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Simulation of Single Fibre Wetting

Abstract
A stationary system composed of a fibre, liquid and air consists of a background for the shape determination of a typical liquid at the liquid-fibre inter-phase. Up to the present, it has not been possible to define this shape by a mathematical function. In this study a differential equation was found and solved analytically, describing the liquid curve at the mentioned inter-phase in the air-fiber-liquid system. This equation was solved and the result calculated by a numerical method, which were then compared with the experimental data obtained by a measurement technique developed by us.

Key words: *wetting, fibre, air-liquid curve, experimental verification.*

Introduction

The Wilhelmy method is one of the most important for the determination of wetting parameters. It is often used for the determination of liquid surface tension. The principal is based on the use of a thin plate immersed in a test liquid. On both sides of the plate a meniscus is created; the shape and maximum height of the liquid that rise along the plate are given by the Laplace equation. The force acting on the plate immersed in the liquid has the following value (1).

$$F = p\,\gamma_{LG} \cos\theta - \rho\, g\, A\, d \qquad (1)$$

where,
p - plate perimeter, m
γ_{LG} - surface tension of the liquid, $N.m^{-1}$
θ - contact wetting angle, deg
ρ - liquid density, $kg.m^{-3}$
A - area of plate base, m^{-2}
d - height of immersion, m

If the end of the plate is placed at the liquid level, then the following relationship of force F is valid(2).

$$F = p\,\gamma_{LG} \cos\theta \qquad (2)$$

The principal of this method is used for measuring the contact wetting angles of fibres immersed in liquid.

Figure 1 presents the inter-phase of the liquid-fibre-air system, which is described by equations (3) to (11). Equation (11) presents the relationship of the geometry of the liquid surface, which was developed and solved by a numerical method (see equation (12) to (16)).

The Young-Dupree equation created based on analysis (3) [5].

$$p = \gamma_{LG} \left(\frac{1}{R_1} + \frac{1}{R_2} \right) \qquad (3)$$

where,
p - Laplace pressure, Pa,

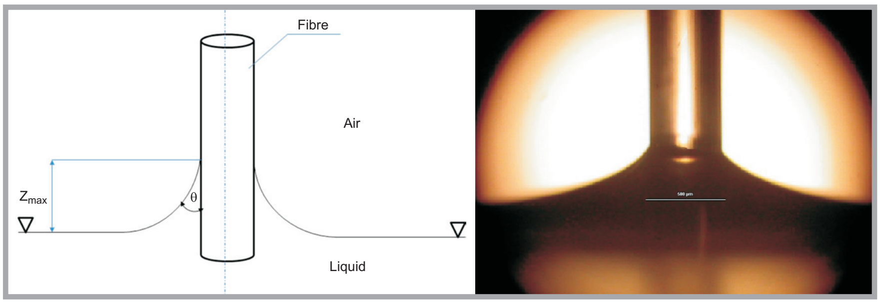

Figure 1. *Scheme of the fibre-liquid-air 3-phase system (a) and photograph of a fibre immersed in a liquid (b), according to [4]; Z_{max} - maximum height of the ascenting liquid, m, θ - contact wetting angle, deg.*

γ_{LG} - Liquid surface tension, N m^{-1},
R_1, R_2 - radii of the curvature, m (see ***Figure 2***).

For a liquid in a static state, the pressure at each point of the liquid is given by equation (4) [6].

$$p = \rho\, g\, z \qquad (4)$$

where,
p - hydrostatic pressure, Pa,
ρ - liquid density, kg m^{-3},
z - height, m.

By substituting equation (4) into eq. (3), we obtain equation (5) [5].

$$\left(\frac{1}{R_1} + \frac{1}{R_2} \right) = k \quad z \qquad (5)$$

where,
k is a constant given by equation (6).

$$k = \rho\, g / \gamma_{LG} \qquad (6)$$

For determination of the radius of curvature R_1, equation (7) was used [1].

$$R_1 = \frac{\left(1 + z'^2\right)^{\frac{3}{2}}}{z''} \qquad (7)$$

z' - first derivative of parameter z

z'' - second derivative of parameter z

The radius of curvature R_2 is based on the definition of Meusnier´s theorem [1], according to which:

$$R_2 = \frac{r}{\cos(\vartheta)} \qquad (8)$$

where,
θ - angle between the normal cut of the plane of a radius described by curvature R_2 and the horizontal level, deg

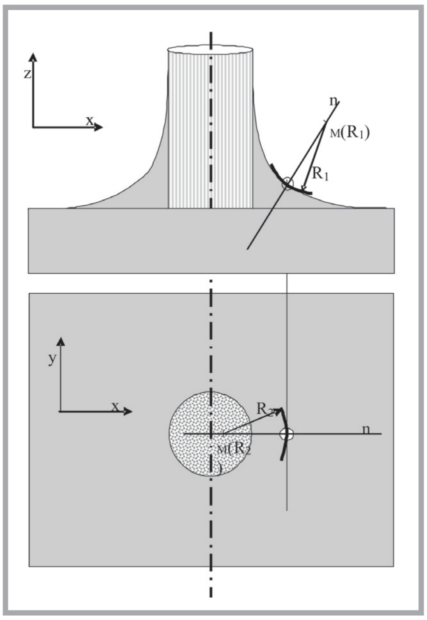

Figure 2. *Scheme of the geometry of the liquid-solid system with radii R_1 und R_2; n - normal to the curvature, M - centre of the curvature radius.*

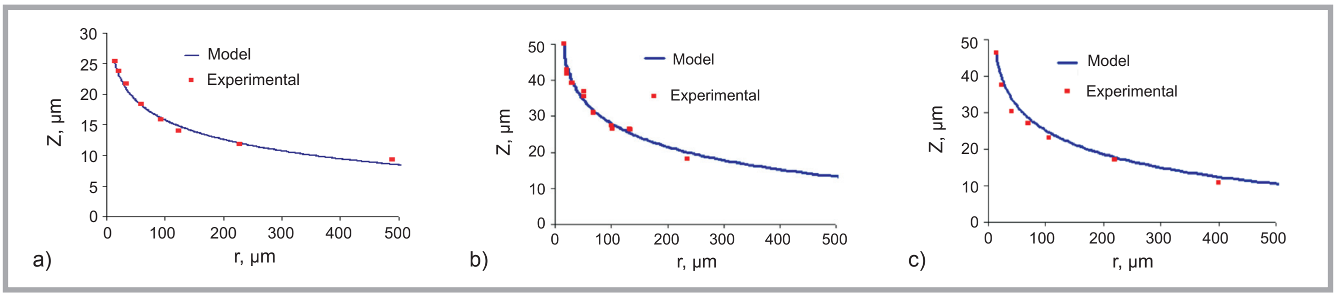

Figure 3. *Model (step 1 µm) and experimental data for the meniscus shape of the distilled water (a), heptane (b) and diiodomethane (c) – interaction system with PES fibre.*

r - horizontal distance from the fibre axis, m

From a geometrical point of view, relationship (9) is valid.

$$\cos(\vartheta) = \sin(\alpha) = \frac{z'}{\sqrt{1+z'^2}} \quad (9)$$

where,

α - angle between the tangent and the cut of the plane of a radius described by curvature R_2 and the horizontal level, deg

After the substitution of equation (9) into equation (8) we obtain relationship (10).

$$\frac{1}{R_2} = \frac{z'}{r\sqrt{1+z'^2}} \quad (10)$$

The differential equation sought arises from the substitution of equations (10) and (6) into eq. (4). Equation (11) presents the final relationship.

$$\frac{z''}{\left(1+z'^2\right)^{\frac{3}{2}}} + \frac{z'}{r\sqrt{1+z'^2}} = k\ z \quad (11)$$

Euler's numerical method was used to solve this differential equation.

Table 1. *Input parameters for the numerical solution of equation (11).*

Parameter	Polyester distill water	Polyester Heptane	Polyester Diiodomethane
Contact angle θ, deg	69.50	29.50	42.30
Fiber diameter r_1, µm	14.25	15.25	14.20
Maximal liquid height Z_{max}, µm	25.40	50.00	46.20
Liquid surface tension γ_{LG}, mN m^{-1}	72.80	20.40	50.80

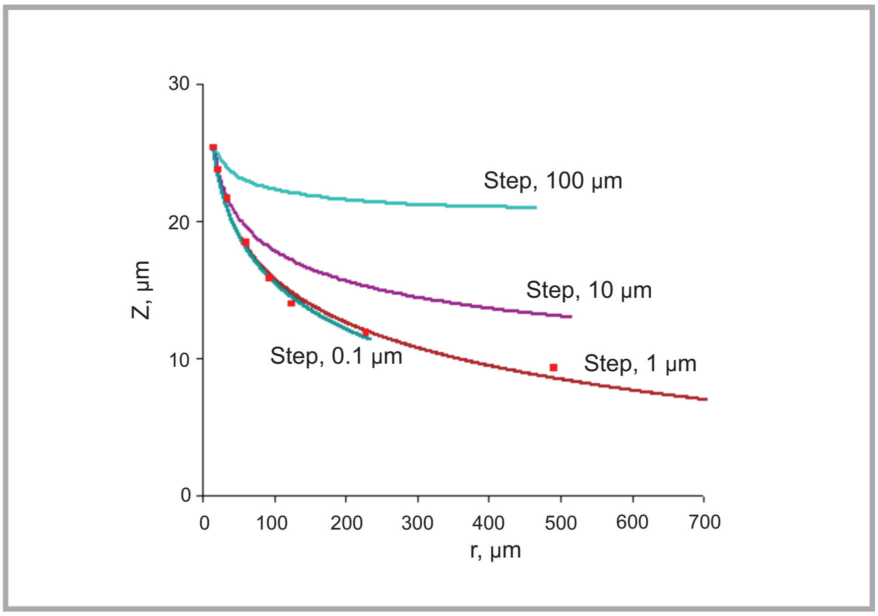

Figure 4. *Models with different steps and experimental data for the meniscus shape of the distilled water system in the contact with PES fibre.*

Figure 2 illustrates the geometry of the liquid-solid system with both radii of the curvature.

Description of Euler's method

The system is given by equation (12) [2].

$$\frac{dy}{dx} = f(x,y) \quad (12)$$

The initial conditions give the solution at point x_0, and subsequently the solutions for points $x_1, \ldots, x_n$ are calculated. The value for point x_{i+1} will be found by the linearisation of the function at point x_i. It can be stated that $h_i = x_{i+1} - x_i$, hence relationship (13) is then valid.

$$y_{i+1} \approx y_i + h_i \left.\frac{dy}{dx}\right|_{x_i} = \\ = y_i + h_i\ f(x_i, y_i) \quad (13)$$

The procedure used to solve differential equation (11) is described by the three equations mentioned below - (14), (15) and (16).

$$z_i'' = \left[1+z_i'^2\right]\left[k\ z_i\sqrt{1+z_i'^2} + \frac{z_i}{r_i}\right] \quad (14)$$

$$z'_{i+1} = z_i' + h\ z_i' \quad (15)$$

$$z_{i+1} = z_i' + h\ z_i' \quad (16)$$

Results and discussion

Examples of liquid meniscus simulation at the inter-phase with polyester fibre are illustrated in ***Figures 3.a, 3.b*** and ***3.c***. Simulated values are compared with the experimental.

Euler's method was also used for the calculation of parameter z. Short steps were chosen (10^{-6} m) in order to achieve high precision. ***Figure 3.c*** shows a comparison of liquid curves for different steps. Particular parts of derivations 2, 1 and 0

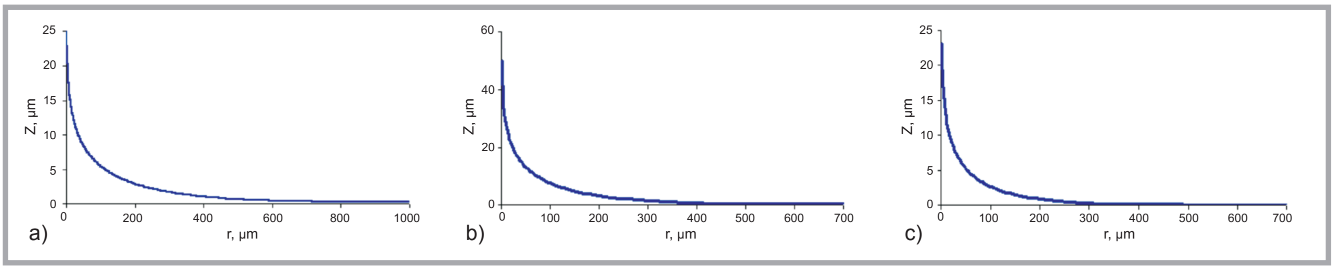

Figure 5. Behaviour of the PES – liquid model: a) water 10 mm distant from the fibre wall, b) water 7 mm distant from the fibre wall, c) diiodomethane model 7 mm distant from the fibre wall.

are calculated in the sequence according to equation (13).

Simulation of the liquid shape in contact with polyester fibre

Values of the input parameters are listed in ***Table 1***.

The solution of the analytically determined differential equation fits very well with the experimental liquid shape. The experimental work was carried out using the measurement equipment described in [7], allowing to make a comparison of the residual variability [3] with the measured variability for experimental and simulated values (***Tables 2, 3, 4***). In ***Figure 3.c*** experimental and simulated values of the meniscus shape of distilled water and polyester fibre are compared.

Figure 4 shows the dependence of the meniscus shape on the step. Lower steps fit better to the experimental values. After analysing the step, 10^{-6}m was found as optimal.

Figures 3.b and ***3.c*** illustrate other examples – polyester fibre in contact with heptane and diiodomethane. The behaviour of the model at high distances from the fibre wall is characterised in ***Figures 5***.

Table 2 presents a variability analysis of the interaction between PES-fibre and distilled water. A variability analysis of the other examples is presented in ***Tables 3*** and ***4*** (heptane with PES-fibre and diiodomethane with PES-fibre). The residual and measured variabilities are, in all cases, very similar, hence it can be stated that good model precision was achieved.

A control was obtained with the purpose of comparing the surface force calculated, according to (14), with that obtained from the model. The integration was made at such a distance from the fibre wall that a horizontal line would

Table 2. *Variability of the interaction of polyester fibre – distilled water; r - distance from fibre wall in m, Ze - experimentally determined liquid height in m, Zm - liquid height calculated from the model.*

r, μm	Ze, μm	Zm, μm	Square residuum, μm²	Variability, μm²
14.25	25.41	25.4	0	0
20.95	23.80	23.5	0.0688	0.0103
34.36	21.74	20.9	0.6696	0.1610
59.50	18.43	18.3	0.0186	0.2000
93.58	15.91	16.2	0.0637	0.0200
123.2	14.00	14.9	0.7460	0.1830
228.0	11.90	12.0	0.0148	0.1330
490.0	9.30	8.6	0.5384	1.9600
Sum, μm²			**2.1198**	**-**
Residual variability, μm²			**0.3028**	**-**
Average variability, μm²			**-**	**0.3329**

Table 3. *Variability of the interaction of polyester fibre – heptane.*

r, μm	Ze, μm	Zm, μm	Square residuum, μm²	Variability, μm²
15.3	50.0	50.0	0	0
20.7	42.8	43.4	0.449	0.374
29.3	39.1	40.0	0.770	0.642
30.6	39.0	39.6	0.389	0.324
51.0	36.9	34.5	5.880	0.490
51.4	35.4	34.3	1.140	0.953
66.8	31.0	31.7	0.529	4.410
68.1	30.9	31.6	0.464	3.870
100.2	27.4	27.9	0.236	1.970
101.2	26.5	27.8	1.830	1.520
132.8	26.3	25.2	1.190	0.995
134.2	26.2	25.2	1.140	0.875
235.0	18.1	20.0	3.550	2.730
Sum, μm²			**17.5695**	**-**
Residual variability, μm²			**1.3515**	**-**
Average variability, μm²			**-**	**1.4734**

Table 4. *Variability of the interaction of polyester fibre – diiodomethane.*

r, μm	Ze, μm	Zm, μm	Square residuum, μm²	Variability, μm²
14	4.62	46.2	0	0
24	3.75	39.3	3.1664	45.5
40	3.04	33.9	12.7287	7.38
70	2.71	28.5	1.8527	22.3
107	2.32	24.4	7.2394	5.11
220	1.70	17.7	30.5993	9.33
400	1.08	12.4	21.3833	8.66
Sum, μm²			**76.9698**	**-**
Residual variability, μm²			**12.8283**	**-**
Average variability, μm²			**-**	**14.04**

Table 5. Comparison of simulated and analytically calculated surface force with the simulated surface force.

Liquid	Simulated surface force, mN	Analytically calculated surface force, mN	Difference, %
Water	2.2595	2.2853	1.13
Heptane	1.8343	1.8674	1.77
Diiodomethane	3.2757	3.3518	2.27

not arise. 10 mm (***Figure 5.a***) and 7 mm (***Figures 5.b*** and ***5.c***) were chosen as examples. The differences determined can be considered as a very good match – under 3% (***Table 5***).

$$F = 2 \pi r \gamma_{LG} \cos \theta \qquad (14)$$

where,
F - wetting force, N m^{-1}
θ - contact angle, deg

The simulated surface force was determined by the integration of the liquid curve.

The analytically calculated surface force was calculated from equation (14).

Conclusion

Based on the analytical description, a differential equation, which was solved by Euler's numerical method, was found. Before solving the initial condition, the contact angle, maximal liquid height and liquid density were determined.

The model's precision was checked and confirmed after detailed analysis of variability. Comparison of the analytically calculated surface force and simulated surface force was the second checking procedure. The model fits well experimental values, as the differences achieved in all cases are within the range of 1.1 to 2.3%.

Knowledge of the meniscus shape has significant importance for further research of the wetting phenomena, hence the model established is of great benefit.

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