquid, these methods can be divided into three classes: Lagrangian, Eulerian, and Lagrangian-Eulerian. Lagrangian methods are used to describe relatively smooth flows with slight deformation of the liquid. In this case the region is divided into cells that move and are deformed together with the liquid. In the case of strong deformations, Eulerian methods are used, in which the cells of the grid remain immovable and the liquid flows through their sides. However, a Lagrangian stage is necessary to follow the free surface even in the case of a fixed grid. In this case the method is Lagrangian-Eulerian.

At present a Lagrangian-Eulerian method on the MAC grid is the most popular [2]. Its advantages are versatility and clarity in description of the motion of the liquid. One of its disadvantages is the basic nonconservativeness of the MAC method induced by the fact that the volume occupied by the liquid is determined from the location of markers whose coordinates are found approximately. Moreover, in order to provide steady-state motion of the free surface of the liquid and to prevent formation of computation-induced voids, it is necessary to introduce a large number of markers, whose coordinates overload the computer storage.

The numerical method described in the present work, which is a conservative Eulerian method (CEM) for calculation of the hydrodynamic parameters of the motion of a liquid with a free surface, is free from these drawbacks. A consequence of the conservativeness of the method suggested is adequate description of fine splash with scales smaller than the scales of the grid, because of which the step of the three-dimensional grid can be increased, decreasing requirements on computer resources. The computations whose results are reported in the present work have been obtained on an IBM PC.

1. Description of the Method. The main idea of the CEM is presented in [3] and consists in the fact that the entire computation region is represented by a density-stratified gas-liquid medium. The proportion of liquid in the volume can be inferred from the value of its density. The location of the free surface is determined from the

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lines of equal density in the medium. In regions fully occupied by the liquid, the medium should be incompressible. In regions partly occupied by the liquid (near-surface areas and splash), the equation of state of the medium should be postulated in a certain way.

In the present work the following simplifying assumptions have been made:

1. There are no phase conversions; gas is not evolved from or absorbed by the liquid.

2. The medium is Newtonian and its effective dynamic viscosity, including the turbulent component, is proportional to the density, $\mu = \nu\rho$, i.e., the effective kinematic viscosity of the medium ν is independent of the density.

3. The equation of state of the medium has the form

$$\rho = \text{const} \quad \text{at} \quad \beta = 1\,, \quad p = \text{const} \quad \text{when} \quad \beta < 1\,; \tag{1}$$

in accordance with this assumption, outside the space fully occupied by the liquid, i.e., near-surface areas, splash, and areas fully free of the liquid, the medium is absolutely compressible. This corresponds physically to a vacuum-liquid medium rather that to a gas-liquid medium.

Due to the assumptions just made, the equations of motion of the medium are separated into two systems:

$$\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V}\nabla)\,\mathbf{V} = \nu\Delta\mathbf{V} + \mathbf{g} - \nabla\tilde{p}\,, \quad \nabla\mathbf{V} = 0 \quad \text{at} \quad \beta = 1\,; \tag{2}$$

$$\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V}\nabla)\,\mathbf{V} = \nu\Delta\mathbf{V} + \mathbf{g}\,, \quad p = \text{const} \quad \text{when} \quad 0 < \beta < 1\,. \tag{3}$$

They are supplemented by the equation

$$\frac{\partial \beta}{\partial t} + \nabla\,(\beta\mathbf{V}) = 0\,, \tag{4}$$

which follows from the equation of mass transfer $\partial\rho/\partial t + \nabla(\rho\mathbf{V}) = 0$ and the relation $\rho = \rho_{\text{liq}}\beta$. Depending on the results of solution of Eq. (4), the integration region is divided into three zones: a liquid zone with $\beta = 1$, where Eqs. (2) are satisfied; a vacuum-liquid zone with $0 < \beta < 1$, for which Eqs. (3) hold; and a vacuum zone with $\beta = 0$. Since the division of the computation region into subzones changes with time, we have a conjugate problem with movable conjugation boundaries. That our approach provides the possibility of describing the dynamics of the vacuum-liquid zone is its distinctive feature that ensures conservativeness of the difference scheme.

In the liquid and vacuum-liquid zones (i.e., throughout the medium considered), Eqs. (2) and (3) equally describe convective and diffusive transfers of momentum and gravity-induced changes in momentum. In using the method of splitting according to physical factors [4], this fact facilitates solution of the stated problem. Indeed, in accordance with this method, the equations of motion of the medium in all the zones can be expressed as a common system of equations

$$\tilde{\mathbf{V}} = \mathbf{V}^n + \tau\,[-(\mathbf{V}^n\nabla)\,\mathbf{V}^n + \nu\Delta\mathbf{V}^n + \mathbf{g}]\,, \tag{5}$$

$$\Delta\tilde{p} = \frac{\nabla\tilde{\mathbf{V}}}{\tau}\,, \tag{6}$$

$$\mathbf{V}^{n+1} = \tilde{\mathbf{V}} - \tau\nabla\tilde{p}\,, \tag{7}$$

where $\mathbf{V}^n$ is the velocity at $t = n\tau$; in this case Eqs. (5)-(7) are solved in the zones where the liquid is present (with $\beta \neq 0$) and Eq. (6) is solved only in the zone fully filled with the liquid (with $\beta = 1$). Thus, Eq. (7) ensures nondivergence of the motion of the medium only in its liquid part.

The conditions of no flow through the surface and free slip are chosen as boundary conditions for the fields of β and V on solid surfaces and symmetry planes (or the axis):

$$\mathbf{n}\nabla\beta = 0\,, \quad \mathbf{n}\nabla V_{\parallel} = 0\,, \quad V_{\perp} = 0\,, \tag{8}$$

and the condition of free flow through the surface is chosen in the inlet and outlet flows:

$$\beta = 1\,, \quad \mathbf{n}\nabla V_{\parallel} = 0\,, \tag{9}$$

Moreover,

$$V_{\perp} = V_s\,, \tag{10}$$

if the flow velocity V_s is given, and otherwise,

$$\mathbf{n}\nabla V_{\perp} = 0 \tag{11}$$

Conditions for $\tilde{p}$ on the boundaries of the computation region are obtained by projecting Eq. (7) onto the normal to the surface n, except for surfaces through which the liquid flows freely and its velocity is not prescribed but is to be calculated (i.e., Eq. (11) is used). On these surfaces the pressure p_s should be prescribed and boundary conditions of the first kind are taken for $\tilde{p}$:

$$\tilde{p} = p_s/\rho_{\text{liq}}\,. \tag{12}$$

Since the vacuum zone is neglected in the calculation of velocities and pressure is calculated only in the liquid zone, boundary conditions for velocities and pressures should be prescribed at the boundaries of the liquid and vacuum zones, respectively. The pressure at the boundary of the liquid zone is assumed to equal the constant value p_a, and at the liquid-vacuum interface free motion of the liquid should be provided, i.e., the conditions of free flow (9) and (11) should be chosen as boundary conditions for the velocities.

The difference approximation of the right-hand sides of the system of equations (5)-(7) is found with a staggered grid [5] by introducing the approximation component of the viscosity in writing down the diffusion term:

$$\nu_a = \frac{d}{\mathrm{Re}_d} V + b^2 d^2 \left| \frac{\partial V}{\partial y} \right|\,, \tag{13}$$

whose parameters Re_d and b along with the isotropic component of the effective viscosity can be used to take account of turbulent motion of the medium.

Whereas at the boundaries of the computation region the difference representation is performed in the standard way [5], on the free surface it is necessary that the conditions of free flow of the liquid be satisfied as accurately as possible, i.e., that the drag of the free surface, which is able to distort its shape and the dynamics of the motion, be absent. To do this, first, it is necessary that velocities on the vacuum sides (separating vacuum cells) be prescribed not for all the velocities calculated but separately for each velocity in accordance with the difference analog of Eqs. (9) and (11) (Fig. 1a). In particular, in calculating a new velocity at point 1, the velocity at vacuum point 0, which should be equated to the velocity at point 1, is used. The same refers to points 2-4. Since in the general case the velocities at points 1-4 are different, one velocity cannot be assigned to point 0 without violating the difference analog of the conditions of free flow, and therefore in calculating each of the velocities 1-4, a new velocity at 0 is prescribed. This makes the calculation slower but does not result in grid-induced deceleration of the liquid on the free surface. Second, on the sides of cells that were vacuum sides and therefore had a zero velocity and to which the liquid comes in a particular time step, velocities should be prescribed. In Fig. 1b point 0 is one such point. Both the velocity of point 1 and that of point 2 can be assigned to it. In such situations the arithmetic mean of the velocities at neighboring nonvacuum points are chosen.

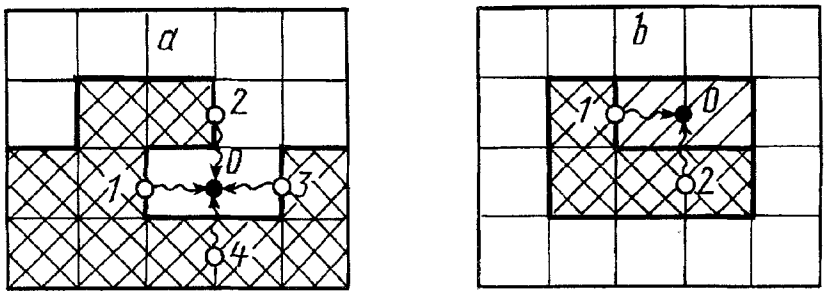

Fig. 1. Prescription of boundary conditions for velocities on the free surface. Cross-hatched cells contain liquid; hatched cells are occupied by the liquid

A constant value p_a in cells that are not filled with the liquid irresepective of the amount of it in them is the boundary conditions for pressure. The difference Poisson equation is solved by the upper relaxation technique [6].

2. A Nondiffusion Method for Solution of the Transfer Equation. Equation (4), determining the division of the calculation region into zones, requires careful choice of a numerical method, since the presence of slight grid diffusion, which usually arises in a difference approximation of a transfer equation, leads to rapid smearing of the liquid-vacuum interface and cannot be followed thereafter. Therefore, to provide the possibility of numerical implementation of the method suggested in the present work for investigation of the hydrodynamics of liquids with a free surface, grid diffusion should be suppressed completely in writing down the difference analog of Eq. (4).

For complete conservation of the liquid (in the free surface, too), a conservative difference scheme will be used for numerical solution of Eq. (4):

$$\beta^{n+1} = \beta^n - \tau\,[(\beta u\sigma)^e - (\beta u\sigma)^w + (\beta v\sigma)^n - (\beta v\sigma)^s], \tag{14}$$

where the superscripts w, e, s, and n refer to the western, eastern, southern, and northern sides of a cell of the grid. On a staggered grid the field of β is prescribed in the center of the cells, determining the proportion of liquid in them. It is necessary to evaluate β, contained in Eq. (14), on the sides of the cells.

In the present case it is impossible to use the arithmetic mean over neighboring cells, irrespective of the time $t \in [n\tau\ (n+1)\tau]$ at which β is taken (i.e., irrespective of the fact that the scheme is explicit or implicit), since grid diffusion will arise. It can be avoided by making the assumption that only void-free liquid with $\beta = 1$ can flow through the sides of the cells. With this assumption, the following rule should be used for choosing values of β on the sides of the cells. When the side separates two cells containing liquid (with $\beta > 0$), $\beta = 1$ should be assumed on it. On sides separating vacuum cells from those partly filled with the liquid (with $0 < \beta < 1$), $\beta = 0$ is assumed. In this case the only exclusion is cells partly filled with the liquid, separated by vacuum cells at two sides along either coordinate axis. If, in correspondence with the given rule, $\beta = 0$ is assumed on the sides perpendicular to this axis, the liquid confined in this cell is not allowed to move along this axis, i.e., the liquid will be artificially brought to stagnation. To prevent this, it is necessary to ensure that passage of the liquid through the sides of such cells is allowed. On the sides separating vacuum cells (with $\beta = 0$) from liquid ones (with $\beta = 1$), the value of β is determined by the velocity of the medium. If the velocity is directed from a liquid cell to a vacuum one, $\beta = 1$ is assumed, otherwise $\beta = 0$.

The present method of solving the transfer equation is completely devoid of grid diffusion, which is confirmed by numerical experiments. For example, a freely falling drop does not change its shape and is not "smeared" throughout falling, irrespective of the value and direction of the initial velocity.

The method of numerical solution of the transfer equation just described can also be used in other cases where network diffusion associated with the convective term should be suppressed. For example, this method can be used for investigation of a homogeneous "spot" in a density-stratified liquid and, in general, in all cases with a movable interface between liquid phases.

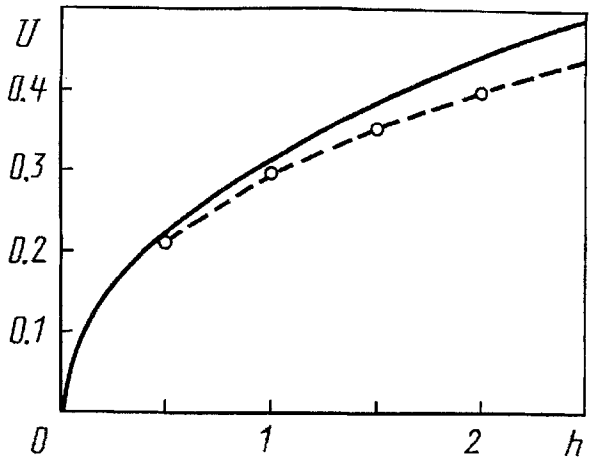

Fig. 2. Plot of the wave velocity versus the depth of the pool; the solid curve is calculated by Eq. (15), the dashed curve is calculated by the CEM. U, m/sec; h, cm.

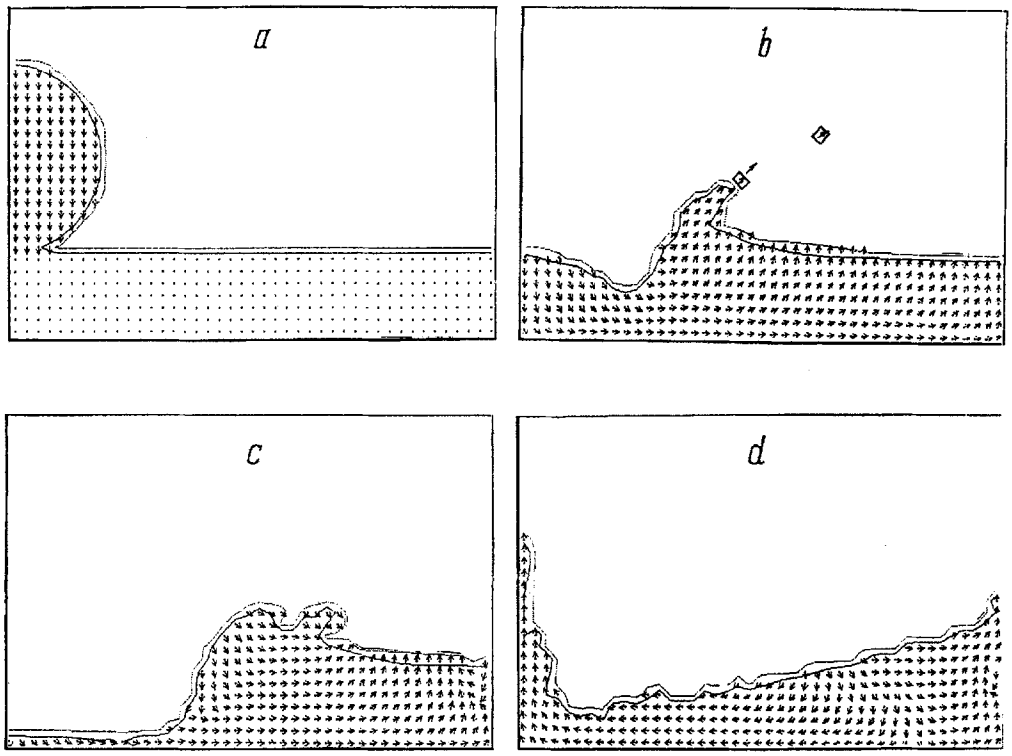

Fig. 3. Dynamics of the liquid in the case of a falling drop 0 (a), 0.555 (b), 0.135, and 0.255 sec (d) after the start of the process. The isoconcentration lines correspond to $\beta = 0.5$ and 0.1; arrows show the direction of motion of the liquid.

3. The adequacy of the Method. The adequacy of the CEM was verified for the first time in the very simple case of a freely falling drop. Moreover, the well-known formula for the velocity of propagation of a gravity wave in a shallow pool [7]

$$U = \sqrt{gh} \tag{15}$$

was verified. Results of this verification are shown in Fig. 2. In general, the computed curve lies below the theoretical one, which can be explained by the presence of grid (approximation) viscosity, which is exhibited more, the higher the velocity.

When the surface is quiet, for example, in the final stages of filling a mold, the hydrodynamic parameters of the motion of the liquid calculated by the present method coincide completely with those calculated by the conventional splitting method [5].

All this proves that models based on the CEM are adequate both qualitatively and quantitatively for simple motions of a liquid.

In order to prove the applicability of the CEM to the modeling of arbitrary motions of a liquid surface, we will consider the problem of a drop falling into a vessel with liquid. In this case the problem has cylindrical symmetry. The initial configuration of the liquid and the directions of the velocities in it are shown in Fig. 3a. The following geometrical dimensions have been chosen: the radius of the vessel is 0.215 m, the radius of the drop is 0.04 m, and the initial depth of the liquid in the vessel is 0.035 m. The velocity of the drop is taken to be 1.5 m/sec. The calculation was conducted on a square grid with a step of $5 \cdot 10^{-3}$ m. The turbulence parameters were chosen following [5].

At the moment of collision of the drop with the liquid, a corona-like splash arises. Fine droplets are separated from the crest of the splash and move over parabolic trajectories toward the wall of the vessel (Fig. 3b). Then, the splash breaks down (Fig. 3c). Subsequently, the liquid starts to move toward the axis of symmetry, an where, as a result of axial symmetry, axial splash arises with possible separation of a drop at its crest (Fig. 3d).

The picture just described coincides with ones that were observed in experiments and obtained by computations performed by other methods [6, 8], which proves that our model is qualitatively adequate for the process considered.

It should be noted that in our opinion, for a complicated process such as the fall of a drop, qualitative adequacy of the model indicates convincingly its quantitative adequacy, since, for example, to obtain the effect of reverse splash with separation of a drop in computations, it is necessary that the proportion of the magnitudes and directions of the velocities in the volume of the liquid be specific, which can only be achieved when they are calculated correctly.

In our opinion, the most promising improvement of the version of the CEM suggested in the present work is the choice of an equation of state of the medium that is less trivial than Eq. (1) for the part not fully filled with liquid. In this way, similarly to [8], it is possible to improve the prescription of theboundary conditions for the pressure on the free surface, which leads to steadier motion of it, and to substitute a gas-liquid medium for the vacuum-liquid one used in the present work.

Conclusions

1. The conservative Eulerian method suggested here is an effective method for numerical investigation of the hydrodynamics of a liquid with a free surface and can be used for computing a broad class of hydrodynamic effects.

2. For processes involving slight deformation of the free surface, the CEM describes adequately the quantitative characteristics of the motion of the liquid and the behavior of the free surface.

3. The CEM provides a qualitatively correct description of motions of a liquid that involve vigorous turbulent effects on the surface.

4. The method considered can be used, for example, for numerical investigation of the filling of ingots and molds with melt.

NOTATION

V, V, u, v, velocity of the medium, its magnitude, and, horizontal and vertical components; $\tilde{V}$, conventional velocity; $V_{||}$, $V_{\perp}$, components of the velocity parallel and perpendicular to the surface; V_s, flow velocity; U, velocity of the wave; g, gravitational acceleration; ρ, ρ_{liq}, density of the medium and the liquid phase; p, pressure; $\tilde{p} = p/\rho_1$; μ, ν, effective dynamic and kinematic viscosities; ν_a, approximation component of the viscosity; Re_d, b, its parameters: grid Reynolds number and ratio of the mixing length to the grid step; y, distance along an axis

perpendicular to the flow; β, volume fraction of the liquid phase; t, time; τ, time step; d, grid step; h, depth of the pool; σ, ratio of the area of the side of a cell to its volume; $\mathbf{n}$, normal unit vector to the surface.

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