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STICK-SLIP BEHAVIOUR OF THE LIQUID DROPS ON AN INCLINED PLANE: A NUMERICAL EXAMPLE

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Abstract. A numerical modelling of the stick-slip effect of the contact line of a liquid droplet, located on a sloping plane is proposed. Our study is based on a continuum model of the contact angle hysteresis [6]. We assume the system to approach an equilibrium state following a specific path. A jerky change of the contact line is obtained in two cases: when the drop volume is increased and when the inclination of a sloping plane is changed.
Key words: stick-slip behaviour, liquid drops, contact line.

1. Introduction

Stick-slip behaviour of equilibrium liquid droplets, located on a sloping plane is a well-known phenomenon [1]. For instance, when the drop volume is increased, the contact line initially appears to be pinned until it is suddenly moved when a certain volume is reached. A similar behaviour is noted for the change of a sloping plane inclination. It is observed even for Superfluid Droplets [2]. This phenomenon is feature of the contact angle hysteresis therefore hysteresis models could be base for analysis of the stick-slip behaviour of the contact line. So, this phenomenon was attributed to potential barriers on the molecular scale [3]. The same phenomenon has also been modelled a priori assuming pinning by surface defects or adding force acts along the contact line [4], or energy related to static friction [5] on the surface between the drop and the solid, the same energy acts as potential barrier too [6].

The hysteresis effect of the contact angle determines the existence of the set of equilibrium shapes with different contact lines of the droplet for its fixed volume and physical-chemical parameters of the system. So, if a definite equilibrium state (with a specific contact line) is violated as a result

of the change of a certain system parameter, the droplet can pass to another equilibrium state with a contact line that significantly differs from the previous equilibrium one. Such a jerky change of the contact line is known as a "stick-slip" effect.

The present paper proposes the stick-slip effect numerical modelling. Consider the contact line of a liquid droplet located on a sloped surface. However, the models employed there cannot be applied for a droplet on a sloping plane without performing some modifications. Regarding the case of a sloping plane, realistic results are obtained only for the droplet equilibrium shapes and stability loss [10–13]. Moreover, the transition to a new equilibrium state, coupled by a jerky change of the contact line, is still not realised. Our study will be based on a continuum model of the contact angle hysteresis [6, 9]. We assume that the system approaches an equilibrium state following a specific path. Furthermore, we assume that the system undergoes a succession of modifications. Each of them decreases the system potential energy and surmounts a potential barrier that is part of the fixed section of the contact line, only. Such an assumption accounts for the fact that the effect of static friction does not hold during motion of the contact line.

In the next section, the model system and equations are described. Further, the numerical technique is briefly described. The result of the simulated stick-slip behaviour is next presented.

2. Model formulation

We consider the liquid/fluid/solid (L/F/S) three-phase system, consisting of a simply connected incompressible liquid drop, which occupies the domain Ω_l with volume V_0 in the fluid medium Ω_f. The drop is located on a sloping rigid body Ω_s (see Fig. 1), α is the surface angle of inclination. In the present work, we consider immiscible material and motionless domain Ω_s. The plane, however, is designed in such a way that the drop volume can be changed quasi-stationary using a thin tube (see Fig. 1).

In accordance with the classic capillary theory (see [5, 14]) the potential energy U of the system can be expressed by the following equation

$$(1)\quad U = \int\limits_{\Sigma_{lf}} \sigma_{lf} d\,\Sigma_{lf} + \int\limits_{\Sigma_{ls}} \sigma_{ls} d\,\Sigma_{ls} + \int\limits_{\Sigma_{fs}} \sigma_{fs} d\,\Sigma_{fs} + \int\limits_{\Omega_l} \rho_l\, U_{gr} d\,\Omega_l + \int\limits_{\Omega_f} \rho_f\, U_{gr} d\,\Omega_f,$$

where l refers to the liquid; f to the fluid ambient; lf, ls and fs to the surfaces liquid/fluid, liquid/solid and fluid/solid, respectively. The volume and density of the droplet and the ambient fluid are denoted by Ω and ρ, while U_{gr} is the

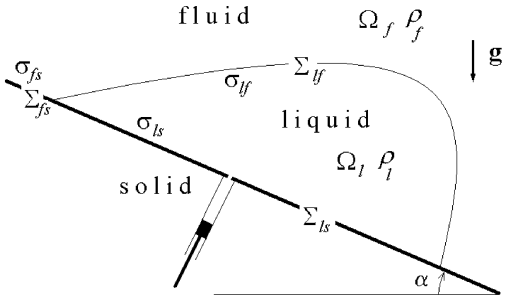

Fig. 1. Schematic drawing of the drop occupying domain Ω_l in the fluid medium Ω_f, on a plane, under the action of the gravity $\mathbf{g}$. The plane, however, is designed in such a way, that the drop volume can be changed by touching the drop contact line, using a thin tube

potential of the gravitation field $\mathbf{g}$ ($\mathbf{g} = -grad\ U_{gr}$). Following the variation approach, a state of equilibrium exists when the virtual work

$$\delta A = -\delta\, U = 0, \tag{2}$$

for all virtual displacements $\Psi = \{\mathbf{R} \mid \mathbf{R} \in \Omega_l \cup \Omega_f\}$ that do not violate the physical constraints: $\Re 1$, the droplet volume is constant; $\Re 2$, the points of the common line remain on it. But fluid motions satisfying condition $\Re 2$ cannot be realised physically. When the common line moves, as it is shown experimentally in [15], the liquid performs a rolling motion. The discrepancy between the motion observed in experiment and the motion under condition $\Re 2$ suggests a change in the class virtual displacements, which would make it possible to describe the possible motions of the liquid more exactly.

We write virtual displacements $\delta\,\mathbf{R}$, $\mathbf{R} = \Omega_l \cup \Omega_f$ as a sum of two terms $\delta\,\mathbf{R} = \delta_1\,\mathbf{R} + \delta_2\,\mathbf{R}$ satisfying the following conditions:

1) The displacements $\delta_1\,\mathbf{R}$ correspond to the change in the configuration. It is this class of displacements that is used in the classical model. The virtual work, which is denoted by $\delta_1 A$, is equal to

$$\delta_1 A = -\delta U;$$

2) The displacements $\delta_2\,\mathbf{R}$ are not connected with the change in the configuration. When the liquid moves away from the surface of the solid, a portion of the liquid leaves the surface of the solid. This type of motion is not described by $\delta_1\,\mathbf{R}$. If $\delta_1\,\mathbf{R} = \Re 1 \cup \Re 2$ is given, then this motion has no effect

on the configuration of the system. Let us describe this motion in terms of $\delta_2 \mathbf{R}$. Let $\delta^-|\Sigma_{ls}|$ and $\delta^-|\Sigma_{fs}|$ be the areas of Ω_l and Ω_f receding from the surface of the solid under the change in the configuration of the system caused by the virtual displacements $\delta_1 \mathbf{R}$. The virtual displacements of points along the surface of the solid satisfy the following relations:

$\delta_1 \mathbf{R} \cdot \mathbf{m}(\mathbf{R}) = 0$, for all points on the L/S surface,
$\delta_2 \mathbf{R} \cdot \mathbf{m}(\mathbf{R}) > 0$, for points on the $\delta^- |\Sigma_{ls}| + \delta^- |\Sigma_{fs}|$ area,
$\delta_2 \mathbf{R} \cdot \mathbf{m}(\mathbf{R}) = 0$, for the other points on the L/S surface,

where $\mathbf{m}(\mathbf{R})$ denotes the unit vector of the Σ_{ls} surface pointing inward into the liquid in $\mathbf{R} \in \Sigma_{ls}$ or the unit vector of the Σ_{fs} surface pointing inward into the fluid in $\mathbf{R} \in \Sigma_{fs}$.

Recently [6, 9] we have modelled the effect of drop hold-up on the sloping surface supposing that the potential energy barrier is connected with the resistance to motion. This energy is related to the fluid particles leaving the solid surface and is proportional to the area of the surfaces receded $\delta^-|\Sigma_{ls}|$ and $\delta^-|\Sigma_{fs}|$ with proportionality coefficients χ_{ls} and χ_{fs}, respectively. Taking into account this hypothesis, virtual work $\delta_2 A$ related to these displacements is

$$\delta_2 A = -\chi_{ls}\delta^-|\Sigma_{ls}| - \chi_{fs}\delta^-|\Sigma_{fs}|. \tag{3}$$

Taking into account this hypothesis, the virtual work δA of the system is

$$\delta A = \delta_1 A + \delta_2 A = -\delta U - \chi_{ls}\delta^-|\Sigma_{ls}| - \chi_{fs}\delta^-|\Sigma_{fs}|,$$

and can be described by energy U^*

$$\delta U^* = \delta U + \chi_{ls}\delta^-|\Sigma_{ls}| + \chi_{fs}\delta^-|\Sigma_{fs}| = -\delta A.$$

The system is in equilibrium when the energy U^* has a local minimum with respect to the class $\bar{\Psi} = \{\delta_1 \mathbf{R} + \delta_2 \mathbf{R} \mid \mathbf{R} \in \Omega_l \cup \Omega_f, \delta_1 \in \Re 1 \cup \Re 2\}$ virtual displacements.

A state of equilibrium exists when

$$\delta U^* = \delta U + \chi_{ls}\delta^-|\Sigma_{ls}| + \chi_{fs}\delta^-|\Sigma_{fs}| \geq 0. \tag{4}$$

for all class $\bar{\Psi}$ of virtual displacements. The latter condition shows that the state of the system can be changed if δU overcomes a potential barrier

$$\delta U < 0; \tag{5}$$

$$\delta U \geq \chi_{ls}\delta^{-}|\Sigma_{ls}| + \chi_{fs}\delta^{-}|\Sigma_{fs}|. \tag{6}$$

Let the system be in a vicinity of an equilibrium state and virtual displacement $\delta\,\mathbf{R}$ satisfies conditions (5), (6). We shall assume that here the real displacement $d\,\mathbf{R}$ corresponds to the virtual displacement in result of which the system passes into a state with the potential energy $U - dU$, kinetic energy $dT = -dU$ is transformed into the friction heat. Let this displacement change the part of contact line $l_\Delta \in l$. For this new state, we search again the variation, which decreases the potential energy and satisfies condition (6). Now for the displaced part of the contact line $l_\Delta \in l$ the coefficient of static friction is zero. If in a process of changes of a configuration there will be not any variation in which the potential energy overcomes potential barrier, this part of contact line $l_\Delta \in l$ becomes motionless again and the coefficient of static friction becomes χ_{ls} or χ_{fs}, respectively.

The number of independent variables in (6) can be reduced, considering that

$$\delta \int\limits_{\Omega_l} d\Omega_l = -\delta \int\limits_{\Omega_f} d\Omega_f, \qquad \delta \int\limits_{\Sigma_{ls}} d\Sigma_{ls} = -\delta \int\limits_{\Sigma_{fs}} d\Sigma_{fs}, \tag{7}$$

and that both parts of (6) hold true, if divided by the positive member σ_{ls}. Putting

$$b = (\rho_l - \rho_f)g/\sigma_{lf},\ \cos\theta_Y = (\sigma_{ls} - \sigma_{fs})/\sigma_{lf},\ \chi_l = \chi_{ls}/\sigma_{ls},\ \chi_f = \chi_{fs}/\sigma_{ls}, \tag{8}$$

we designate the angle θ_Y (Young), in a Cartesian coordinate system (x, y, z), where $\mathbf{z} = -\,\mathbf{g}\,/\|\,\mathbf{g}\,\|$, (6) is reduced to

$$\chi_l\delta^{-}|\Sigma_{ls}| + \chi_f\delta^{-}|\Sigma_{fs}| \geq -\delta\left[\cos\theta_Y \int\limits_{\Sigma_{ls}} d\Sigma_{ls} + \int\limits_{\Sigma_{lf}} d\Sigma_{lf} + b\int\limits_{\Omega_l} z d\Omega_l\right], \tag{9}$$

while, instead of the potential U, the potential $\bar{U}$ can be used

$$\bar{U} = -\int\limits_{\Sigma_{ls}} \cos\theta_Y d\Sigma_{ls} + \int\limits_{\Sigma_{lf}} \Sigma_{lf} + b\int\limits_{\Omega_l} z d\Omega_l. \tag{10}$$

3. Solution technique

The base of the numerical method is the finite dimensional approximation of the set of three-phase system virtual displacements and the calculation

of the drop volume changes, the potential energy changes, the area of the contact movement as the result of these displacements. It allows to realise a sequence of its changes that decreases the system potential energy taking into account the conditions (6). So, we obtain series of surfaces. The series converges to a surface that satisfies (4) for all small disturbances of a chosen class of displacements. This method uses the fact that the virtual displacements of the drop free surface determine the change of the system configuration, the variation of the potential energy, the areas through which the drop flows. Hence, the system potential energy is the function of the drop free surface, the class of surface drop small displacements approximates the set of virtual displacement of the system. Numerical approach was developed by Iliev [16].

1. The liquid drop free surface Γ 12 in the 3-D space is approximated by a surface Γ being a mesh of M triangles. Part of the triangle nodes $\mathbf{p}^1, \mathbf{p}^2, \ldots, \mathbf{p}^N$ are internal for the L/F surface, while nodes $\mathbf{p}^{N1+1}, \mathbf{p}^{N1+2}, \ldots, \mathbf{p}^N$ lie on the three-phase contact line l

$$\bar{\Gamma} = \bigcup_{j=1}^{M} e^j = \\ = e^1(\mathbf{p}^{1_1}, \mathbf{p}^{1_2}, \mathbf{p}^{1_3}) \bigcup e^2(\mathbf{p}^{2_1}, \mathbf{p}^{2_2}, \mathbf{p}^{2_3}) \bigcup \cdots \bigcup e^M(\mathbf{p}^{M_1}, \mathbf{p}^{M_2}, \mathbf{p}^{M_3}), \tag{11}$$

where e^j denotes a triangle with nodes $\mathbf{p}^{j_1}, \mathbf{p}^{j_2}, \mathbf{p}^{j_3}$. We have that

$$\bar{\Gamma} = \bar{\Gamma}(e^1, \ldots, e^M) = \bar{\Gamma}(\mathbf{p}^1, \ldots, \mathbf{p}^N); \tag{12}$$

2. $\bar{\Gamma}$ and the solid surface $\partial\Omega_s$ determines the drop domain Ω_l;
3. Nodes $\mathbf{p}^1, \ldots, \mathbf{p}^i_\Delta, \ldots, \mathbf{p}^N$

$$\mathbf{p}^i_\Delta = \mathbf{p}^i + \varepsilon_i \mathbf{N}_i, \quad \| \mathbf{N}_i \| = 1, \tag{13}$$

where $\mathbf{N}_i$ is outnormal to the surface $\bar{\Gamma}$ in $\mathbf{p}^i$ and determines the surface $\bar{\Gamma}^i_\Delta$, which is the small deformation of the surface $\bar{\Gamma}$ with centre in $\mathbf{p}^i$. The formulas for calculating the drop volume variation $\Delta V = V(\bar{\Gamma}^i_\Delta) - V(\bar{\Gamma})$, energy variation $\Delta\bar{U} = \bar{U}(\bar{\Gamma}^i_\Delta - \bar{U}(\bar{\Gamma})$, the variation of the solid-liquid surface $\Delta P = P(\bar{\Gamma}^i_\Delta) - P(\bar{\Gamma})$ for displacement (13) are given in [16].

We may present the deformation $\bar{\Gamma}_\Delta$ of the surface $\bar{\Gamma}$ as sequence of unit deformations:

$$\bar{\Gamma}_\Delta = \bar{\Gamma}^{i_1}_\Delta(\bar{\Gamma}^{i_2}_\Delta(\ldots \bar{\Gamma}^{i_N}_\Delta(\bar{\Gamma}))).$$

So, the changes of volume, energy and the other components of the system are reduced to the formulas for unit deformation.

Iterative algorithm

1. Let Γ^0 be the initial drop surface. Fix $N = N_0, \varepsilon = \varepsilon_0$. Obtain $\mathbf{p}_0^1, \mathbf{p}_0^2, \ldots, \mathbf{p}_0^N$ such that $\bar{\Gamma}^0\left(\mathbf{p}_0^1, \mathbf{p}_0^2, \ldots, \mathbf{p}_0^N\right)$ is a triangulation of the initial surface. To each change of the contact line determined by the deformation (13) of the points $\mathbf{p}^{N1+1}, \mathbf{p}^{N1+2}, \ldots, \mathbf{p}^N$ we connect friction factor $\chi^{N1+1}, \chi^{N1+2}, \ldots, \chi^N = 1$.

2. Step k, $k > 0$. Let $\bar{\Gamma}^{k-1}$ be obtained in the current $k-1$-iteration.

2.1. Choose i; $1 \le i \le N$, obtain unit deformation $\bar{\Gamma}_\Delta^{k-1^i}$.

2.2. Choose $j \ne i$, $1 \le j \le N$, obtain unit deformation $\bar{\Gamma}_\Delta^{k-1^j}(\bar{\Gamma}_\Delta^{k-1^i})$; $\mathbf{p}_\Delta^j = \mathbf{p}^j - \varepsilon_j \mathbf{N}_j$ such that the summary change of drop volume is zero.

Calculate $\Delta\bar{U}(\bar{\Gamma}_\Delta^{k-1^j}(\bar{\Gamma}_\Delta^{k-1^i}))$, $\Delta PP(\bar{\Gamma}_\Delta^{k-1^j}, \Delta P(\bar{\Gamma}_\Delta^{k-1^j}(\bar{\Gamma}_\Delta^{k-1^i}))$.

If $\Delta\bar{U}(\bar{\Gamma}_\Delta^{k-1^j}(\bar{\Gamma}_\Delta^{k-1^i})) < 0$, and

$$|\Delta\bar{U}(\bar{\Gamma}_\Delta^{k-1^j}(\bar{\Gamma}_\Delta^{k-1^i}))| \ge \chi^i\chi_f|\Delta P(\bar{\Gamma}_\Delta^{k-1^i})| + \chi^j\chi_l|\Delta P(\bar{\Gamma}_\Delta^{k-1^j}(\bar{\Gamma}_\Delta^{k-1^i}))|,$$

then $\mathbf{p}_{k-1,\Delta}^1, \mathbf{p}_{k-1,\Delta}^2, \ldots, \mathbf{p}_{k-1,\Delta}^N$ are obtained in the current k-iteration and the

$\chi^i = \chi^j = 0$.

Else

if we have compared $\bar{\Gamma}_\Delta^{k-1^j}(\bar{\Gamma}_\Delta^{k-1^i})$ to all $j \ne i$, $1 \le j \le N$ then $\chi^i = 1$.

If we have compared $\bar{\Gamma}_\Delta^{k-1^i}$ to all i; $1 \le i \le N$,

then $\bar{\Gamma}^{k-1} = \bar{\Gamma}^{k-1}(\mathbf{p}_{k-1}^1, \mathbf{p}_{k-1}^2, \ldots, \mathbf{p}_{k-1}^N) = \bar{\Gamma}^*(N, \varepsilon)$ is the (N, ε) solution of the equilibrium state. Go to 3.

Else choose other i; $1 \le i \le N$, and go to 2.2.

3. If $N = N_0$ and $\varepsilon = \varepsilon_0$,

then change parameter $\varepsilon = \varepsilon/2$ and go to 2.1 using a new value of ε.

Else compare this solution to the recently obtained solution with different N and (or) ε. Change ε and go to 2 or close the process.

We begin the iterative process for $\varepsilon = 0.02$ and stop it for $\varepsilon = 0.00001$, keeping N and employing a remeshing procedure.

4. Numerical results

First, consider the contact line stick-slip behaviour when the drop volume is increased. The similar example for the axisymmetric drops on a horizontal plane is considered in [9]. Therefore, here we choose the same system parameters

$$\theta = 60^\circ,\ b = 1,\ \chi_l = 0.2,\ \chi_f = 0.2. \tag{14}$$

Let the unit contact line be as in [9] a circle with radius

$$R = 0.72. \tag{15}$$

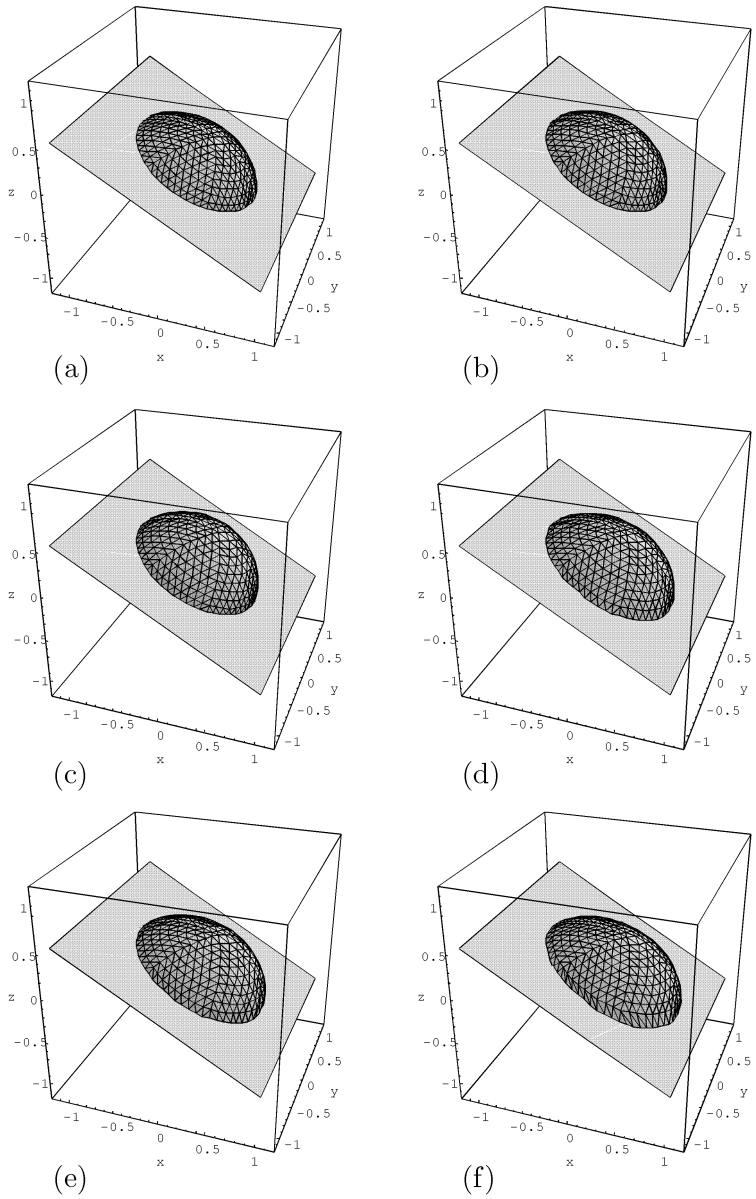

Fig. 2. Shape of a equilibrium drop ($\theta_Y = 60°$, $b = 1$, $\chi_l = 0.2$, $\chi_f = 0.2$) on a plate inclined at 30° for drop volume (a), 0.35 (b), 0.41 (c), 0.42 (d), 0.45 (e), 0.46 (f)

Let the drop be located on a surface with slop angle $\alpha = 30^\circ$. Start the iterative method with surface Γ^0, which is axisymmetric equilibrium state with the drop located on a horizontal surface:

(16) $$\theta_Y = 60^\circ,\ b = 1,\ \chi_l = 0.2,\ \chi_f = 0.2,\ R = 0.72,\ V = 0.3.$$

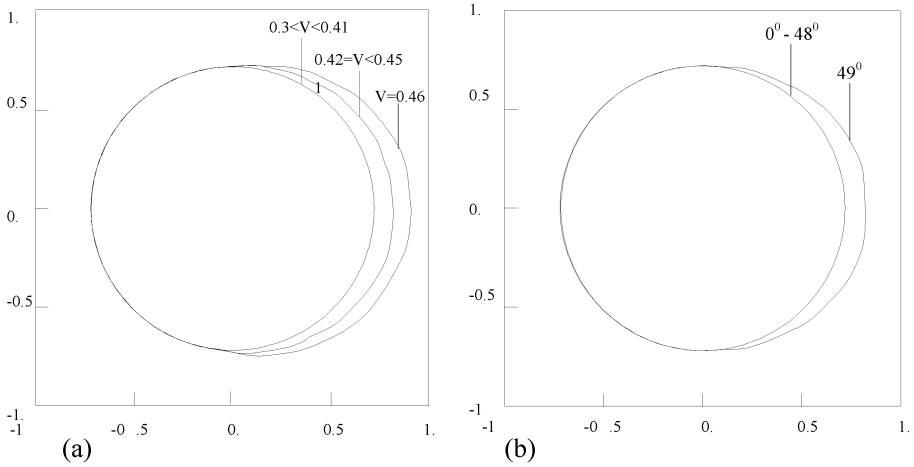

Fig. 3. Contact lines of drops shown in figure 2 (a) and figure 4 (b)

This shape is numerically obtained as it is described in [16]. The equilibrium surface obtained by step-by-step numerical method is shown in Fig. 2a. The contact line corresponding to the solution is shown in Fig. 3a. The contact line is not changed and remains the same as the drop axisymmetric equilibrium shape on a horizontal plane. We gradually increase the drop volume and follow whether the obtained equilibrium states, for a drop contact line radius $R = 0.72$, are stable. We increase the volume by $\Delta V = 0.01$ by set of displacements (13):

$$\mathbf{p}^i_\Delta = \mathbf{p}^i + \varepsilon_i \mathbf{N}_i, \quad \| \mathbf{N}_i \| = 1, \quad i = 1, \ldots, N1.$$

And then this obtained form we take as initial one for iterative algorithm and we obtain new equilibrium form.

Numerical results show that for a wide range of the drop volume from $V = 0.3$ to $V = 0.41$ the liquid drop, with a contact line radius $R = 0.72$, is in an equilibrium state. Solutions for $V = 0.35$ and $V = 0.41$ are shown in Figs

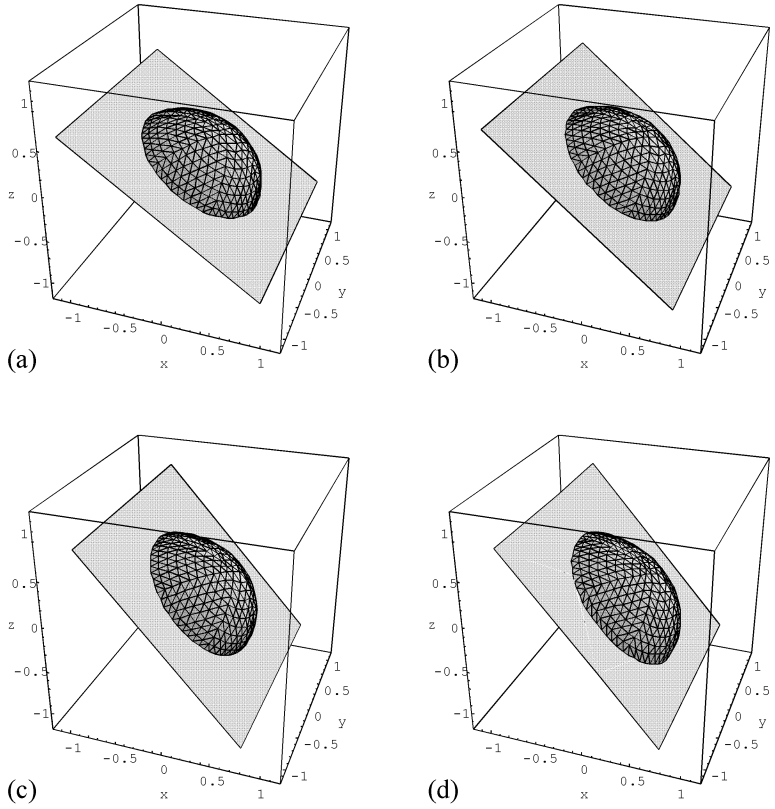

Fig. 4. Shape of an equilibrium drop ($\theta_Y = 60°$, $b = 1$, $\chi_l = 0.2$, $\chi_f = 0.2$) on a plate inclined at (a) 35°, (b) 40°, (c) 48° and (d) 49°

2b and 2c. For $V = 0.42$ the drop contact line starts to move and drop comes over in equilibrium state with different contact line. Obtained drop shape for $V = 0.42$ is shown in Fig. 2d. At further increase of the volume up to $V = 0.45$ the line remains without change. Drop shape for $= 0.45$ is shown in Fig. 2e. For $V = 0.46$ there is the contact line repeated change. Obtained drop shape for $V = 0.46$ is shown in Fig. 2f. In Fig. 3a are shown the contact lines from $V = 0.3$ to $V = 0.46$. The jerky change of the contact line is seen. The obtained result shows that under resistance to shift and for a gradual volume increase the drop cannot change its contact line and then can sharply pass into a new state with significantly increased contact line.

Consider now the stick-slip behaviour of contact line realised for drop with fixed volume when the inclination of a sloping plane is changed. We investigate this effect for obtained above equilibrium drop shape with volume

$V = 0.35$ located on a surface with slop angle $\alpha = 30°$. Increasing an inclination on the solid surface with on one degree by using the step-by-step algorithm, the sequence of equilibrium forms is obtained. The obtained equilibrium surface of the drop for a preceding smaller slope angle is taken as an initial surface for each successive angle. Numerical analysis proves that the angle 48° is critical one for the circle contact line with radius $R = 0.72$. The contact line remains the same till this slope angle as the initial equilibrium shape. The drop equilibrium states are shown in Fig. 2b, Figs 4a – 4c, for slope angles of 30°, 35°, 40° and 48°, respectively. For slope angle of 49° the drop contact line starts moving and drop passes into an equilibrium state with another contact line. This equilibrium drop shape is shown in Fig. 4d. Numerical results show that for the further increase of a slope angle the contact line remains without changes. The contact lines, corresponding to the equilibrium shapes for angles of inclination between 0° and 49°, are given in Fig. 3b. It is well seen as in the previous case that the change of a contact line is jerky.

5. Conclusions

The present study proceeds with the test of the equilibrium model given in [6, 9]. Numerical examples show that the resistance-to-shift component, well-known from the classical theory of capillary, gives contact line stick-slip behaviour of the liquid droplet located on a sloping plane. Numerical analysis shows that the stick-slip behaviour of the contact line depends on shape and volume of initial drop, gravitation and static friction coefficients.

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