Application of polynomial approximation method to water drop evaporation

Nina Bogdanova and Stefan Todorov

Institute of Nuclear Research & Nuclear Energy, BAS, Bulgaria
Email: nibogd@inrne.bas.bg, stef2006t@inrne.bas.bg

The paper proposes a new application of our orthonormal polynomial expansion method-OPEM[1], based on Forsythe three term relation[2]. Some special features of the method are developed for this purpose.

1.PHYSICAL DATA

Up to now the wetting properties of liquids present a high interest for research. This is not only because of the various applications in industry, but also due to some unsolved topics in the theory of liquid wetting [3].

Here we discuss the kinetics of the wetting angle of water drop of deionized water placed on a non wettible substrate (hostaphan). In the course of evaporation of the drop, as the drop’s contact angle changes, we measure the frequency of appearance f(θ) of such angles θ within prescribed angle intervals. One can say that in this way the “state spectrum” with respect to the contact (wetting) angle is obtained of the corresponding thermodynamically open system.

For this purpose one measures at regular time intervals (here every 2 minutes) the values for several drops (to enable drawing statistical conclusions). In this way one obtains a set of discrete values {f(θi), i=1,2..} – the frequencies of occurrence of θ.

One determines θ by microscope observations using the optical method of Antonov [4].

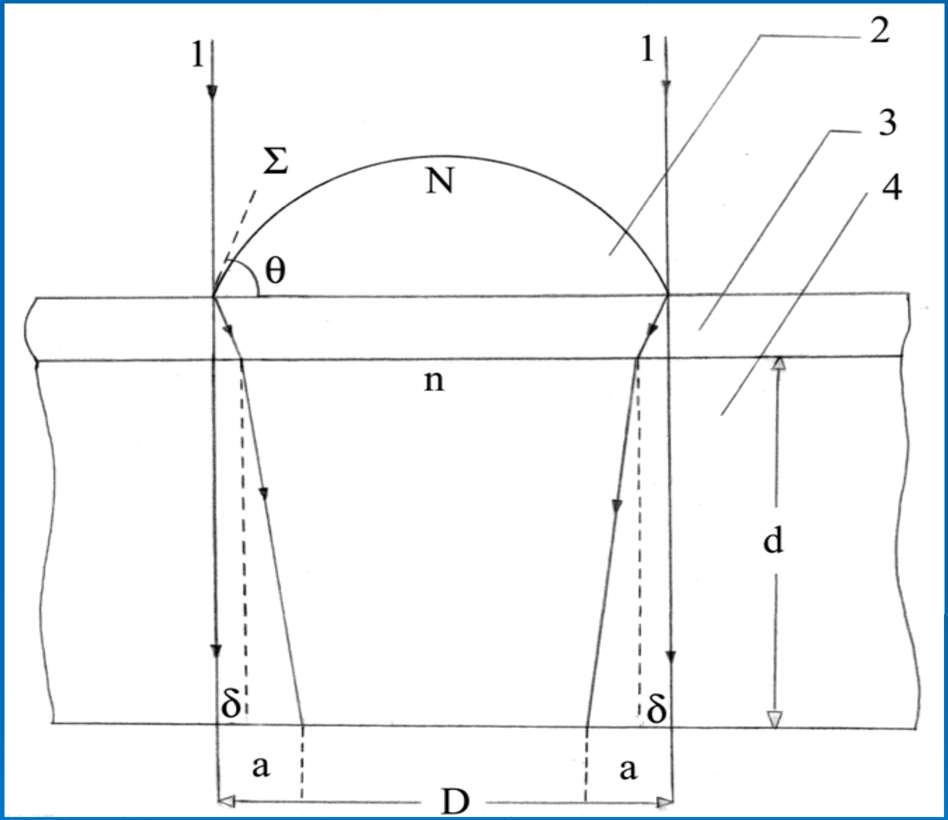

Figure 1.Experimental setup of contact water angle measurement-the water drop and the substrate with the light beam passing trough the drop and producing the light pattern

- One measures the width of a light refraction pattern in the form of a dark ring produced around the drop (Fig.1) by light beams 1 passing near the boundary of the drop 2 which is situated on the non wetting folio 3 and kept at a constant room temperature. The folio is situated on a glass plate 4 having a refraction index **n** and thickness **d**. The width **a** is measured by microscope observations. The laws of geometric optics give **tg(θ)** as a function of **a** by the formula:
- $tg(\theta) = n/[(N^2\Delta - n^2)^{1/2} - \Delta]^{1/2}$; $\Delta = 1 + d^2/(a-\delta)^2$,
- where **N** is the water refraction index and the dimension **δ** denoted on. Fig. 1 is usually neglected in the above formula since **δ<<a** .

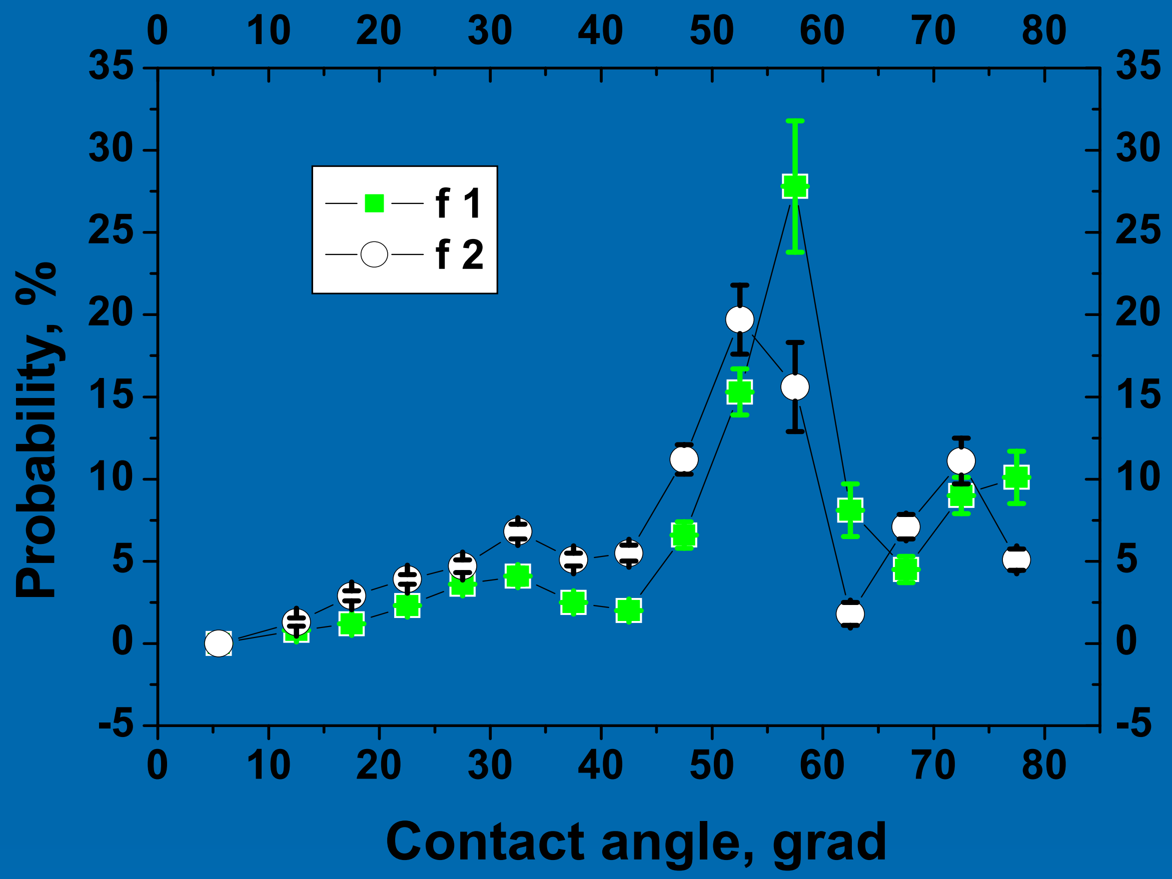

Figure 2. Experimental probability (in %) of contact angle of deionized treated (squares) f1 and non treated f2 (circles) water data (with experimental errors)during the evaporation

The circles correspond to non treated water sample. The squares - to treated by **γ - rays**. The source of **γ** rays is Co- 60(65 krad/h). The period of treatment - 2 minutes.

2.Mathematical method. Generalized OPEM.

Consider [5] [6] (as Bevington) the square of total uncertainty (total variance) $S^2(\theta, f)$ associated with (θ, f) and their errors

$$(2) \quad S^2(\theta, f) = \sigma^2(f) + (\partial f / \partial\theta)^2 \sigma^2(\theta)$$

$$(3) \quad [f - S(\theta, f), f + S(\theta, f)]$$

$$(4) \quad [f - \sigma(f), f + \sigma(f)]$$

1. The first criterion - the fitting curve passes within the errors corridors (4) or (3).
2. The second criterion –the fitting curve minimizes the (5):

$$(5) \quad \chi^2 = \Sigma_{i=1}^{M} [f^{appr}(\theta_i) - f(\theta_i)]^2 / S^2(\theta_i, f_i)$$

(6) $$f^{(m)appr}(\theta) = \sum_{i=1}^{L} a_i P_i^{(m)}(\theta) = \sum_{i=1}^{L} c_i \theta^i$$

(7) $$a_i = \sum_{k=1}^{M} f_k w_k P_i^{(m)}(\theta_k)$$

(8) $$P_{i+1}^{(m)}(\theta) = \gamma_{i+1}[(\theta - \mu_{i+1}) P_i^{(m)}(\theta) - (1 - \delta_{io}) v_i P_{i-1}^{(m)}(\theta) + m P_i^{(m-1)}(\theta)]$$

Ref .[7] and [8] for inherited errors in $\{a\}$ and $\{c\}$.

(9) $$\Delta a_i = (\sum_{k=1}^{M} P_i^2(\theta_k) w_k (f_k - f_k^{appr}))^{1/2}, \quad \Delta c_i = (\sum_{k=i}^{L} (c^{(k)}{}_i)^2) \Delta a_i$$

where coefficients $c^{(i)}{}_k$ **are defined explicitly in [7].**

The second criterion for the fitting curve $f^{appr}(\theta)$ is that the expression (5) should be minimal:

(5) $$\chi^2 = \sum_{i=1}^{M} [f^{appr}(\theta_i) - f(\theta_i)]^2 / S^2(\theta_i, f_i).$$

More detailes of the calculational procedure are given in Bogdanova and Todorov (2001).

Our procedure gives results for approximating function by two expansions: of orthogonal $\{a_i\}$, and usual coefficients $\{c_i\}$ (calculated from orthogonal) with optimal degree L:

(6) $$f^{(m)appr}(\theta) = \sum_{i=1}^{L} a_i P_i^{(m)}(\theta) = \sum_{i=1}^{L} c_i \theta^i .$$

The orthogonal coefficients are evaluated by the given values f_k, weights and orthogonal polynomials:

(7) $$a_i = \sum_{k=1}^{M} f_k w_k P_i^{(m)}(\theta_k).$$

The main three-term recurrence relation for generating orthonormal polynomials and their derivatives (m=1,2…) are carried out by:

(8) $$P_{i+1}^{(m)}(\theta)=\gamma_{i+1}[(\theta-\mu_{i+1})P_i^{(m)}(\theta)-(1-\delta_{io})\nu_i P_{i-1}^{(m)}(\theta)+mP_i^{(m-1)}(\theta)],$$

where μ_i and ν_i are recurrence, and γ_{i+1} is a normalizing coefficient.

The inherited errors in usual coefficients are given by the inherited errors in orthogonal coefficients by $\Delta c_i=(\sum_{k=i}^{L}(c_i^{(k)})^2)^{1/2}\Delta a_i$,

where coefficients $c_i^{(k)}$ are defined explicitly in [7] and

(9) $$\Delta a_i=(\sum_{k=1}^{M}P_i^2(\theta_k)w_k(f_k-f_k^{appr})^2)^{1/2}.$$

Two criteria are used to select the optimum series length in Eq.(6) in the next steps:
First, the fitting curve lies:
i) inside the error corridor with $\sigma(f)$

$$[f-\sigma, f+\sigma]$$

ii) and after calculating derivatives the fitting curve has to lie inside big corridor with $S(\theta, f)]$

$$[f-S, f+S].$$

2) Second, we extend the above algorithm OPEM to include the total version **S** in OPEM in two stages:

(i). Here one neglects the errors in **θ** variable, i.e. the chi –squared (5) is minimized, using as weights

$$1/\sigma^2(f).$$

(ii) The chi- squared (5) is minimized, using as weights the

$$1/S^2(\theta, f).$$

The preference is given to the first criterion and when it is satisfied, the search for the minimal chi-squared stops. The procedure is iterative and the result of the consequtiente **k** - th iteration, **k>**1, is called below the **k**-th approximation (see [7][8]) **.**

3.Approximation results.
(i) Non treated deionized water data.

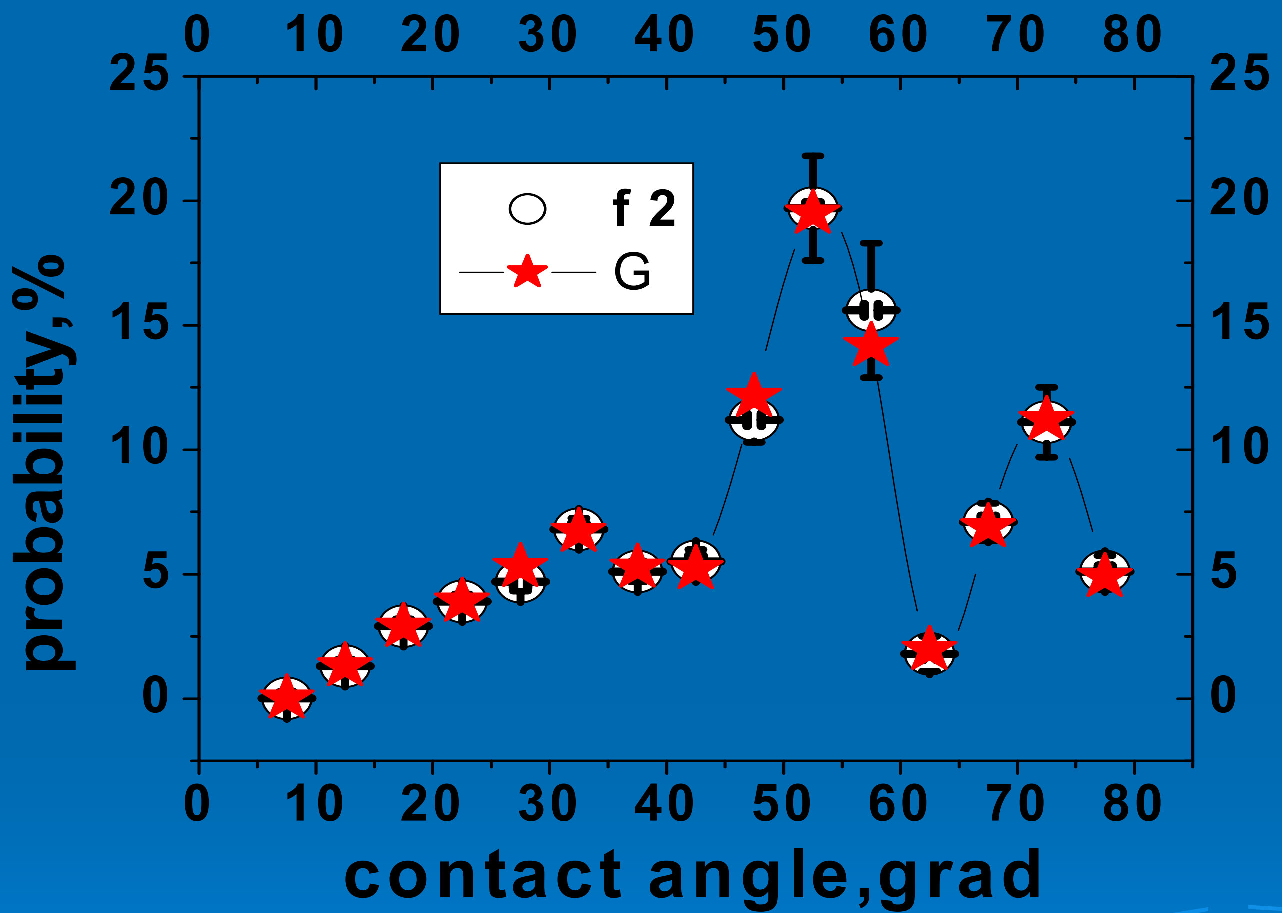

Figure 3. *The OPEM approximation G by 11-th degree polynomials (stars) of contact angle probability for non treated deionized water (circles) f2*

(ii) Treated deionized water data

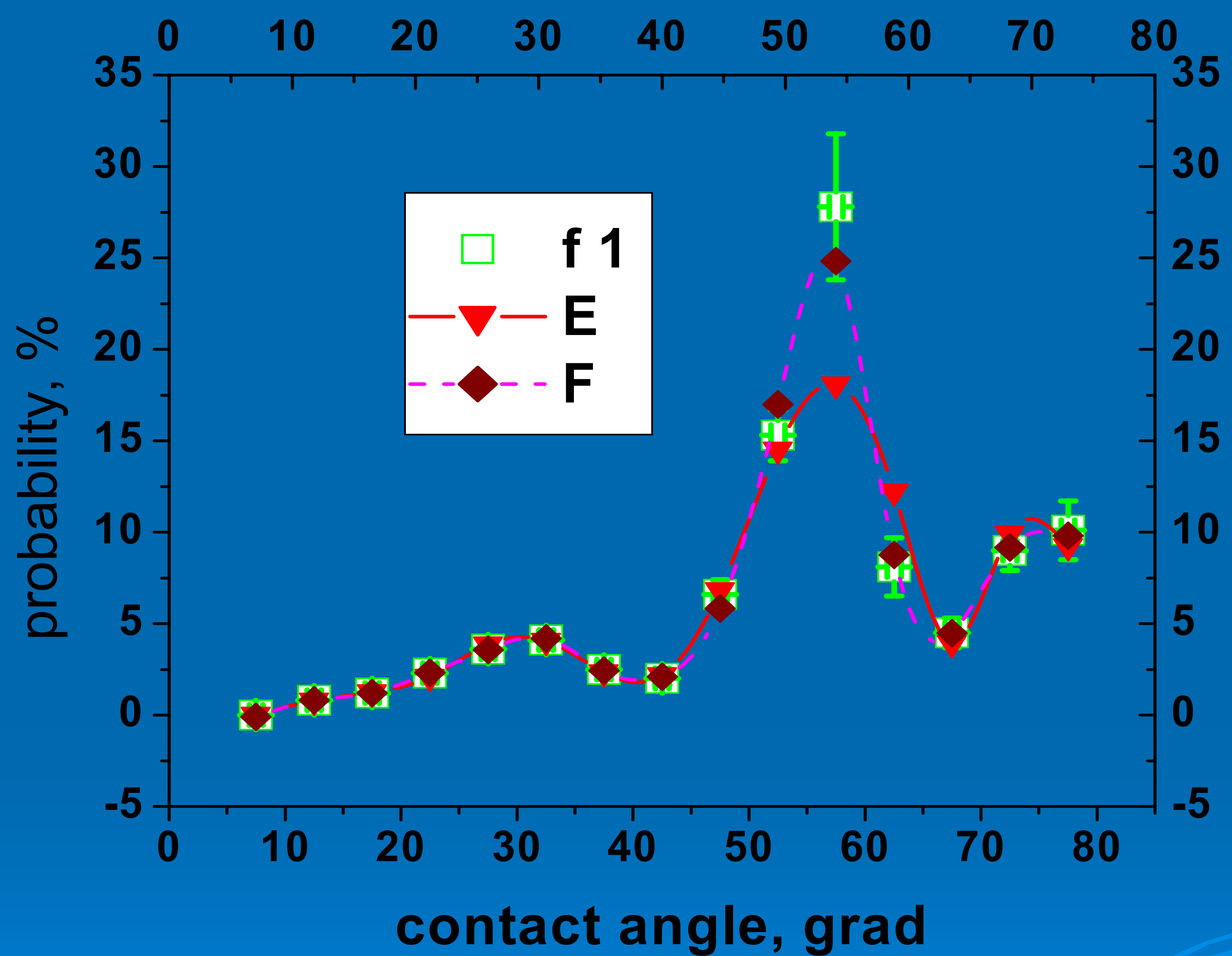

Figure 4. *The OPEM approximation E by 9-th (triangles) and 13-th degrees polynomials (rhombs) F of contact angle probability for treated deionized water f1 (squares)*

Table 1: *OPEM approximation of contact water angle-given and approximating values*

No	θ	f	$\sigma(\theta)$	$\sigma(f)$	$f^{appr,9(a_k)}$	$f^{appr,9(c_k)}$	$f^{appr,13(a_k)}$
1	7.5	0.1	0.6	0.001	0.01380	0.01381	0.10468
2	12.5	0.8	0.6	0.200	0.78957	0.78957	0.81378
3	17.5	1.2	0.6	0.250	1.23899	1.23927	1.19310
4	22.5	2.3	0.6	0.350	2.08552	2.08592	2.30828
5	27.5	3.6	0.6	0.400	3.80385	3.86199	3.55922
6	32.5	4.1	0.6	0.540	0.05056	4.04787	4.19897
7	37.5	2.5	0.6	0.320	0.34706	2.34459	2.43052
8	42.5	2.0	0.6	0.350	2.17360	2.16459	2.09021
9	47.5	6.6	0.6	0.860	6. 82522	6.79850	5.83620
10	52.5	15.3	0.6	1.400	14.51524	14.49400	16.98400
11	57.5	27.8	0.6	4.000	18.08124	18.02445	24.82427
12	62.5	8.1	0.6	1.600	12.22944	12.12178	8.76558
13	67.5	4.5	0.6	0.800	3.92818	3.71804	4.37418
1 4	72.5	9.0	0.6	1.100	9.91328	9.81663	9.16343
15	77.5	10.1	0.6	1.600	9.23731	9.23587	9.10499

Conclusions

The approximating results with optimal degrees of OPEM orthonormal polynomials for contact wetting angle founded by orthogonal and usual coefficients show good accuracy, demonstrated from Figures 3 and 4 and Table 1(3rd iteration step). The approximating curves are chosen to satisfy the proposed criteria (3),(4) and (5). We have received good descriptions of the angle variations useful for further physical and mathematical investigations.

References:

1. Bogdanova N., *J .Comp. Appl. Mathem.*,14, (1986), 345.
2. Forsythe G., *J Soc. Ind. Appl. Mathem.*, 5, 74, (1957).
3. Bonn, D., D. Ross, Wetting transitions, *Rep. Progr. Phys*. ,64 (2001) 1085.
4. Antonov, A., *Comptes Rendus de l'Academie bulgare de Sciences*, 37, 1199 (1984).
5. Bevington P. R., Data Reduction and Error Analysis for the Physical Sciences, (McGrow-Hill, New York, 1969)
6. Jones G., Preprint TRI-PP-92-31, A(1992).
7. Bogdanova N., Todorov St., *IJMPC, 12, No.1(2001)pp.117-127.*
8. Bogdanova N., *Commun.JINR, Dubna,* E11-98-3(1998).