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IDENTIFICATION OF THE PROPERTIES OF HYDROPHOBIC LAYERS AND ITS USAGE IN TECHNICAL PRACTICE

VYSOKÉ UČENÍ TECHNICKÉ V BRNĚ
Fakulta strojního inženýrství
Energetický ústav
Odbor fluidního inženýrství Victora Kaplana

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IDENTIFICATION OF THE PROPERTIES OF HYDROPHOBIC LAYERS AND ITS USAGE IN TECHNICAL PRACTICE

IDENTIFIKACE VLASTNOSTÍ HYDROFOBNÍCH VRSTEV A JEJICH VYUŽITÍ V TECHNICKÉ PRAXI

ZKRÁCENÁ VERZE HABILITAČNÍ PRÁCE
V OBORU KONSTRUKČNÍ A PROCESNÍ INŽENÝRSTVÍ

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Teaching experience:

- In the bachelor’s degree program giving lectures in Hydromechanics, Hydraulic processes and Hydraulic machines
- In the master’s degree program giving lectures in Fluids engineering, Fluid machines and for Erasmus students Hydraulic machines (in English)
- Supervisor of 5 diploma and 10 bachelor theses, all successfully defended
- Involved in further training of industrial researchers (courses of applied fluid mechanics for Honeywell GDC Brno)

Research activities:

- Co-author of **5** patents, **8** utility designs and **11** engineering products
- Successfully finished a post-doc grant project of the Czech Science Foundation **GP101/06/P044** (The extra corporal pump optimization)
- In 2015 finished a grant project of the Czech Science Foundation **GA13-20031S** (The properties of hydrophobic surfaces in interaction with the fluid) as a principal investigator
- Since 2015,co-investigator on a grant project of the Czech Science Foundation **GA15-06621S** (Modelling of smart damping elements of rotating systems utilizing the physical properties of magnetorheological fluids)
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NOMENCLATURE

$\boldsymbol{c}\ (c_i)$	velocity vector	$[m \cdot s^{-1}]$
c_φ	peripheral coordinate of the velocity vector	$[m \cdot s^{-1}]$
c_r	radial coordinate of the velocity vector	$[m \cdot s^{-1}]$
d	pipeline diameter	$[m]$
$f;\ F_S$	static force of separation	$[N]$
$\boldsymbol{F}\ (F_i)$	force vector	$[N]$
$\boldsymbol{g}\ (g_i)$	gravity acceleration vector	$[m \cdot s^{-2}]$
H	distance between the plates	$[m]$
k	adhesive coefficient	$[Pa \cdot s \cdot m^{-1}]$
$\boldsymbol{n}\ (n_i)$	nominal vector	$[-]$
p	pressure	$[Pa]$
Q	flow rate	$[m^3 \cdot s^{-1}]$
R_2	stator radius	$[m]$
S, Γ	surface	$[m^2]$
$\bar{S}$	droplet contact area	$[m^2]$
t	time	$[s]$
$\boldsymbol{u}\ (u_i)$	annular velocity vector	$[m \cdot s^{-1}]$
V	droplet volume	$[m^3]$
$\boldsymbol{x}\ (x_i)$	Cartesian coordinates, $i = 1,2,3$	$[m]$
α	angle of the plane inclination	[°]
δ_{ij}	Kronecker delta	$[-]$
η	dynamic viscosity	$[kg \cdot m^{-1} \cdot s^{-1}]$
ν	kinematic viscosity	$[m^2 \cdot s^{-1}]$
Π_{ij}	irreversible stress tensor	$[Pa]$
ρ	density	$[kg \cdot m^{-3}]$
σ	shear stress	$[Pa]$
σ_{ij}	shear stress coordinates	$[Pa]$
σ_S	static prestress	$[Pa]$
θ	contact angle	[°]

1 INTRODUCTION

Nowadays in the time of modern technologies, advances in nanotechnology and materials engineering, research fields dealing with the so-called wettability have been developing dynamically. It is not only the issue of surface finishing of the materials, their manufacture and use in technology, but also the mathematical description and subsequent simulation of fluid flow along these surfaces. The utilization of specific properties of these surfaces has an impact on the construction of modern hydraulic machines, fluids transport over long distances, the treatment of internal parts of water reservoirs and swimming pools, and more.

The scope of the work undertaken arose largely from the requirements of the Czech Science Foundation and Ministry of Trade and Industry research projects, where the author figured as a principal investigator, respectively a co-investigator.

The subject has to be seen and evaluated interdisciplinary. It is not only the interest of material or fluids engineering. First and foremost, it is necessary to understand the principle of hydrophobic materials, their effect on the fluid and the way this is defined. Subsequently, to find and establish a way how to describe and evaluate the interaction between the surface layer and the liquid. Finally, to implement this knowledge into commercial software, validate it experimentally and introduce into practical use.

The implications of using hydrophobic materials in technical practice greatly depend on the possibilities that are opened by computational modeling of the flow. Given that each hydraulic design nowadays starts with simulations, it is surprising that commercial software does not include hydrophobicity and the zero velocity on the wall is considered a standard boundary condition. This makes the path towards understanding the function and importance of hydrophobicity uneasy.

2 SUMMARY OF WORK

The thesis can be divided into several parts. The first introduces the phenomenon of hydrophobicity and rationalizes the choice of the methods of solution used. The second deals with the definition of boundary conditions on the hydrophobic surface. Selected examples show the effect of the new boundary conditions on the dissipation function and comparison of the hydrophobic with commonly used hydrophilic assumption. Planar examples of flow between two plates are followed by extension to a more complex system of long journal bearings, represented by a stationary and non-stationary flow in the annulus. Solution for the journal bearings model logically leads to the popular field of FSI (Fluid Structure Interaction), which characterizes the interaction of the body and fluid. In these systems, the fluid flow affects the motion of the body in it (in the given case it was a rotation with possible eccentricity). A kinematics solution of this problem leads on to the complex problem of mechanics, where the results are matrices of additional damping and stiffness. These vary according to the type of surface and thus the selected boundary conditions, thus showing a possibility of development in the design and construction of journal bearings. Using a hydrophobic coating on the static parts of the bearing can reduce the stiffness of the liquid layer in half and damping in quarter, which could affect the size of the gap and possibly also the type of liquid used in the bearing. The hydrophobic surface also affects cavitation in the bearing and the formation of vortex structures. This was not part of this work, but it is a logical continuation of the issue. The selected example of a journal bearing was modeled by Matlab software. The obtained results make it easier to visualize the effect of the hydrophobic surface on the velocity field inside the bearing. The altered velocity field also indicates a decrease in the dissipation function and hence a reduction of losses in the bearing.

To ensure that the results could be applied in practice, it was necessary to describe the behavior of a hydrophobic surface and implement this in the theoretical solutions. The hydrophobic surface is characterized by a non-zero velocity of the liquid on the wall, thus slippage of the liquid occurs. This slippage is described via the adhesion coefficient k, which is however too complicated to measure directly. Therefore it was necessary to create a new methodology for the evaluation of the adhesion coefficient, depending on easily measurable quantities. For hydrophobic materials, these typically include water contact angle and surface energy. The theory of a droplet motion on an inclined plane of a defined hydrophobic material led to the determination of the adhesion coefficient depending on the droplet velocity and angle of the plane α.

The results of the experiments led to a set of values of adhesion coefficients depending on the angle of inclination, the water contact angle and the surface energy. During the measurements, it was shown that the coefficient will be dependent not only on the contact angle, but also on the static force of separation. This occurs more or less in all hydrophobic materials and changes the flow character in the vicinity of hydrophobic surfaces. This fact leads to another idea with which the presented theory will be extended and that is a mathematical model containing the initial preload, just as in the case of Bingham fluids model.

As it was previously mentioned, the 21st century is dependent on computer simulations, and therefore the newly derived boundary condition was implemented into the most commonly used commercial software for flow simulation – ANSYS Fluent. The results of the simulations already show good applicability in modeling of the flow over hydrophobic walls.

The use of hydrophobic materials is currently one of the most interesting research topics and the area of interaction of such materials with liquids still provides numerous unanswered questions. It is an interdisciplinary area and therefore the clear and precise definition of the problem is rather challenging. Where material science obtains great results in terms of the contact angle, the low mechanical resistance of accordingly produced layers is insufficient for actual practical use and experiments in the harsh conditions of real hydraulic devices. Where nature is perfect and with inherent elegance uses hydrophobicity in the world of plants (lotus flower, rice leaf) and animals (inner surface of vascular bloodstreams, ie cell membranes), there engineering and technology encounters problems that appear during the investigation of the effects associated with flow and hydrophobicity.

And that is the biggest motivation in research to understand concepts established and used elsewhere, in order to help reduce energy losses, increase utilization of available resources and improve currently used technologies.

3 LIQUID FLOW BETWEEN TWO PARALLEL PLATES

Since the properties of hydrophobic surfaces are generally little known, the conventionally used hydrophobic surface boundary condition is mentioned in the form that it was introduced by Navier [1], but further extended to the general curvilinear surface [16].

Note that on an impermeable surface, this boundary condition should also respect the term $\boldsymbol{c} \cdot \boldsymbol{n} = 0$ (on a stationary surface), which is identically fulfilled by the hydrophilic surface, wherein $\boldsymbol{c} = 0$.

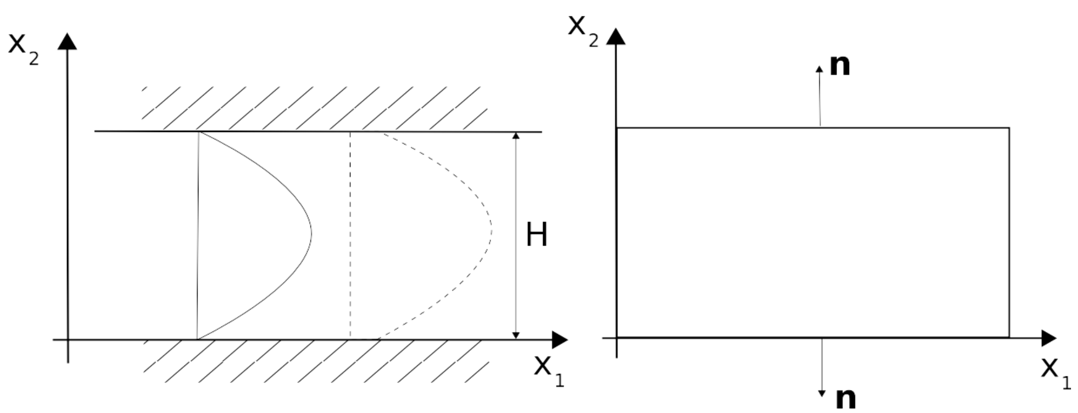


Fig. 1Flow of the Newtonean liquid between two parallel plates

3.1 NEW BOUNDARY CONDITION

When fluid passes over a curved hydrophobic surface moving with velocity $\boldsymbol{u}$, a slip of the liquid occurs.

Within the work described in [15], a new boundary condition was derived for a shear stress vector whose definition is given by the following equation (1):

$$\boldsymbol{\sigma}_A = (\boldsymbol{\sigma} \times \boldsymbol{n}) \times \boldsymbol{n} = k(\boldsymbol{c} - \boldsymbol{u}) \tag{1}$$

where *k*, is adhesion coefficient whose value is given by the contact angle and corresponding surface energy [14].

To illustrate the validity of the derived relations and to demonstrate the impact of hydrophobicity, initially a simple case was selected of Newtonian fluid flow between two parallel plates. The simulation of the actual velocity profile and the velocity course depending on the adhesion coefficient was done within [21], see Fig. 2.

The change in the shape of the velocity profile with visible non-zero velocity at the wall shows the influence of hydrophobic boundary condition on the dissipation function, ie hydraulic losses.

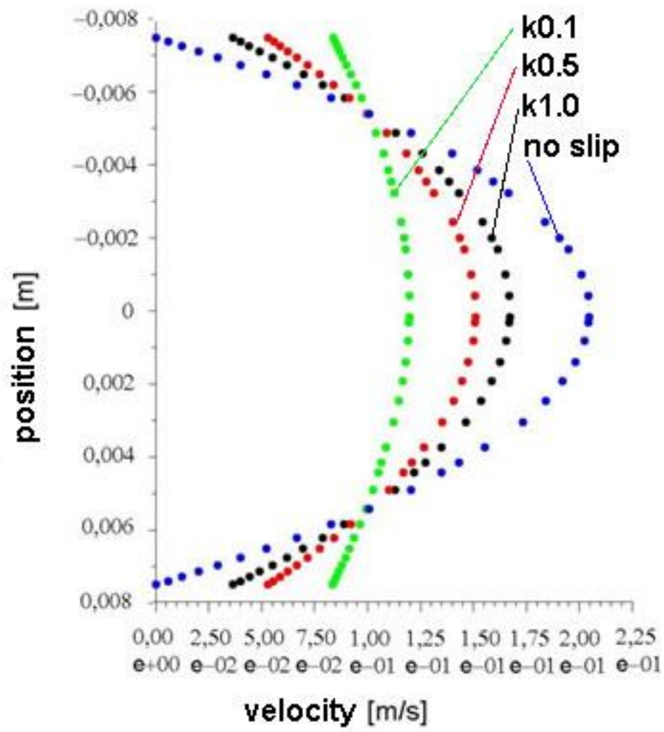


Fig. 2 Velocity profile with different values of adhesion coefficient on the wall (ANSYS Fluent)

Velocity close to the hydrophilic surface can be for the parallel plates defined as a dependence on the pressure gradient:

$$c_1 = -\frac{\partial p}{\partial x_1}\left(\frac{H}{2\eta}\right)x_2 + \frac{1}{2\eta}\frac{\partial p}{\partial x_1}x_2^2 \tag{2}$$

Compared to the same case with hydrophobic surface on both plates:

$$c_1 = -\frac{\partial p}{\partial x_1}\frac{H}{2k} - \frac{\partial p}{\partial x_1}\left(\frac{H}{2\eta}\right)x_2 + \frac{1}{2\eta}\frac{\partial p}{\partial x_1}x_2^2 \tag{3}$$

From the comparison of (2) and (3), an impact of the adhesion coefficient on the velocity profile shape is evident. Due to the first term of the equation where the coefficient of adhesion occurs (at the hydrophilic surface, the adhesion coefficient approaches ∞, therefore the entire first term is equal to zero) the velocity changes the course and magnitude.

3.2 DISSIPATION FUNCTION

Hydraulic losses in the system can be described by the **dissipation function**, which is defined as:

$$2D = \int_V \Pi_{ij} \frac{\partial c_i}{\partial x_j} dV = \int_V 2\eta c_{ij} \frac{\partial c_i}{\partial x_j} dV \tag{4}$$

Flow rate and pressure gradient is derived in the thesis for both types of boundary conditions (hydrophilic and hydrophobic). These are used for the determination of the corresponding dissipation function. In the case of planar flow we obtain a comparison of the dissipation function with a clear influence of adhesion on the wall:

$$2D_{\substack{hydrophobic\\surface}} = \frac{1}{\left(1 + \frac{6\eta}{Hk}\right)^2} 2D_{\substack{hydrophilic\\surface}} \tag{5}$$

k (adhesion coefficient) value therefore strongly positively affects the hydraulic losses.

In a similar way, the validity of the derived relations and the impact of hydrophobicity will be demonstrated for a more complex problem of a planar liquid flow with the solid/liquid interaction.

4 LIQUID FLOW IN THE ANNULUS

In the past ten years there has been a noticeable effort in the literature to find a solution for the interaction of bodies of different physical character; especially the interactions of liquid, magnetic field and solid body.

This is also what the problematic shown in this thesis is concerned with. Based around the unsteady motion of the rotor in a journal bearing with hybrid characteristics. These characteristics are given by the mutual interaction of the liquid, hydrophilic and hydrophobic surface.

4.1 THEORY OF LONG JOURNAL BEARINGS

The classical theory of journal bearings is clearly shown for example in monography [2].

All the shown problems were solved with the assumption of a **hydrophilic** surface with zero velocity vectors on the motionless surface and zero relative velocity vectors on the moving surface.

Owing to the technological progress in the area of surface layers it is not necessary anymore to assume the surface of the solid/liquid interaction to be hydrophilic.

It is nowadays possible to generalize the solution of hydrodynamic problems and assume **hydrophobic** character of the surface in the solid/liquid interaction. That means slipping of the liquid on the hydrophobic surface. This characteristic of the surface to repel liquid was assumed by Navier [1] 200 years ago. For liquid on hydrophobic surface, he predicted the shear stress to be proportional to the slipping velocity.

Other authors also interested in the solution of this problematic were focused especially on the determination of the adhesive coefficient and friction losses. A complex study of the dependence of the liquid flow on the hydrophobic surface is presented in [20] where the effect of hydrophobic surface on the creation of cavitation is emphasized. Recent research in this field is shown for example in works [7] - [9], [18], [23] and [26]. An application for the journal bearing is mentioned within [24] and [25].

The solution of the classical problem of a hydrodynamic journal bearing with cylindrical lining and hydrophilic surface and a journal bearing with conductive liquid and hydrophilic surface leads to the Reynolds equation [7] and its modification [2]. The effect of the hydrophobic surface results again in the modified Reynolds equation [24].

For all these problems the generalized Reynolds equations are given and the force vector in dependence on the vector of translation and velocity of the shaft motion is determined.

From these equations, it is possible to define the matrices of stiffness and damping of the bearing.

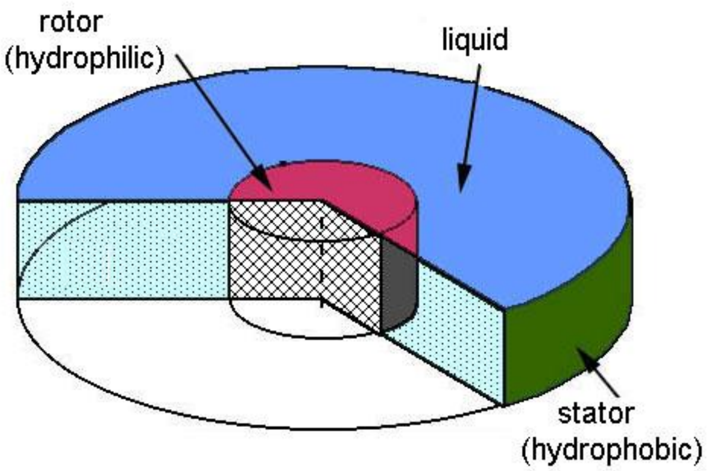


Fig. 3 Planar example of a journal bearing with hydrophobic lining on the stator

It makes sense for journal bearings to choose the rotor surface as hydrophilic and the motionless surface of the bearing lining as hydrophobic. By this we accept certain slippage of liquid on the surface of the lining, see Fig. 3.

The term $\boldsymbol{c} = 0$ for the velocity vector holds on the hydrophilic surface of the lining.

Hence for the velocity components in the tangential and radial direction, it can be written:

$$c_\varphi = 0; \qquad c_r = 0 \tag{6}$$

For $k \to \infty$, the term (1) applied on the motionless lining of the bearing changes into (6). From a practical point of view, the boundary condition (1) has an exceptional importance, since the total energy dissipation in the journal bearing is dependent on the adhesive coefficient k. By an appropriate choice of the coating of the inner lining of the journal bearing, it is possible to significantly lower the hydrodynamic losses, maintaining the stiffness and damping abilities of the bearing, as it is shown below.

4.2 HYDROPHOBIC SURFACE EFFECT ON THE MATRICES OF ADDED STIFFNESS AND DAMPING

The generalized Reynolds equation was the basic mathematical model for the determination of the stiffness and damping matrices. Its universal form is shown for the simplification of the laminar flow.

Within the thesis a detailed analysis of the mathematical theory of the classical journal bearing is shown and compared to the effect of the hydrophobic lining. Presented were only the results for non-cavitating bearings. As a result we obtain the velocity and pressure fields, the force effect on the shaft and the matrices of added damping and stiffness in the journal bearing with and without a hydrophobic lining. The resulting comparison shows an exemplary effect of a hydrophobic surface on the matrices of additional stiffness and damping.

Stiffness of an ideally hydrophilic surface (S) relative to an ideally hydrophobic surface (N):

$$\boldsymbol{K}_N = \frac{1}{2}\boldsymbol{K}_S \tag{7}$$

Damping of an ideally hydrophilic surface (S) relative to an ideally hydrophobic surface (N):

$$\boldsymbol{B}_N = \frac{1}{4}\boldsymbol{B}_S \tag{8}$$

4.3 MODEL PROBLEM

This theory was tested by a simple problem modeling using Matlab software. This task showed significant changes in flow inside the non-cavitating bearing due to the use of hydrophobic lining.

The solution comes from the same assumptions as in the classic bearings, changing only the boundary condition on the radius R_2 at the point of the bearing lining.

For the comparison of the results of simulations (Matlab) for the velocity field of non-cavitating journal bearings with hydrophobic/hydrophilic surface of the lining, see Fig. 4 and Fig. 5

From Fig. 4 a fluid slip along the lining of the journal bearing is apparent. Compare it with Fig. 5 applicable for the hydrophilic surface of the lining. Lower hydraulic losses correspond to this velocity field.

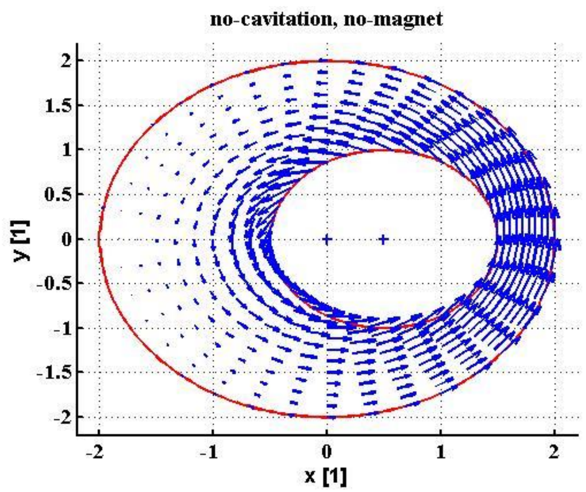


Fig. 4 Velocity field for non-cavitating bearing, k=10

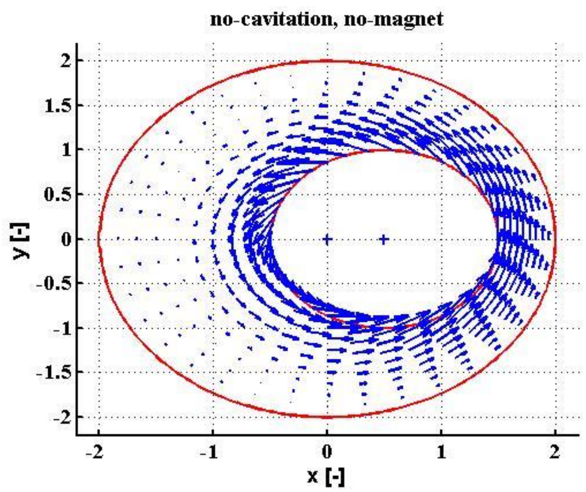


Fig. 5 Velocity field for non-cavitating bearing

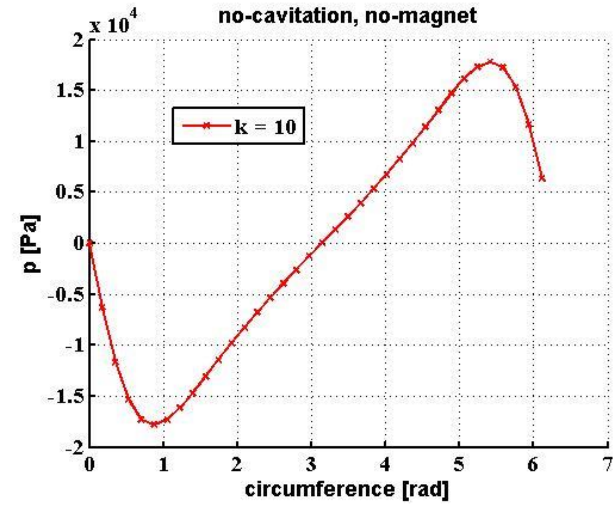


Fig. 6 Circumferential pressure distribution for non-cavitating bearing, k=10

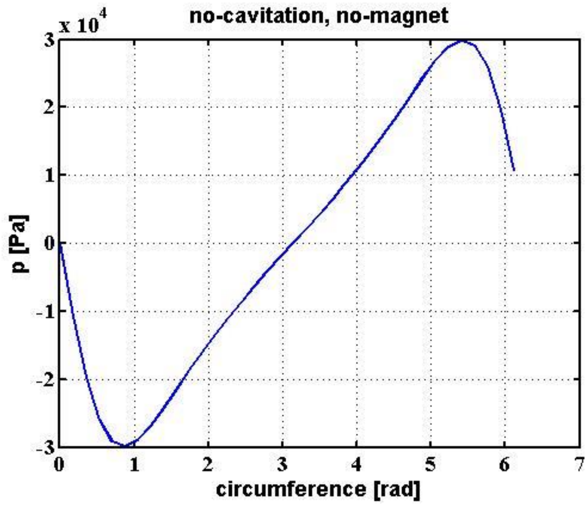


Fig. 7 Circumferential pressure distribution for non-cavitating bearing

A comparison of the Matlab simulations results for the pressure field of non-cavitating journal bearings with hydrophobic, respectively hydrophilic lining is visible from Fig. 6 and Fig. 7.

5 NEW BOUNDARY CONDITION IMPLEMENTATION IN COMMERCIAL SOFTWARE

It was already mentioned that the standard boundary condition used in mathematical simulations of flow assumes a zero velocity on the wall. When creating CFD mathematical model it is sometimes necessary to improve, refine or modify some of the standard features that are defined in the program by default. If we want to use commercial software packages for computational simulations of flow around the hydrophobic surface, this must be added to the program.

There are several approaches how to implement this. The smartest method is the use of the User-defined function (UDF). UDF function uses **C++** for the additional programming of required functions. UDF function in CFD program has only a few restrictions and the scope of its use is evident from the following list: creating custom boundary conditions, definition of material properties, choice of reaction volume dependencies, defining various sources (thermal, volume, weight, etc.), diffusion function, treatment of the calculated values for the different iterations, etc. First, you need to correctly program **C++** code of the given functional dependence, for example in Microsoft Visual studio and the like. It is also necessary to comply with the requirements and commands of the developers as stated in the UDF manual. After the assembly a so called hooking of the feature into the environment of ANSYS Fluent software must be performed. There are two basic approaches: Compiled, Interpreted. Advantages and disadvantages of these approaches are not in the scope of this thesis (it is in detail in the UDF manual, which is freely available). For simpler tasks, it is preferable to use function Interpreted. UDF additional programming features for ANSYS Fluent software are now available for free on the website of BUT - Victor Kaplan Department of Fluids Engineering.

Subsequent comparison of the results with and without influence of hydrophobic surface should investigate the influence of hydrophobic surface on the flow field behavior. The test case was a straight pipeline modeled in 2D, see Fig. 8. The geometry was considered as axisymmetric. The densification is carried out to a solid wall. The wall is considered as stationary. Entry in the mathematical model is considered as a velocity inlet and output as the pressure outlet.

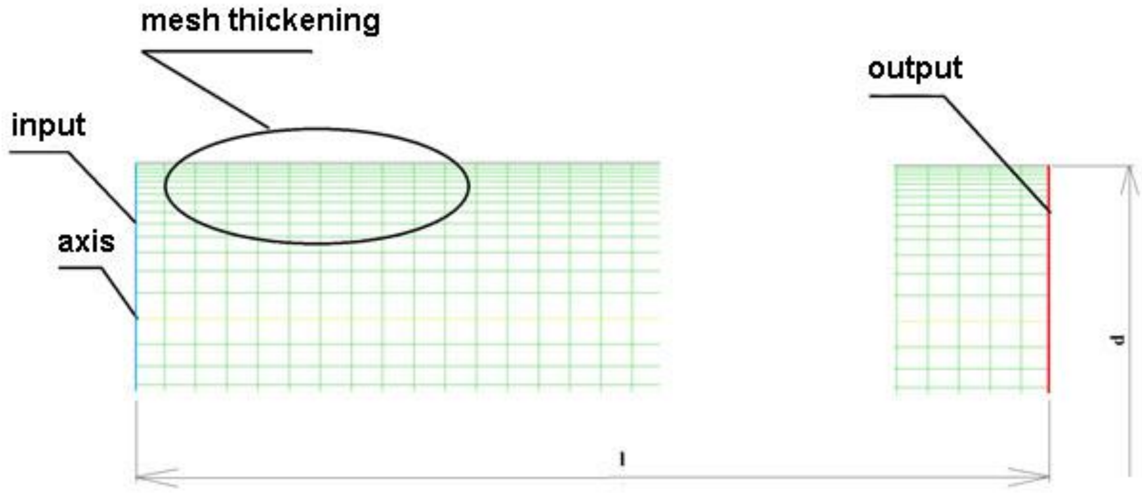


Fig. 8 The geometry of the examined pipeline

The influence of hydrophobic surface in two flow modes - laminar and turbulent flow regime mode was investigated. This had the fundamental influence on the choice of boundary conditions. Accordingly were also selected the input velocities.

Laminar flow regime

$$Re = \frac{c \cdot d}{\nu} = \frac{0{,}03 \cdot 0{,}05}{10^{-6}} = 1500 \leq 2320 \tag{9}$$

For laminar flow velocity $c = 0{,}03\, m.s^{-1}$ has been selected. As it is evident from the calculation, the value of the Reynolds number is lower than the critical value and therefore a laminar flow is confirmed.

Turbulent flow regime

$$Re = \frac{c \cdot d}{\nu} = \frac{1 \cdot 0{,}05}{10^{-6}} = 50000 \geq 2320 \tag{10}$$

For turbulent flow velocity $c = 1\, m.s^{-1}$ was chosen. Again, it was verified by Reynolds number calculation. Its value was greater than the critical one, and hence it is really a turbulent flow.

Additionally, it is necessary to define the different kinds of a hydrophobic surface. Hydrophobicity is understood as the slipping of the fluid on the surface and thus the relative velocity of the liquid on the wall is nonzero. The degree of hydrophobicity in this case is proportional to an adhesion coefficient *k* [$Pa \cdot s \cdot m^{-1}$].

◆ no slip	■ 0,01	▲ 0,05	✖ 0,1	★ 0,5	● 1,0	*k* [$Pa \cdot s \cdot m^{-1}$]

Tab. 1 The adhesive coefficient variants (markers on the spline lines in following figures Fig. 9-14 correspond with the markers in table)

5.1 SIMULATION RESULTS

Laminar flow | *Turbulent flow*

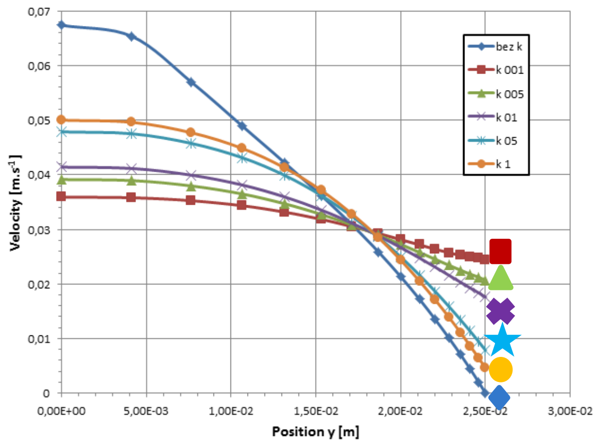


Fig. 9 Velocity profile

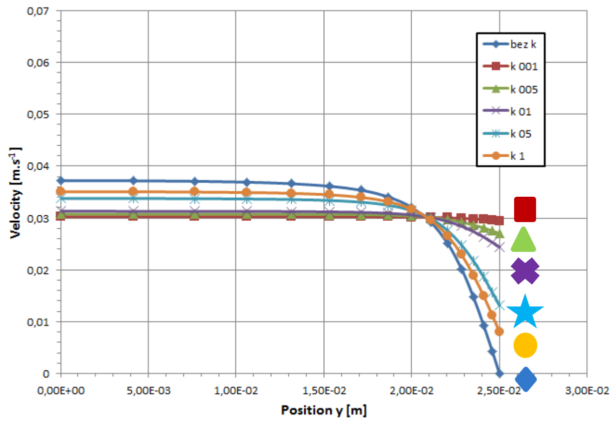


Fig. 10 Velocity profile

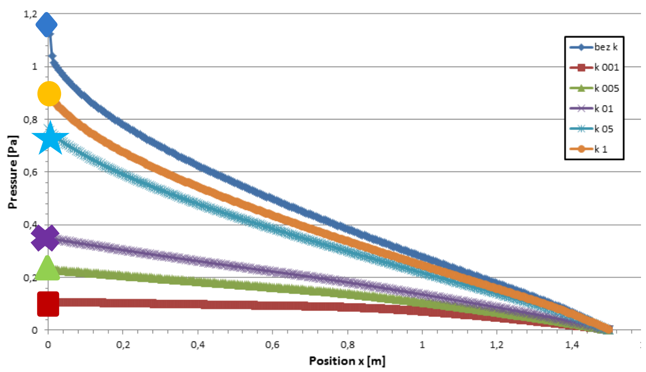


Fig. 11 Pressure losses

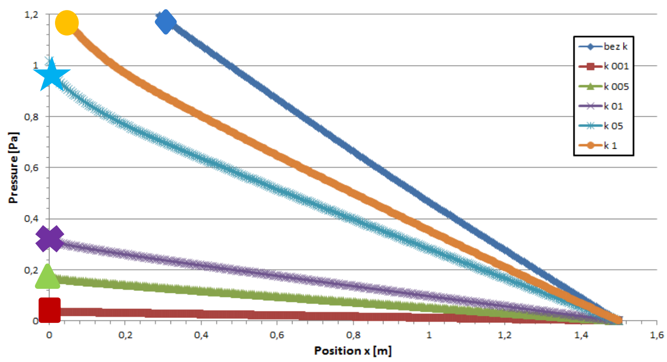


Fig. 12 Pressure losses

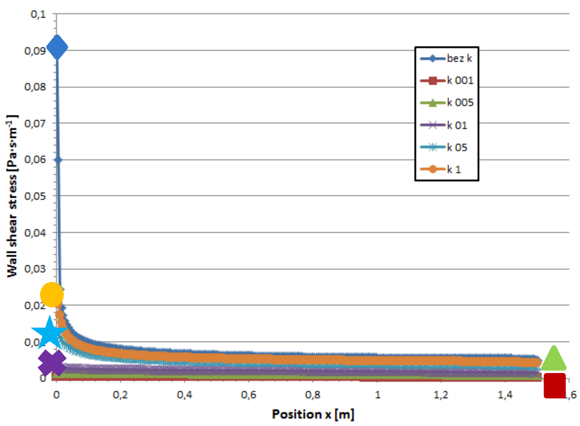


Fig. 13 Shear stress on the wall

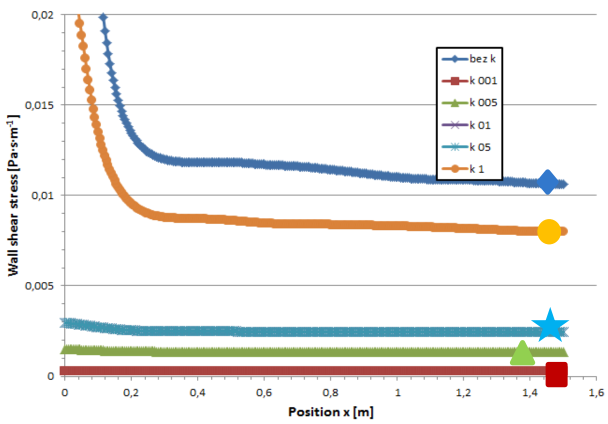


Fig. 14 Shear stress on the wall

6 EXPERIMENTAL SETTING OF ADHESION COEFFICIENT

For an effective use of the newly derived theory in commercial software, the value of the adhesion coefficient must be determined for each material. Direct measurement of the adhesion coefficient for different surfaces is complicated. Therefore, in the experiment not only the adhesion coefficient was observed, but especially its dependency on the easily measurable quantities, such as the contact angle or surface energy. Then it is easier to study its influence on the flow losses, velocity profiles and overall flow behavior.

6.1 THEORETICAL BASIS

According to [17], a mathematical model of the adhesive force is derived based on the droplet motion on an inclined plane. Fig. 15 shows the droplet motion along an inclined plane, where the translational motion of the droplet along the axis x_1, with the speed c_1 in each point of the motion is considered.

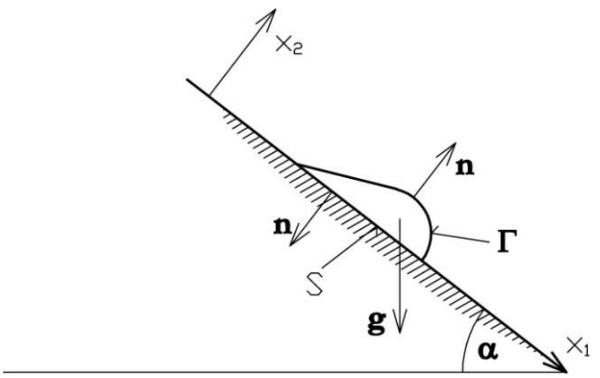


Fig. 15 Droplet motion on an inclined plane

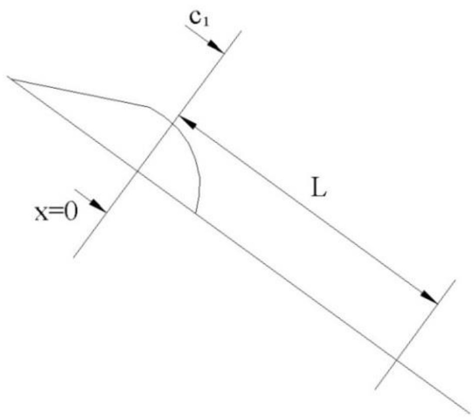


Fig. 16 Droplet on an inclined plane, initial conditions (23)

Navier-Stokes equations represent a mathematical expression of the law of conservation of momentum in the flowing fluid. This is a differential equation describing the generally turbulent flow of Newtonian fluids. An incompressible liquid and the continuity equation are assumed.

$$\frac{\partial c_i}{\partial x_i} = 0 \tag{11}$$

Then the Navier-Stokes equations can be written in the shape:

$$\rho \frac{\partial c_i}{\partial t} + \rho \cdot \frac{\partial c_i}{\partial x_j} \cdot c_j - \frac{\partial \sigma_{ij}}{\partial x_j} = \rho \cdot g_i \tag{12}$$

The equation for the adhesive force acting on the rigid body surface can be derived from its solution:

$$F_i = -\rho \cdot \int_V \frac{\partial c_i}{\partial t} dV - \rho \cdot \int_\Gamma c_i \cdot c_j \cdot n_j d\Gamma + \int_\Gamma \sigma_{ij} \cdot n_j d\Gamma + \rho \cdot g_i \cdot V \tag{13}$$

6.2 STATIC ADHESIVE FORCE

From the equation (13) follows that the static part of the adhesive force can be written as:

$$F_{iS} = \int_{\Gamma} \sigma_{ij} \cdot n_j d\Gamma + \rho \cdot g_i \cdot V \tag{14}$$

When the shear stress is expressed as a pressure function $\sigma_{1j} = -\delta_{1j} \cdot p$ and we consider the pressure dependence:

$$p = p_A + \sigma \cdot \mathrm{div}\boldsymbol{n} \tag{15}$$

Then considering the fact, that the droplet is in the gravity field, $i = 1$ and $\alpha = \alpha_0$, the static adhesive force in the direction x_1 can be written as:

$$F_{1S} = f = -\sigma \int_{\Gamma} div\mathbf{n} \cdot n_1 d\Gamma + m \cdot g \cdot sin\alpha_0 = const. \tag{16}$$

Analogically for the static force in the direction x_2:

$$F_{2S} = -p_A \cdot S - \sigma \int_{\Gamma} div\mathbf{n} \cdot n_1 d\Gamma + m \cdot g \cdot sin\alpha_0 = const. \tag{17}$$

When $\alpha_0 = \alpha_{0krit}$, the droplet starts to move.

6.3 DYNAMIC ADHESIVE FORCE

The translational motion of the droplet along the axis x_1, with the speed c_1 in each point of the motion is considered, see Fig. 16.

The equation for the adhesive force in the direction $i = 1$ according to (13) will be in the form:

$$F_1 = -\rho \cdot \int_{V} \frac{\partial c_1}{\partial t} dV - \rho \cdot \int_{\Gamma} c_1^2 \cdot n_1 d\Gamma - \int_{\Gamma} p \cdot \delta_{1j} \cdot n_j d\Gamma + \rho \cdot g_1 \cdot V \tag{18}$$

Considering (15) it can be written:

$$F_1 = -\rho \cdot \int_{V} \frac{\partial c_1}{\partial t} dV - \rho \cdot \int_{\Gamma} c_1^2 \cdot n_1 d\Gamma - p_A \int_{\Gamma} n_1 \, d\Gamma + \mathrm{m} \cdot g \cdot sin\alpha \tag{19}$$

When we consider constant angle α of the inclined plane and the shape of the droplet in motion does not change then (16) can be used and written:

$$F_1 = -m \cdot \frac{\partial c_1}{\partial t} + f \tag{20}$$

When the adhesive force and movement velocity are proportional, then:

$$dF_1 = -\sigma_{ij} \cdot n_j dS = -k \cdot c_1 dS$$

$$F_1 = -\int_S \sigma_{1j} \cdot n_j dS = \int_S k \cdot c_1 dS = k \cdot c_1 dS \tag{21}$$

Here it is assumed that the adhesive coefficient k is not dependent on the initial velocity c_1 . After adjustment, the solution of equation (21) is in the form:

$$F_1 = -m \cdot \frac{\partial^2 x_1}{\partial t^2} + f = k \cdot c_1 dS$$

After adjustment:

$$F_1 = -m \cdot \frac{\partial^2 x_1}{\partial t^2} + S \cdot k \cdot \frac{\partial x_1}{\partial t} = f \tag{22}$$

Solution of the equation (22) will be in the form:

$$x_1 = B \cdot e^{-\frac{S \cdot k}{m} \cdot t} + A \cdot \frac{1}{S \cdot k} + \frac{f \cdot m}{S^2 \cdot k^2} \cdot \left(\frac{S \cdot k}{m} \cdot t - 1\right)$$

Initial conditions - see Fig. 16:

$$t = 0\colon\ x_1 = 0;\ \dot{x}_1 = c_1 \tag{23}$$

In the time $t = 0$ we obtain the integration constants A and B and the relation for velocity:

$$c_1 = \frac{A}{m} - \frac{f}{S \cdot k} + \frac{f}{S \cdot k} \Rightarrow A = m \cdot c_1$$

$$B = \frac{f \cdot m}{S^2 \cdot k^2} - \frac{m \cdot c_1}{S \cdot k}$$

$$\dot{x}_1 = \left(c_1 - \frac{f}{S \cdot k}\right) \cdot e^{-\frac{S \cdot k}{m} \cdot t} + \frac{f}{S \cdot k} \tag{24}$$

The adhesive coefficient k was detected numerically from an exponential function of measured velocities that correspond with the equation (24). The form of the solved equation is:

$$y = A \cdot e^{Bt} + C \tag{25}$$

The unknown coefficients A, B and C from the equation (25) were determined by the method of least squares that enables the calculation of the unknowns: k, c_1, f from (24).

6.4 EXPERIMENT

Experimental verification serves as a more accurate prediction for a further description of hydrophobic materials and their properties. The obtained result is experimentally determined adhesion coefficient k at an initial velocity c_1 and the corresponding value of the function f. For this experiment, described in details within [30], only water was used as a testing substance.

The chosen coated metal sheet was treated before each measurement sequence by technical gasoline and dried with cotton, in order to minimize the error of copying the motion trajectory of previous droplets.

Droplets of different sizes were deposited on the surface of the plate with a pipette in two ways - in a horizontal position and a tilted position. The results of both of these methods are comparable. It was only necessary to pay attention to the initial velocity in the case of the inclined plate to not allow the separation of the droplet (problem with leaving an imprint →droplet volume decreasing→droplet velocity distorted). In horizontal position it was easier to place the droplet on the plate, but more difficult to observe the moment of droplet separation during the inclination.

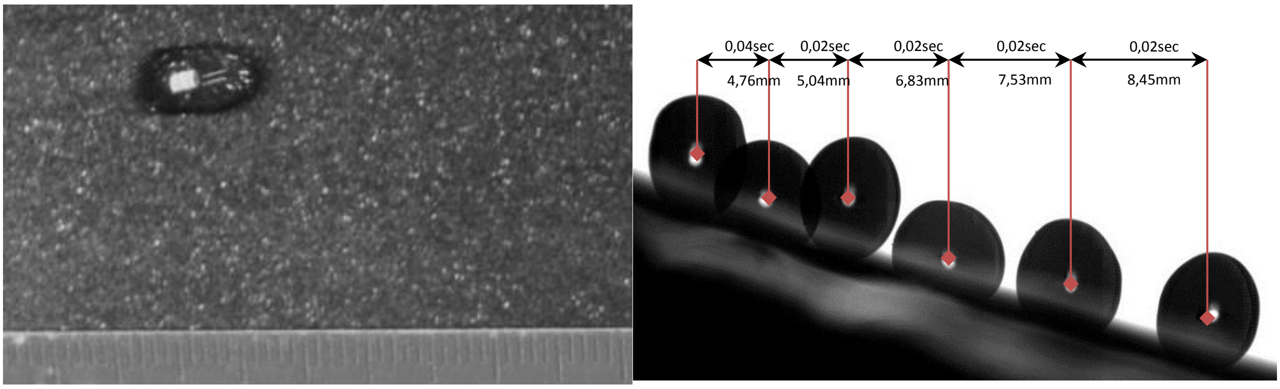


Fig. 17 Droplet captured in motion on the inclined plane – droplet detail on the right side picture, Shadowgraph from Technical University of Liberec (cooperation during the GAČR project solution) – visible air layer formed and bonded to the hydrophobic surface

From the camera records, individual images were created and the positions of droplets in time were deducted. The velocity was calculated from the position and the time using central differences. The adhesive coefficient *k*, the initial velocity c_1 and the corresponding value for function *f* (see [15]) was obtained from the calculated values of the droplet speed using the method of least squares. Data approximation of equation (25) for the measured data was carried out in Matlab software using nonlinear regression.

One of the assumptions of the derived mathematical model was that the shape of the moving droplets on an inclined plane does not change, as described in the equation (16). It is very difficult to keep this premise in normal laboratory conditions; however, any possible change in the size of the contact area of the droplet with the surface has been monitored to minimize errors. In the calculation, the droplet contact area *S* was then defined as the mean value on the whole interval, i.e. $\bar{S}$. The droplet weight *m* has been known through the use of pipettes.

6.5 EXPERIMENTAL RESULTS

The measured values of contact angle and surface energies are shown in Tab. 2 for water at two ambient temperatures (taken from [13]).

The adhesive coefficient values *k* for all three measured materials are shown in the following Tab. 3, Tab. 4 and Tab. 5.

The angle of the inclination of the plane α was not firmly held to the same extent, the inclination was dependent on the behavior of droplets and their separation. However, this fact did not affect the essence of the experiment.

Material	θ [°]	θ [°]	γ [mJ/m²]	γ [mJ/m²]
	t = 18° C	t = 28° C	t = 18° C	t = 28° C
TC 1191 (black)	63,0 ± 6,2	77,5 ± 6,4	39,6	40,7
TC 3072 (metal black)	74,7 ± 7,4	95,4 ± 8,2	24,3	24,9
TC 4111 (green)	88,9 ± 6,3	78,8 ± 6,4	25,7	34,8

Tab. 2 Contact angle θ and surface energies for measured materials

TC1191	$\bar{S}$ [m²]	m [kg]	α [°]	k [Pa·s/m]	f [N]	c_1 [m/s]
DSC_7864	4.871E-05	6.494E-05	26	1.051	2.47E-06	0.0167
DSC_8070	3.853E-05	6.494E-05	27	1.7469	2.98E-06	0.0128
DSC_7833	4.467E-05	6.494E-05	28	1.8784	6.65E-06	0.0173
DSC_7834	4.467E-05	6.494E-05	29	1.552	5.18E-06	0.0134
DSC_7831	4.808E-05	6.494E-05	32	1.7772	5.89E-06	0.0492
mean				**1.6011**		

Tab. 3 The adhesive coefficient values k for given angle α and material TC1191

TC3072	$\bar{S}$ [m²]	m [kg]	α [°]	k [Pa·s/m]	f [N]	c_1 [m/s]
DSC_7901	4.270E-05	6.494E-05	26	1.9691	3.43E-06	0.0196
DSC_7905	4.839E-05	6.593E-05	27	1.2766	3.06E-06	0.0332
DSC_7960	5.571E-05	6.593E-05	28	1.0066	4.29E-06	0.0169
DSC_7948	4.235E-05	6.494E-05	29	1.244	4.76E-06	0.0278
DSC_7956	4.729E-05	6.593E-05	30	1.1938	6.67E-06	0.0326
DSC_7981	4.983E-05	6.494E-05	31	1.3309	7.42E-06	0.0184
mean				**1.3368**		

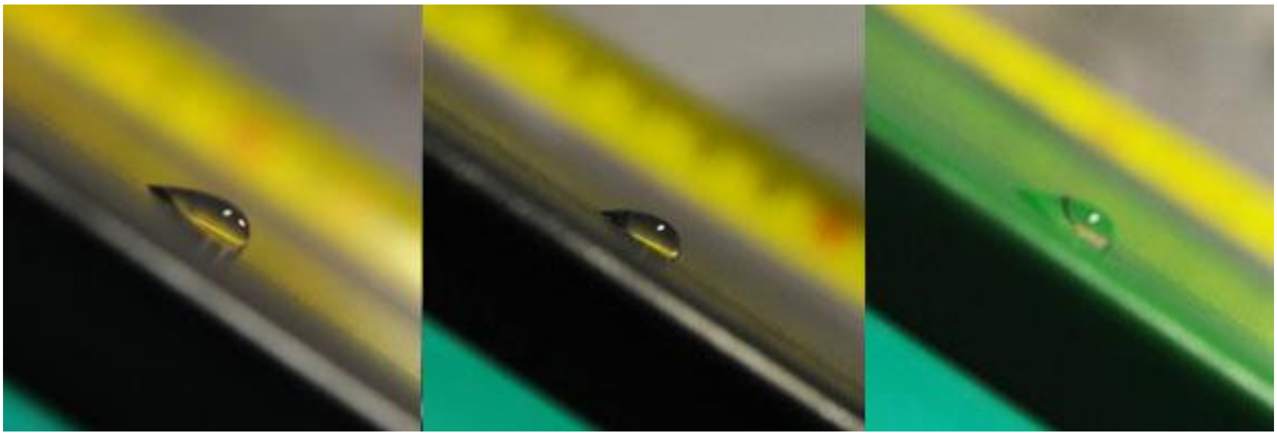
Tab. 4 The adhesive coefficient values k for given angle α and material TC3072

TC4111	$\bar{S}$ [m²]	m [kg]	α [°]	k [Pa·s/m]	f [N]	c_1 [m/s]
DSC_7820	4.115E-05	6.194E-05	27	2.4439	8.59E-06	0.0463
DSC_7715	4.048E-05	5.495E-05	28	1.1464	1.36E-06	0.0115
DSC_8090	3.821E-05	6.593E-05	29	1.0552	1.26E-06	0.0174
DSC_7713	5.000E-05	5.994E-05	30	1.0797	2.95E-06	0.0321
DSC_8083	4.206E-05	6.494E-05	31	0.9048	2.11E-06	0.0335
mean				**1.326**		

Tab. 5 The adhesive coefficient values k for given angle α and material TC4111

The value of the calculated function f (static force F_s) should match the droplet shape. The recording of the droplets was made at approximately the same time interval as their picture was taken. These were taken perpendicularly to the material surface due to the determination of the contact area $\bar{S}$.

The individual shapes of droplets on measured materials are shown in Fig. 18.



TC1191 (black plate) | TC3072 (metal black plate) | TC4111 (green plate)

Fig. 18 Droplet size 65mm^3, angle of plate inclination $\alpha = 30°$

6.6 CONCLUSIONS FROM THE EXPERIMENTAL RESULTS

The dependence of the adhesion coefficient on the inclined plane angle α is evaluated in Tab. 6. The droplet of identical volume $V = 74\,\boldsymbol{mm^3}$ flows down the plane. It is clear that the adhesion coefficient changes depending on the angle of inclination of the plane, indicating its dependence on the velocity (or Reynolds number). Based on the knowledge obtained from these experiments, the mathematical model of the non-wettable surface will be extended with the initial stress. This stress (σ_S), respectively the static force of the separation ($F_s=f$) differs for different materials (Newtonian fluid on the hydrophobic surfaces behaves like Bingham fluid).

material	m [kg]	S $[m^2]$	α [°]	k $\left[\frac{Pa\cdot s}{m}\right]$	f [N]	v_0 $\left[\frac{m}{s}\right]$	$\sigma_S\left[\frac{N}{m^2}\right]$	θ [°]
TC4111	7.39E-05	4.96E-05	26	2.1201	4.26E-06	0.0216	8,59E-02	90
AE2	7.39E-05	3.88E-05	40	1.874	4.02E-06	0.0329	10,8E-02	110
AL1	7.39E-05	4.02E-05	45	1.9077	2.24E-06	0.0462	5,57E-02	125
DR-B	7.39E-05	1.69E-05	5	0.9784	2.77E-05	0.2046	163,9E-02	140

Tab. 6 Static force of separation (f), adhesion coefficient (k) and static prestress (σ_S)
In the dependence on the inclined plane angle (α) and water contact angle (θ)

7 CONCLUSION

The implications of using hydrophobic materials in technical practice greatly depend on the options that are provided by computational modeling of the flow. Given that nowadays hydraulic design begins with simulations, it is necessary to enrich the simulations with the latest research findings. Zero speed on the wall is regarded as the standard boundary condition, but it is denied by hydrophobic materials.

In the presented thesis, the new boundary condition was derived which confirms the hydrophobic surface influence on the losses in the hydraulic systems and refutes the argument that a reduction in losses does not occur [18].

The examples show the influence of new boundary conditions on the dissipation function and comparison of the hydrophobic with commonly used hydrophilic assumption. Planar examples of flow between two parallel plates are followed by a more complex problem of the planar journal bearing. Journal bearing is represented by a stationary and unsteady flow in the annulus. Solution for the journal bearing model logically leads to the popular field of FSI (Fluid Structure Interaction). FSI is the mutual interaction of the body and the fluid. In these systems, where the fluid flow affects the movement of the body in it (in the given case the rotation with possible eccentricity) kinematics solution of the motion leads on to the complex problem of mechanics, where the obtained result are matrices of additional damping and stiffness. These are significantly changing according to the type of the surface and accordingly also the selected boundary conditions. Thus it shows an opportunity for development in the design and construction of journal bearings. Using a hydrophobic coating on the stationary part of the bearing can reduce the stiffness of the liquid layer to about a half (7) and damping to a quarter (8). This can affect the size of the gap, but also the type of liquid used in the bearing. The hydrophobic surface also affects cavitation in the bearing and the formation of vortex structures, which were not part of this work, but are a logical continuation of the study of the issue.

To ensure that the results would be useful in practice, it was necessary to further describe the behavior of a hydrophobic surface and implement this into a mathematical model. The hydrophobic surface is characterized by nonzero velocity of the liquid at the border, known as slippage of the liquid. This slippage is described via the adhesion coefficient k. To measure the adhesion coefficient directly is too complicated, therefore it was necessary to create a new methodology for evaluating the adhesion coefficient depending on the easily measurable quantities typical for materials that are in contact with water, such as contact angle and surface energy. The theory for moving droplets on an inclined plane of a defined hydrophobic material led to the determination of the adhesion coefficient depending on the velocity and the angle of the inclined plane α.

The experimental results led to a set of values of adhesion coefficients depending on the angle of inclination, the contact angle and surface energy. During the measurements it was shown that the coefficient will be dependent not only on the contact angle, but also on the static force of separation, which occurs on all hydrophobic materials to a greater or smaller extent. This dependence can change the natural behavior of the flow in the vicinity of a hydrophobic wall. This fact leads to another idea by which this theory will be extended. The mathematical model will be widened of the initial preload, just as in models for Bingham fluids.

As it was already mentioned, the 21st century is characterized by abundant use of computer simulations, and therefore the newly derived boundary condition is implemented into commercial, most commonly used software for flow simulations - ANSYS Fluent. The comparison of the simulation results with experiments has already proven the usefulness of the modeling of flow close to hydrophobic surfaces.

Another observed property, which must be taken into account in the modeling of flow in the vicinity of hydrophobic layers, is the ability of the hydrophobic layer to bind molecules of air, see Fig. 17. This ability disappears during the transition into turbulent flow regime. The ability of the hydrophobic surface to bind air (“aerofilia”), can also be used for a gentle aeration without gas bubbling through the liquid. This type of application has already been tested in the laboratory OFI VK with very good results. Measurements of the velocity profile were done within the GACR project, where author was a principal investigator, at the co-investigator laboratory (Technical University of Liberec) using PIV (Particle Image Velocimetry) and clarified in the vicinity of the wall using micro PIV. Significant effect on the velocity profiles and existence of the wall slippage represented the final results of the grant project, but are not part of this thesis. Nevertheless, the results obtained were used for the verification of the appropriateness of the proposed methodology fort the description of the behavior of hydrophobic layers. The mutual influence of the thickness of the air layer and velocity (respectively Reynolds number) was investigated qualitatively in microchannels. With the increase of the Reynolds number, the thickness of the air layer decreases and with reaching a turbulent flow is completely extinguished. However the velocity profile still differs compared to a hydrophilic surface. This leads to the idea of formulating a new boundary condition with varying viscosity near the hydrophobic wall, which is yet to be confirmed. Returning to computer simulations, it will be necessary to rephrase or supplement the turbulence models, which will be different for different degrees of hydrophobicity. Research on the ability of the hydrophobic surfaces to change the character of the flow, the formation of vortex structures and the concentration of gases in liquids shows a vast field of possible further investigations. A move to the reduction of hydraulic losses, material savings and thus savings in the production and operation costs is always a positive movement. In this direction hydrophobicity can advance the technical practice, and therefore it is sensible to continue and further develop the above mentioned theories.

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ABSTRAKT

V současné době moderních technologií, pokročilých možností v oblasti nanotechnologií a materiálového inženýrství se dynamicky rozvíjí obory zabývající se tzv. smáčivostí. Jedná se nejen o problematiku povrchových úprav materiálů, jejich výrobu a využití v technice, ale také o matematický popis a následnou simulaci proudění kapalin po těchto površích.

Danou problematiku je třeba vnímat a hodnotit mezioborově, není to jednoznačně zájem pouze materiálového či fluidního inženýrství. Prvotně je třeba pochopit princip funkce hydrofobních materiálů, jejich vliv na kapaliny a způsob jakým tento vliv definovat. Následně najít a stanovit způsob, jakým lze vzájemnou interakci povrchové vrstvy a kapaliny popsat a vyhodnotit. A v neposlední řadě tyto znalosti zapracovat do komerčních softwarů, experimentálně ověřit a prakticky používat. A to bylo cílem habilitační práce.

Význam využití hydrofobních materiálů v technické praxi výrazně závisí na možnostech, které dává počítačové modelování proudění. Vzhledem k tomu, že v dnešní době hydraulické návrhy začínají u simulací, je nutné tyto obohatit o znalosti posledního výzkumu. Nulová rychlost na stěně je považována za standardní okrajovou podmínku, kterou ale hydrofobní materiály popírají. V předložené práci byla odvozena nová okrajová podmínka, která vliv hydrofobního povrchu na rychlostní profil a rychlost na stěně zahrnuje.

Na příkladech je ukázán vliv nové okrajové podmínky na disipační funkci a srovnání hydrofobního s běžně užívaným hydrofilním předpokladem. Rovinné příklady proudění mezi dvěma deskami jsou následovány složitějším systémem rovinné úlohy kluzných ložisek, tedy stacionárním i nestacionárním proudění v mezikruží. Řešení modelu kluzného ložiska logicky vede na populární obor FSI (Fluid Structure Interaction), což je vzájemná interakce tělesa s kapalinou. V těchto systémech, kdy proudění kapaliny ovlivňuje pohyb tělesa v ní (v řešeném případě rotace s možnou excentricitou), vede řešení kinematiky pohybu na komplexní problém mechaniky, kdy výsledkem jsou matice přídavných tlumení a tuhostí. Tyto se podle typu povrchu a tím i zvolené okrajové podmínky výrazně liší a ukazují tak na možný vývoj v návrzích a konstrukci kluzných ložisek. Použitím hydrofobního nátěru na nepohyblivé části ložiska můžeme snížit tuhost kapalinové vrstvy o polovinu a tlumení až o čtvrtinu, což může ovlivnit velikost mezery, eventuálně i typ používané kapaliny v ložisku. Hydrofobní povrch také ovlivní kavitaci v ložisku a tvorbu vírových struktur.

K tomu, aby byly teoretické výsledky použitelné v praxi, bylo dále nutné popsané chování hydrofobního povrchu zavést do matematického modelu. Hydrofobní povrch je charakteristický tím, že rychlost kapaliny na jeho hranici není rovna nule, dochází k tzv. prokluzu kapaliny. Tento prokluz je popsaný pomocí adhezního součinitele *k*. Měřit přímo adhezní součinitel je příliš komplikované, proto byla vytvořena nová metodika vyhodnocování adhezního součinitele v závislosti na snáze měřitelných veličinách typických pro materiály, co jsou v kontaktu s vodou.

Teorie stékání kapky po nakloněné rovině definovaného hydrofobního materiálu vedla na určování adhezního součinitele v závislosti na rychlosti a úhlu naklonění roviny α.

Výsledky experimentů vedly na soubor hodnot adhezních součinitelů v závislosti na úhlu naklonění roviny, kontaktním úhlu a povrchové energii. Během měření se ukázalo, že koeficient bude závislý nejen na kontaktním úhlu, ale také na statické síle odtržení, která se vyskytuje u všech hydrofobních materiálů ve větším či menším měřítku a mění charakter proudění v blízkosti hydrofobní stěny.

Nově odvozená okrajová podmínka byla implementována do komerčního softwaru nejčastěji používaného pro modelování proudění – ANSYS Fluent. Výsledky simulací srovnané s experimentem ukázaly na dobrou využitelnost při modelování proudění kolem hydrofobních povrchů. Takto obohacený software je dále využíván na Odboru Fluidního inženýrství Victora Kaplana při řešení reálných problémů při spolupráci s průmyslem i v rámci projektů Grantové Agentury České Republiky a Technologické Agentury České Republiky.

Další pozorovanou schopností, kterou bylo nutno zohlednit v modelování proudění v blízkosti hydrofobních vrstev, je schopnost hydrofobní vrstvy vázat molekuly vzduchu. Tato se vytrácí při přechodu do turbulentního režimu proudění. Schopnost hydrofobního povrchu vázat vzduch, tedy „aerofilie“, se dá využít i k účinné aeraci bez nutnosti vytváření mikrobublin plynu. Tento druh použití byl v rámci řešení projektu TAČR testován v laboratoři OFI VK s velmi dobrými výsledky a také autorkou publikován.

Výzkum schopností hydrofobních povrchů měnit charakter proudění, vznik vírových struktur i koncentraci plynu v kapalinách ukazuje na ohromné pole dalšího možného zkoumání. Posun ke snížení ztrát, úsporám materiálů a tím i nákladů na výrobu a provoz je vždy posun pozitivní. Tímto směrem hydrofobie technickou praxi posunout může, a proto má smysl pokračovat a rozvíjet výše zmíněné teorie dál.