Simulation of a liquid drop on a vibrating hydrophobic surface

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Abstract. Mathematical simulation is used to study processes describing a liquid droplet oscillation on a solid surface. The pattern of generated internal flows is characterized by complex interaction between capillary and gravity waves, free surface and contact angle. Interaction process factors are analysis. The given results are compared with the experimental ones.

Introduction
Problem of a solid heaving with Faraday wave’s generation in a liquid is an example of complex dynamic interaction in solid – liquid system [1]. When liquid layer with free surface oscillates in heave we can observe surface capillary waves – Faraday wave’s. Its dynamics depends on the system control values such as: viscosity, surface tension and liquid density as well as external action characteristics. Such waves are initiated after they reach some threshold amplitude of oscillation.

Let’s consider preliminary stage of the phenomenon with small amplitudes that endure liquid heave oscillations on its surface to initiate capillary – gravity waves. The present thesis is concerned with a research on internal flows in a small amount of liquid - a droplet and its influence on generation and initiation threshold of waves.

Most articles in experimental hydrodynamics on studying a parametrical resonance in a liquid research have the same model in common, i.e. as a rule an oscillating vessel is considered. [2, 3]. Frequency range of gravity waves initiation on a free surface in a liquid droplet is experimentally studied in scientific works [4, 5, 6, 7]. Thus, the work [4], is concerned with problems of detection of various oscillation modes for free surface of a droplet placed on a vibrating water proof surface with small hysteresis of a contact angle, as well as with contact angle and hysteresis impact on liquid oscillation modes research. Works [5, 6, 7] study oscillations of a liquid of extra small volume (5 µl) laying on a solid surface vibrating at a low frequencies (less than 800Hz) and with small amplitudes (up to 22 µm). Data on droplet free surface depending on the vibrating surface location are provided, instant droplet profiles and internal capillary flows obtained using PIV method are also considered. Moreover, articles [5, 6, 7] represent obtained droplet shapes corresponding to the various surface vibration modes.

There are only few studies [3, 8, 9, 10] that are dedicated to the solid surface vibration with a liquid of various volume simulation problems. At the same time problems of mathematical simulation of a single droplet placed on vertically vibrating at low frequencies and small amplitudes (solid) surface are concerned only in article [10] that study oscillation and spraying of a single liquid droplet of 30µl on a solid rod. In this study the physical thesis statement has several rather strong assumptions: the
initial droplet configuration was determined as half sphere, in addition to this the possible movement of a contact line was not considered and the state on the border of a solid surface was assumed as sticking; in hydrodynamic equations cycling acceleration of a body is added to the gravity acceleration (system parameter) considered in equation factors or boundary conditions. Navier-Stokes equations in axially symmetrical statement are solved by marker and cell projection method. The equation system is approximated by space with the finite volume method on a structured grid. Flow reconstruction on the cell edges is performed using central difference schemes and the convective terms sampling was performed using hybrid Nichols difference scheme. The solution of given algebraic systems was achieved under Cholesky conjugate gradient scheme.

Experimental researches prove that internal flows in a droplet are characterized by a clear three-dimensionality, and wetting angle is one of the key parameter in a system. Solution methods of such tasks concerning free liquid surface require high resolution of thin layers (gas-liquid-solid contact point) and developed free surfaces implementation.

The given study is set in a following way. First chapter provides the problem description and general assumptions. Second chapter observes the features of calculating the free surface using the control volume method and VOF. Third chapter provides both results of selected schemes and algorithms tests with the task [6] having experimental description as an example, and analysis of obtained instant capillary flows patterns in an oscillating droplet, it also concerns typical topological features of flows.

1. Problem statement
We consider the problem of liquid droplet motion caused by vertical movements of a solid surface. Let the area \( \Omega \subseteq \mathbb{R}^3 \) (fig. 1) be filled with biphasic medium and \( \Omega = \Omega_1 \cup \Omega_2 \). We consider subdomain \( \Omega_2 \) being a gas, and \( \Omega_1 \) — being a liquid; \( \Gamma_0 \) is a phase boundary, \( \Gamma_1 \) — atmospheric boundary of computational region. At the initial instant \( t = 0 \) the surface starts to vibrate at a given frequency and amplitude. A liquid drop placed on the surface also starts to make vertical oscillations.

![Figure 1. Computational region: droplet crosses section initial profile.](image)

The experimental apparatus is described in article [6], the surface was carefully cleaned and covered by hydrophobic coating. De-ionised water droplet of 5\( \mu \)l volume was placed in a center of a surface (on a center line of a rigid surface, fig. 1) using a dropper, thus the wetting angles were equal to \( \theta = 115 \pm 1 \), and the contact diameter and droplet height — 2.02 mm and 1.52 mm, respectively. Needless to say, vertical oscillations of a solid surface obtained in the study [6] are not harmonic but due to insignificance of the differences they were considered as sinusoidal oscillations under the numerical experiment.
2. Methods and algorithms

The given problem can be considered as a system of two immiscible incompressible viscous fluids the motion of each is described by Navier-Stokes equations and continuity equation

\[
\frac{\partial (\rho U)}{\partial t} + \nabla \cdot (\rho U U) = -\nabla p + \nabla \cdot \mathbf{\tau} + \rho \mathbf{g},
\]

(1)

\[
\nabla \cdot \rho_i U_i = 0,
\]

(2)

where \( \mathbf{e} \) — unit normal, external to the \( \Omega_0 \), \( K \) — surface curvature \( \Gamma_0 \), \( \sigma \) — surface tension coefficient, \( \Theta \) - wetting angle. In this study the wetting angle value will be determined basing on empirical model of dynamic contact angle [11]

\[
\Theta = \Theta_0 + (\Theta_A - \Theta_R) \tanh \left( \frac{u_w}{u_0} \right),
\]

where \( \Theta_0 \) — static contact angle, \( \Theta_A \) — maximum permitted value of the contact angle (for the given problem \( \Theta_A = 116 \)), \( \Theta_R \) — maximum value of the contact angle (for the given problem \( \Theta_R = 114 \)), \( u_w \) — solid interface velocity, \( u_0 \) — a constant, well-behaved as scale of contact angle change rate, for the given problem \( u_0 = 1 \), while the problems of impact of dynamic angle changing model on simulation results are not considered.

Geometrical characteristics of phase interface \( \Gamma_0 \) are unambiguously determined as

\[
e = \frac{\nabla \alpha}{|\nabla \alpha|}, \quad K = \frac{\nabla \cdot \nabla \alpha}{|\nabla \alpha|},
\]

where \( \alpha \) — is scalar function.

\[
\alpha(t, x) = \begin{cases} 
1, & x \in \Omega_1, \\
0, & x \in \Omega_2 \cup \Gamma_0,
\end{cases}
\]

in this case having the meaning of volume concentration of a liquid. By doing so we determine density, pressure and viscosity functions as \( \rho = \rho_2 + (\rho_1 - \rho_2) \alpha \), \( p = p_2 + (p_1 - p_2) \alpha \) and \( \mu = \mu_2 + (\mu_1 - \mu_2) \alpha \) respectively, and rewrite the system (1), (2) considering (4), (3) as following

\[
\frac{\partial \rho U}{\partial t} + \nabla \cdot (\rho U U) = -\nabla p + \nabla \cdot \tau - \sigma K V \alpha \delta(\alpha)(1 - \cos \Theta) + \rho \mathbf{g},
\]

(5)

\[
\nabla \cdot U = 0.
\]

(6)

System (5), (6) is added by transfer equation for \( \alpha \)

\[
\frac{\partial \alpha}{\partial t} = \mathbf{U} \cdot \nabla \alpha.
\]

(7)

We pass on to the modified pressure

\[
p_d = p - \rho g h, \quad \nabla p_d = \nabla p - \rho g,
\]

(8)

Then the equation (5) is written as

\[
\frac{\partial \rho U}{\partial t} + \nabla \cdot (\rho U U) = -\nabla p_d + \nabla \cdot \tau - \sigma K V \alpha \delta(\alpha)(1 - \cos \Theta).
\]

(9)

Surface tension force acting in a thin transient layer, that in the limit is thin infinite and corresponded to the \( \Gamma_0 \), can be converted to volume one [12]

\[
\mathbf{G} = -\sigma K V \alpha \delta(\alpha)(1 - \cos \Theta).
\]
The system (6), (9), (7) was numerically solved using control volume method for the sampling of the original equations. In order to simplify the further stage we pass in the conventional manner on to the dimensionless variables, in this case only written form of the equation (9) will be changed

$$\frac{\partial u}{\partial t} + \nabla \cdot uu = -\nabla p + \frac{1}{\rho} \nabla \cdot \nabla u + \mathbf{G}.$$  \hspace{1cm} (10)

Let's write an approximation of the equations (6), (10) in semi-discrete form

$$\sum_{f \in N_M} S_f \cdot u_f^{n+1} = 0,$$  \hspace{1cm} (11)

$$\frac{3u_M^{n+1} - 4u_M^n + u_M^{n-1}}{2\Delta t} V_M + \sum_{f \in N_M} F_f u_f^{n+1} - \sum_{f \in N_M} \frac{1}{\rho} S_f \cdot (\nabla u^{n+1})_f = - (\nabla p)_M V_M,$$  \hspace{1cm} (12)

where $u_M^n$ — velocity in the centre of a cell numbered $M$ on $n$ time interval; $V_M$ — cell volume; $F_f$ — flow through the edge with number $f$, $N_M$ — set of neighboring cells numbers; $S_f$ — outward normal vector to the edge with number $f$, in absolute value equal to the area of this edge.

Numerical solution of incompressible fluid dynamics equations of type (9), (6) require application of special methods to obtain velocity and pressure fields meeting the conditions of conservation and continuity by time on each step. In this study pressure implicit procedure with splitting of operator offered by Issa [13] called PISO is used.

Discretization of convective terms by area is performed using second order Van Leer's scheme. Reconstruction of flows on the edges of cells is performed using TVD scheme where approximation is based on central differences, and Van Leer's limiter [14] is applied as required limiter function. The obtained algebraic equation system is solved numerically using conjugate gradient method with incomplete Cholesky diagonal preconditioner.

The equation (7) is solved on each time step after system (9), (6) solution. In order to do so it is more convenient to rewrite (7) in conservative form

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (u \alpha) + \nabla \cdot (\alpha (1 - \alpha) u_r) = 0,$$  \hspace{1cm} (13)

where $u_r = u - \bar{u}$ — is velocity of the relative phase motion on the interface $\Gamma_0$. In initial model $\Gamma_0$ is infinitely thin and $u_r = 0$, however due to the numerical diffusion in calculations transition zone inevitably appears. Following the method of control volume we write an approximation (13)

$$\frac{3\alpha_M^{n+1} - 4\alpha_M^n + \alpha_M^{n-1}}{2\Delta t} + \sum_{f \in N_M} F_f (\alpha_M^{n+1}) + \sum_{f \in N_M} (1 - \alpha)_M^n F_f^* (\alpha_M^n) = 0,$$  \hspace{1cm} (14)

where

$$F_f^*(\alpha) = c_\alpha \max_{\Omega} \left| \frac{e \cdot S_f}{|S_f|} \right| e,$$

When solving the equation (14) a convective term approximation is performed is performed to that described above. And scalar coefficient $c_\alpha$ serves to control the artificial compression in the area of dispersion to compensate the numerical diffusion effect, in this study the coefficient $c_\alpha = 1$.

### 3. Numerical simulation

This study investigates low-frequency ($\approx 85$ Hz) oscillation of a water drop $5 \, \mu l$ in volume on a rigid surface, that is experimentally described [6], including the analysis of droplet profile and data on time-to time variation of free surface height change.

Mathematical simulation of liquid motion under oscillations was performed using volume-of-fluid method in a cell in two stages: first — the solution of liquid droplet stabilization on a horizontal rigid
surface problem; second – the vibration of the surface with a stabilized droplet on it. Droplet was set into equilibrium considering contact angle change, stabilization of the droplet from a cylindrical column of liquid of given volume under gravitation and surface tension was investigated. The droplet configuration was compared to the experimental by profile height, 3 phase contact diameter and wetting angle real value.

A Low-frequency oscillation of a liquid drop on a rigid surface simulation was performed on a grid consisting in 364140 hexagons. Let’s consider methods of accounting of the contact angle in a 3 phase gas-liquid-surface contact line. Wetting angle \( \Theta \) is determined not only by physical and chemical properties of a liquid but by surface material properties and is not constant even in case of liquid and surface stability. As the dynamic component of the contact angle during surface oscillations is not zero it is possible to estimate its effect both on oscillating droplet profile and on droplet local height. Fig. 2 shows diagram of the droplet height change in time resulting from vibration process simulation considering the dynamic change of wetting angle (curve 1, fig. 2) and using only static contact angle model (curve 2, fig. 2).

![Figure 2. Droplet height variation diagrams: a) considering: 1 — dynamic wetting angle; 2 — static contact angle b) for mode 2: 1 — experiment [6], 2 — calculation.](image)

Given curves have similar quantities and qualitative values but the amplitude difference on peaks reach up to 15%. Thus, static wetting angle consideration alone leads to droplet height amplitude lowering. Needless to say, oscillation frequency increase leads to contact angle determination method impact increase. Free droplet surface oscillation forms on a vibrating at frequency of 85 Hz surface (fig.3) were determined, i.e. one circle nodal line on a free surface corresponding to the oscillation second mode [6] was discovered.

![Figure 3. Droplet forms for the second mode: a) numerical; b) experimental [6].](image)

As shown on fig. 3, the simulation with set up parameters provides oscillation modes equal to the experimental ones, but local values of calculated phase interface motions (fig. 3 a) are less that
experimental ones (fig. 3 b) that results from discovered differences of equilibrium profiles and can be solved using additional algorithms of free surface reconstruction. Let’s consider diagrams of droplet height change on a vibrating surface (fig. 2 b). Time-dependencies of droplet height change obtained during simulation match in qualitative values with experimental values. However, droplet oscillation amplitude values are significantly (up to 41%) less than experimental values due to small qualities of free surface motion (fig. 3).

To study the internal flow peculiarities we generated instant patterns of droplet velocity vectors at various moments of time (fig. 4).

As shown on fig. 4 the flows in a droplet are mainly determined by surface motion direction. Thus at initial moment of surface lifting on a 4th period ($4t^* + 3\pi/4$ - lowest position of the surface and $4t^* + 0.775$ - beginning of a surface lifting) we observe velocity vectors relocation and flow direction change. Paired symmetrical whirls are clearly visualized. In this case, when at the initial moment of flowerets surface location 5 pairs of symmetrical whirl structures (three on various heights close to the droplet center line and two paired whirls at the periphery close to a free surface) and one special point of saddle type are detected the following surface lifting ($4t^* + 0.775$) leads to integration of lower whirls into large symmetrical paired whirl with two clearly defined drip lines, and integration of previously detected side whirl structures is observed. Thus internal liquid flows have delayed response to the surface motion direction change and start to change their direction from lower layers directly interacting with the surface. Interaction of differently directed internal flows results in circulation zones formation and interaction of turning flows results in drip lines and saddle point formation.

Furthermore, at the moment of time related to the fifth period ($5t^*$) beginning and highest ($5t^* + \pi/4$) position of the surface irrotational flows are observed in the drop, and at the moment of time related to the fifth oscillation period beginning, we detect final relocation of velocity vectors, two drip lines directed along with the spreading pressure.
4. Conclusion
The studied problem of liquid droplet oscillation on a solid surface under heave low-frequency oscillations is one of the few studies that have experimental description that allows numerical schemes and algorithms testing. Comparison of the numerical simulation results and experimental data shows that applied VOF method provides appropriate description of surface-to-droplet energy transfer processes. In addition, detected significant differences of calculated drop oscillation amplitude values from experimental ones indicate a need for more detailed account of both surface forces and dynamic contact angle range. Thus algorithms for surface forces and dynamic contact angle change determination in air-liquid-surface triple point require additional improvement and testing.

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