

**2-бөлім****Раздел 2****Section 2****Механика****Механика****Mechanics**

UDC 517.958:532.546

Kudaikulov A.A.<sup>1\*</sup>, Josserand C.<sup>2</sup>, Kaltayev A.<sup>1</sup><sup>1</sup>Al-Farabi Kazakh National University, Republic of Kazakhstan, Almaty<sup>2</sup>Sorbonne Universit'es, Institut D'Alembert, CNRS and UPMC UMR 7190, 4 place Jussieu, 75005

France, Paris

\*E-mail: aziz.kudaikulov@gmail.com

**Numerical investigation of interface motion between two immiscible fluids in a channel**

The main difficulty of the modeling of two immiscible viscous fluids flow in the channel (pipe, etc.), is the choice of the boundary condition on the line (contact line) formed by intersection of the interface between fluids with the solid surface. If the no-slip condition is used on the solid boundary to determine the flow produced when a fluid interface moves along a solid boundary, the viscous stress is approached to infinity at the vicinity of the contact line. It seems, unreasonable to continue to apply a continuum model at the vicinity of the contact line. Thus an inner region, close to the contact line, could be examined, where the molecular interactions between the two fluids and the solid must be studied, and this region matched to an outer region, where the Navier-Stokes equations would apply. Such an analysis would be very difficult, but it has been suggested that the likely outcome would be equivalent to replacing the no-slip boundary condition by a slip condition, and continuing to employ the Navier-Stokes equations. The effect of the slip on the interface motion is numerically investigated in this work. Also relation between steady-state contact angle and capillary number is investigated in this paper and compared with work [8].

**Key words:** Navier-Stokes equations; Flow of two immiscible fluids; Gerris program; Slip boundary condition; Volume-of-fluid (VOF) method; Contact line; Contact angle; Capillary number.

Кудайкулов А.А., Жозеранд К., Калтаев А.

**Численное моделирование движения границы раздела двух несмешивающихся жидкостей в канале**

Основной проблемой моделирования течения двух несмешивающихся вязких жидкостей в канале (трубе и т.д.) является постановка граничного условия на линии (контактной линии), образованной пересечением поверхности раздела жидкостей с твердой поверхностью. Если выбрать граничное условие прилипания на твердой границе, тогда при движении поверхности раздела жидкостей по твердой поверхности, в окрестности контактной линии, вязкие напряжения стремятся к бесконечности. Видимо, применение модели сплошной среды в области, близкой к контактной линии, является необоснованным. Таким образом, в области, близкой к контактной линии, необходимо исследовать молекулярное взаимодействие между двумя жидкостями и твердой поверхностью, и эту область связать с областью вдали от контактной линии, где можно применить уравнения Навье-Стокса. Такой анализ будет очень сложным, но он позволяет подтвердить предположение, что вместо граничного условия прилипания можно использовать граничное условие проскальзывания.

В данной работе численно исследовано влияние проскальзывания жидкости по твердой поверхности на движение поверхности раздела жидкостей. Также исследована связь между контактным углом и капиллярным числом, при установившемся течении жидкости, и полученные результаты сравнены с результатами работы [8].

**Ключевые слова:** Уравнения Навье-Стокса; Течение двух несмешивающихся жидкостей; программа Gerris; Граничное условие проскальзывания; Метод объема жидкости; Контактная линия; Контактный угол; Капиллярное число.

Кудайкулов А.А., Жозеранд К., Калтаев А.

### Каналдағы екі араласпайтын сұйықтардың бөліну шекарасының қозғалысын сандық арқылы модельдеу

Каналдағы екі араласпайтын сұйықтардың бөліну шекарасының қозғалысын сандық арқылы модельдеудің негізгі қиындығы - қатты беттегі шекаралық шарттарды таңдау болып табылады. Егер қатты шекарада жабысқақ шекаралық шартты таңдасақ, онда бөліну шекарасы қатты бет бойынша қозғалғанда, тұтқырлық кернеуі шексіздікке ұмтылады. Түйіскен сызықпен қатты бет арасындағы аймақта ағындар молекулярлық масштабта өтсе, тұтас орта моделін қолдану әлбетте дұрыс емес. Сонымен, түйіскен сызықпен қатты бет арасындағы аймақта екі сұйықпен қатты беттің молекулярлық өзара әрекетесуін зерттеу қажет және осы аймақты Навье-Стокс теңдеуін қолдануға болатын түйіскен сызықтан шет аймақпен байланыстыру керек. Осындай талдау өте күрделі болады, бірақ Навье-Стокс теңдеуін шешу үшін жабысқақ шекаралық шарттың орнына сырғанақ шекаралық шартты қолдануға болады деген жорамалымызды растауға мүмкіндік береді. Осы жұмыста каналдағы екі араласпайтын сұйықтардың ағыны үшін Навье-Стокс теңдеуін шешуге сұйық көлем әдісін қолданған. Сонымен қатар осы мақалада түйіскен бұрышпен капиллярлық сан арасындағы байланыс зерттеледі.

**Түйін сөздер:** Навье-Стокс теңдеулер; Екі араласпайтын сұйықтардың ағыны; Gerris бағдарлама; Сырғанақ шекаралық шарт; Сұйық көлем әдісі; Түйіскен сызық; Түйіскен бұрыш; Капиллярлық сан.

## Introduction

When an interface between two immiscible fluids joins a solid boundary, a line is formed. This line is sometimes known as the three-phase line or the contact line. A moving contact line can be found in many different situations; some cases in which it plays a central role are the spreading of adhesives, the flowing of lubricants into inaccessible locations, the coating of solid surfaces with a thin uniform layer of liquid, the displacement of oil by water through a porous medium, etc. However, the dynamics of the fluid surrounding the contact line, and hence the contact line itself, are poorly understood. The main difficulty of the modeling of the contact line motion is the choice of the boundary condition on the solid surface. If the no-slip condition is used on the solid boundary to determine the flow produced when a fluid interface moves along a solid boundary, a viscous stress is approached to infinity [1-3], nevertheless the no-slip boundary condition has been verified for a number of liquid-solid combinations by careful experimental studies [4]. It seems, unreasonable to continue to apply a continuum model at the vicinity of the contact line. Thus an inner region, close to the contact line, could be examined, where the molecular interactions between the two fluids and the solid must be studied, and this region matched to an outer region, where the Navier-Stokes equations would apply. Such an analysis would be very difficult, but it has been suggested that the likely outcome would be equivalent to replacing the no-slip boundary condition by a slip condition, and continuing to employ the Navier-Stokes equations. Introduction of the precursor film into the model clearly allows one to remove the viscous stress singularity [2]. Experiments

indicate that this is not always the case and is in fact unlikely when the observed value of the contact angle is not small. The physical mechanisms of slip for smooth solid surfaces are still not completely understood, with possible explanations including formation of a layer of gas or small-scale bubbles between the liquid and the solid [4,5]. Significant slip can be achieved for flows near structured surfaces [6]. There are exist many models to simulate slip flow along the solid surface but one of the most popular is the Navier slip boundary condition, which in our 2D Cartesian coordinates is written as:

$$u = \lambda \frac{\partial u}{\partial y}, \text{ at } y = 0, \quad (1)$$

where  $u$  is the horizontal velocity component in the x-direction, and  $\lambda$  is a constant called the slip length. The latter can be interpreted as the distance below the solid-liquid interface at which the velocity  $u(y)$  extrapolates to zero, as sketched in fig. 1. The viscous stress singularity is avoided when this condition is used instead of the classical no-slip condition [7]. The effect of the slip on the interface motion is numerically investigated in this work. The incompressible, two immiscible, viscous fluids flow in 2D channel is considered in this article. In order to find the shape and location of the interface between two fluids, the volume-of-fluid method is used in this work [9,10,13]. The Navier-Stokes equations are numerically solved using projection method on non-staggered grid to find the velocities and pressure of the two fluids flow in the channel [11]. The relation between steady-state contact angle and capillary number is investigated in this paper and compared with work [8]. All numerical calculations are performed using Gerris program [14].

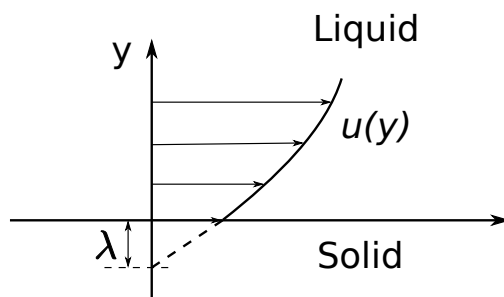


Figure 1 – Navier slip boundary condition

### Formulation of the problem

We numerically solve the Navier-Stokes equations for incompressible, two immiscible, viscous fluids flow in 2D channel:

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla p + \nabla \cdot (2\mu E), \quad (2)$$

$$E = \frac{1}{2}(\nabla \vec{u} + \nabla \vec{u}^T), \quad (3)$$

$$\nabla \cdot \vec{u} = 0, \quad (4)$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0, \quad (5)$$

$$\rho = F\rho_1 + (1 - F)\rho_2, \quad (6)$$

$$\mu = F\mu_1 + (1 - F)\mu_2, \quad (7)$$

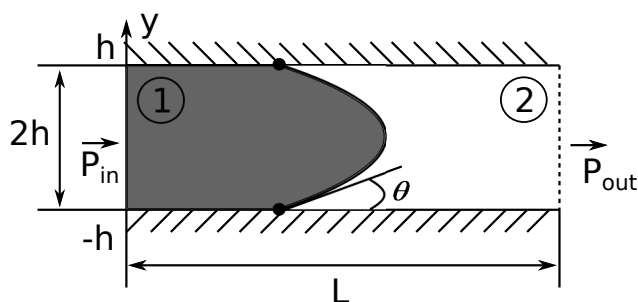
where  $F$  is the parameter that identify a given fluid  $i$  ( $i=1$  or  $2$ ) is present at a particular location  $\mathbf{x}$ :

$$F(x) = \begin{cases} 1, & \text{if } x \text{ is in fluid } i \\ 0, & \text{if } x \text{ is not in fluid } i \end{cases} \quad (8)$$

If we substitute the equation (6) into the equation (5), we have that:

$$\frac{\partial F}{\partial t} + \vec{u} \cdot \nabla F = 0. \quad (9)$$

In order to find the shape and location of the interface between the two fluids, we use the volume-of-fluid method and advect this interface using equation (9). Equations (2, 4 and 9) numerically solved using the projection method on non-staggered grid [11] and the following boundary conditions were used (see fig. 2):



**Figure 2** – The steady movement of a interface between two fluids in a channel

1) Inlet boundary condition:

$$\frac{\partial u_{in}}{\partial x} = 0, \quad (10)$$

$$v_{in} = 0, \quad (11)$$

$$p_{in} = 1. \quad (12)$$

2) At the walls of the channel:

$$u_w = \lambda \frac{\partial u}{\partial \vec{n}}, \quad (13)$$

$$v_w = 0, \quad (14)$$

$$\frac{\partial p_w}{\partial y} = 0, \quad (15)$$

where  $\lambda$  is the slip length and  $\vec{n}$  is the normal vector to the wall.

3) At the interface between the two fluids -  $S$ :

$$[\vec{u}]_S = 0, \quad (16)$$

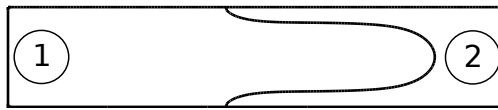
$$-[-p + 2\mu\vec{n} \cdot E \cdot \vec{n}]_S = \sigma k, \quad (17)$$

$$k = -\nabla \cdot \vec{n}, \quad (18)$$

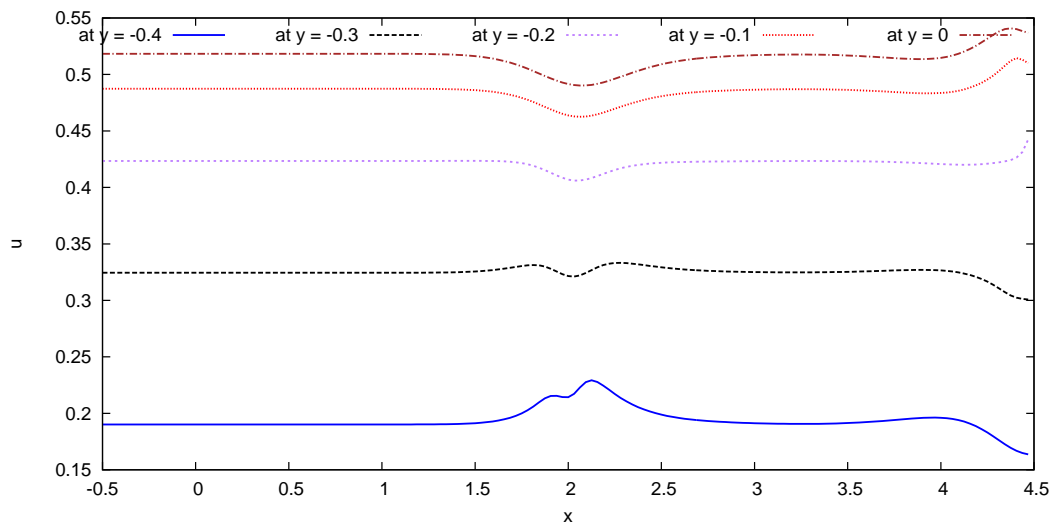
$$-[2\mu\vec{t} \cdot E \cdot \vec{n}]_S = \vec{t} \cdot \nabla_S \sigma, \quad (19)$$

where  $\sigma$  is the surface tension,  $k$  is the curvature,  $\vec{n}$  is the normal vector to the interface  $S$  and  $\vec{t}$  is the tangent vector to the interface  $S$ . In order to solve the equations (2, 4 and 9) we need set outlet boundary conditions too. The outflow conditions are not known a priori. But nevertheless, we need to prescribe suitable conditions to make the problem determinate. An analysis of outflow boundary conditions is given in the literature [12]. Here the following outlet boundary conditions were used:

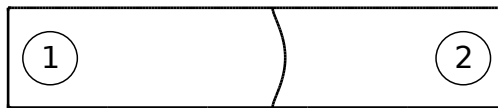
$$\frac{\partial u_{out}}{\partial x} = 0, \quad (20)$$



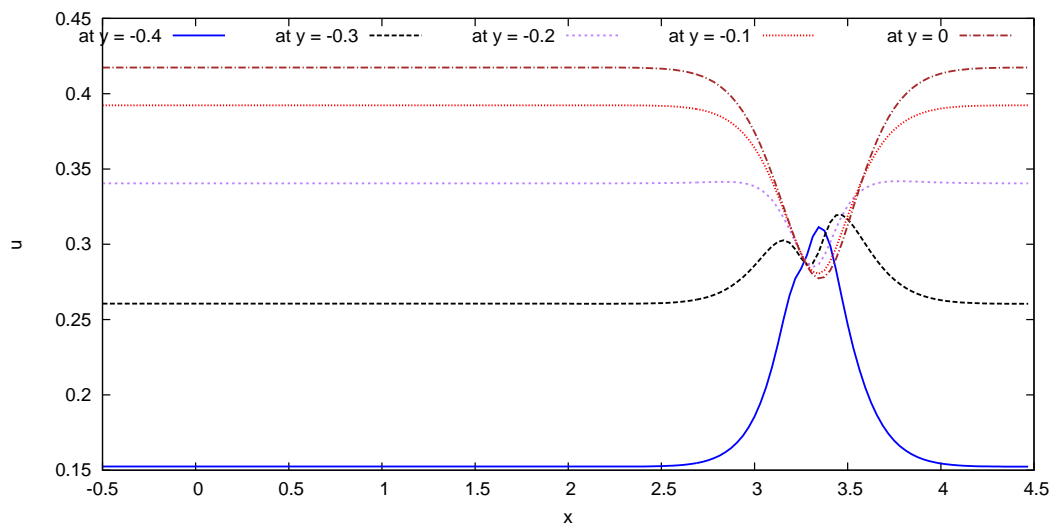
**Figure 3** – Formation of fingering pattern in unstable interface between two fluids, when  $\mu = 1$ ,  $\sigma = 1$  and  $\lambda = 0.01$



**Figure 4** – Profile of horizontal component velocity, when  $\mu = 1$ ,  $\sigma = 1$  and  $\lambda = 0.01$



**Figure 5** – Shape of the interface between two fluids, when  $\mu = 1$ ,  $\sigma = 5$  and  $\lambda = 0.01$



**Figure 6** – Profile of horizontal component velocity, when  $\mu = 1$ ,  $\sigma = 5$  and  $\lambda = 0.01$

$$v_{out} = 0, \quad (21)$$

$$p_{out} = 0. \quad (22)$$

## Results

The steady state solution of the equations (2, 4) with boundary conditions at the walls of the channel (13 - 15) and with boundary conditions at the interface between the two fluids (16 - 19) can be obtained by neglecting the viscous force on the interface between the two fluids (19):

$$u = \frac{p_{in} - p_{out} - p_c}{\mu L} \left( \frac{h^2 - y^2}{2} + \lambda h \right), \quad (23)$$

where  $p_c$  is the capillary pressure. The value of capillary pressure can be obtained from Young-Laplace equation and for 2D case (see fig. 2):

$$p_c = \frac{\sigma \cos \theta}{h}. \quad (24)$$

The average value of (23):

$$\bar{u} = \frac{p_{in} - p_{out} - p_c}{\mu L} \left( \frac{h^2}{3} + \lambda h \right). \quad (25)$$

The value of the steady state contact angle  $\theta$  is unknown in the equation (23) or (25). The numerical investigation of interface motion between two immiscible fluids in a channel is performed in this paper to find this contact angle. In this work the equations (2 - 9) are dimensionless. The width of the channel is  $2h = 1$  and length of the channel is  $L = 5$  (see fig. 2). The viscosities of the two fluids are the same:  $\mu = \mu_1 = \mu_2 = 1$ . Initially, the contact angle equals 90 degrees. The apparent contact angle is introduced in this article, and it is difference between initial contact angle and steady state contact angle:

$$\theta_{app} = 90^\circ - \theta. \quad (26)$$

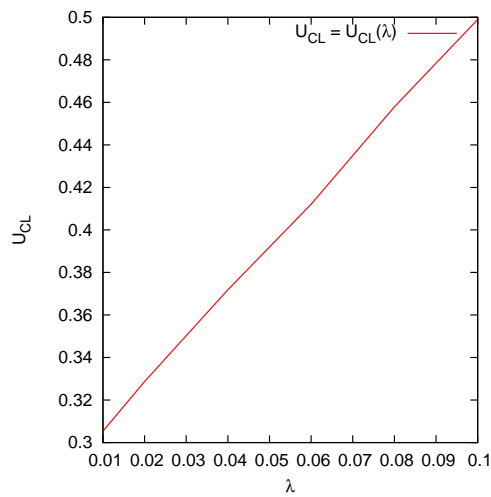
When the surface tension is sufficiently small the fingering pattern is formed in unstable interface between two fluids (see fig. 3), and as can be seen in fig. 4, the velocities are different along the transverse section of the channel at the interface between two fluids. However, if we increase the surface tension, the fingering pattern is no longer formed in the interface between two fluids (see fig. 5), and the velocities are same along the transverse section of the channel at the interface between two fluids (see fig. 6). In this paper we only considered the

case when the fingering pattern is not formed in the interface between two fluids. Three cases considered in this article to verify the relation between apparent contact angle and capillary number, which is investigated in [8]:

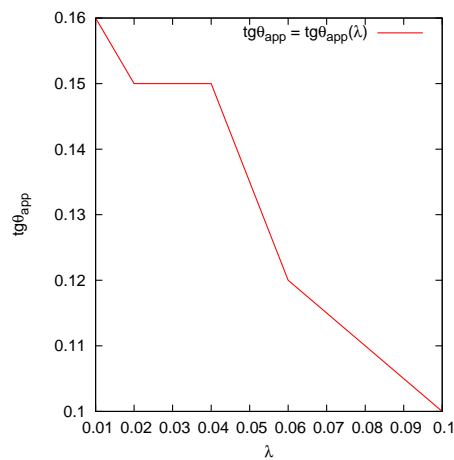
$$\theta_{app}^3 \sim Ca, \quad (27)$$

where  $Ca$  is the capillary number. Capillary number is the ratio between viscous force and surface tension force:

$$Ca = \frac{\mu U_{CL}}{\sigma}, \quad (28)$$

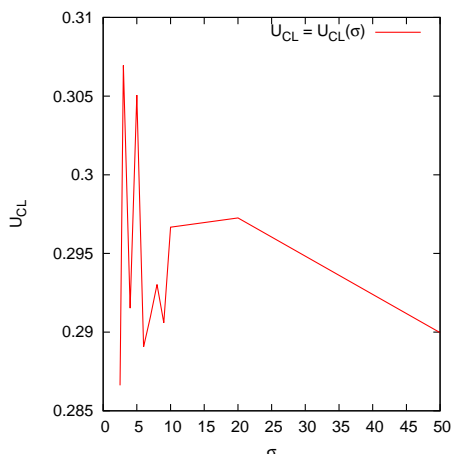


**Figure 7** – Relation between contact line velocity and slip length, when  $\mu = 1$ ,  $\sigma = 5$

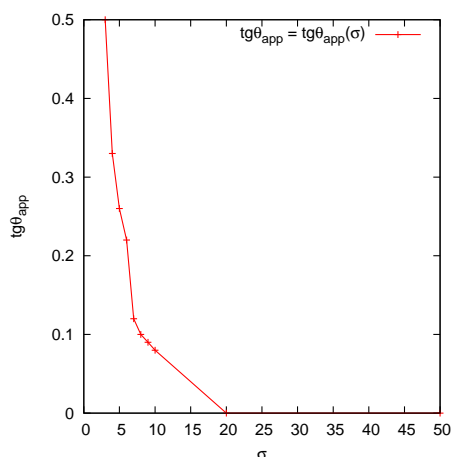


**Figure 8** – Relation between apparent contact angle and slip length, when  $\mu = 1$ ,  $\sigma = 5$



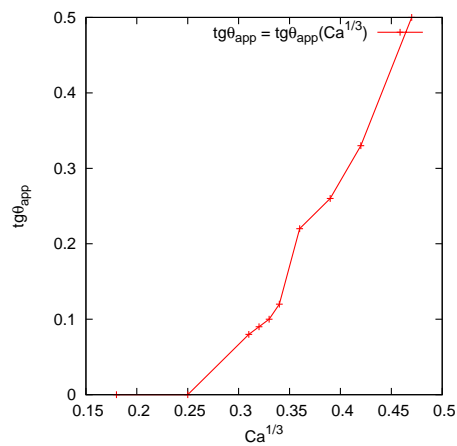


**Figure 9** – Relation between contact line velocity and surface tension, when  $\mu = 1$  and  $\lambda = 0.01$

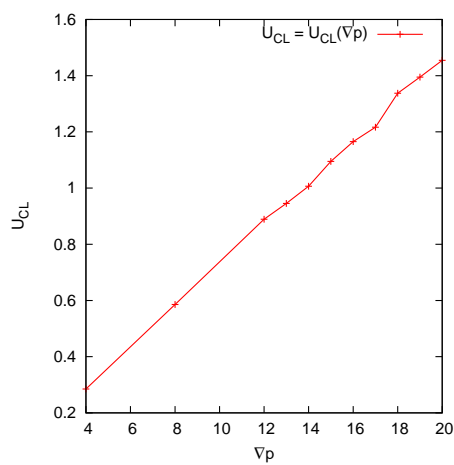


**Figure 10** – Relation between apparent contact angle and surface tension, when  $\mu = 1$ ,  $\lambda = 0.01$

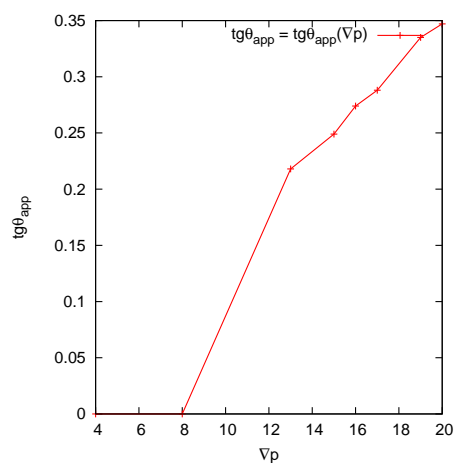
where  $U_{CL}$  is the contact line velocity. In the first case, the surface tension is constant, and relation between the apparent contact angle and slip length is investigated. As can be seen in fig. 7, the contact line velocity are linearly depends on the slip length, so it is mean that the viscous stress is constant at the walls of the channel. Since the viscous stress is constant at the walls of the channel (1) and surface tension is constant too, therefore as can be seen in fig. 8, the apparent contact angle almost doesn't depend on the slip length. In the second case, the slip length is constant, but the surface tension is changed, and relation between the apparent contact angle and surface tension is investigated (see fig. 10). As can be seen in fig. 9, the contact line velocity is slowly changed when surface tension is greater than 5, so in this region the viscous stress at the walls is almost constant. We can verify the relation between the apparent contact angle and capillary number for this case (see fig. 11). In the third case, the slip length and surface tension is constant, but the pressure drop is changed, and relation between the apparent contact angle and pressure drop is investigated (see fig. 13). The relation between the apparent contact angle and capillary number also verified for this case (see fig. 14).



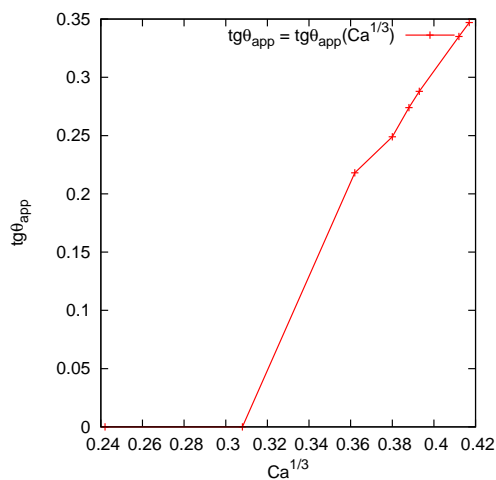
**Figure 11** – Relation between apparent contact angle and capillary number, when  $\mu = 1$ ,  $\lambda = 0.01$



**Figure 12** – Relation between contact line velocity and pressure drop, when  $\mu = 1$ ,  $\sigma = 20$ ,  $\lambda = 0.01$



**Figure 13** – Relation between apparent contact angle and pressure drop, when  $\mu = 1$ ,  $\sigma = 20$ ,  $\lambda = 0.01$



**Figure 14** – Relation between apparent contact angle and capillary number, when  $\mu = 1$ ,  $\sigma = 20$ ,  $\lambda = 0.01$

## Conclusion

A moving contact line can be found in many different situations; some cases in which it plays a central role are the spreading of adhesives, the flowing of lubricants into inaccessible locations, the coating of solid surfaces with a thin uniform layer of liquid, the displacement of oil by water through a porous medium, etc. In most cases it is necessary to calculate the steady state contact angle, to find the capillary pressure (24) or at least find the relation between steady state contact angle and other parameters (surface tension, viscosity etc.). In this article the relation between steady state contact angle and capillary number is numerically investigated, and this relation is reasonably good matched with [8].

## Acknowledgments

This work was supported by the Committee of Science of Ministry of Education and Science of the Republic of Kazakhstan, grant №1735/ГФ4 МОИ РК.

## References

- [1] *Dussan V.E.B.* On the spreading of liquid on solid surfaces: static and dynamic contact lines // *Annu. Rev. Fluid Mech.* - 1979. - Vol.11. - P. 371-400.
- [2] *de Gennes P.G.* Wetting: statics and dynamics // *Rev. Mod. Phys.* - 1985. - Vol. 57. - P. 827-863.
- [3] *Huh C. and Scriven L.* Hydrodynamic model of steady movement of a solid/liquid/fluid contact line // *J. Coll. Interf. Sci.* - 1971. - Vol. 35. - P. 85-101.
- [4] *Lauga E., Brenner M.P., Stone H.A.* Microfluidics: The no-slip boundary condition, in *Handbook of Experimental Fluid Dynamics* (Chapter 19) // Springer, 2007.
- [5] *Vinogradova O.I.* Slippage of water over hydrophobic surfaces // *Int. J. Mineral Processing.* - 1999. - Vol. 56. - P. 31-60.
- [6] *Teo C.J., Khoo B.C.* Analysis of Stokes flow in microchannels with superhydrophobic surfaces containing a periodic array of micro-grooves // *Microfluid Nanofluid.* - 2009. - Vol. 7. - P. 353-382.
- [7] *Greenspan H.P.* On the motion of a small viscous droplet that wets a surface // *J. Fluid Mech.* - 1978. - Vol. 84. - P. 125-143.

- [8] *Bonn D., Eggers J., Indekeu J., Meunier J. and Rolley E.* Wetting and spreading // *Rev. Mod. Phys.* - 2009. - Vol. 81. - P. 739-805.
- [9] *Pilliod J.E., Jr. and Puckett E.G.* Second-order accurate volume-of-fluid algorithms for tracking material interfaces // *J. Comput. Phys.* - 2004. - Vol. 199. - P. 465-502.
- [10] *Scardovelli R. and Zaleski S.* Analytical relations connection linear interfaces and volume fractions in rectangular grids // *J. Comput. Phys.* - 2000. - Vol. 164. - P. 228-237.
- [11] *Brown D.L., Cortez R. and Minion M.L.* Accurate projection methods for the incompressible Navier-Stokes equations // *J. Comput. Phys.* - 2001. - Vol. 168. - P. 464-499.
- [12] *Christer B. and Johansson V.* Boundary Conditions for Open Boundaries for the Incompressible Navier-Stokes Equation // *J. Comput. Phys.* - 1993. - Vol. 105. - P. 233-251.
- [13] *Tryggvason G., Scardovelli R. and Zaleski S.* *Direct Numerical Simulations Of Gas-Liquid Multiphase Flows* // Cambridge University Press, 2011.
- [14] *Popinet S.* The Gerris Flow Solver: <http://gfs.sourceforge.net>