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Application of Polynomial Approximation Method to Drop Water Evaporation

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In the paper our method for construction of orthonormal polynomials — orthonormal polynomial expansion method [OPEM] — is applied to water contact angle variations. Some special features of the method are developed for this purpose. The total variance method is demonstrated to include the errors in both dependent and independent variables. Two polynomial expansions are presented for approximating function: orthonormal and "usual" ones.

Key words and phrases: orthonormal and usual polynomial approximation, drop water evaporation.

1. Introduction

The phenomena related to liquid-solid contact are at present intensively investigated. This is not only because of the various applications, but due to some unsolved problems in the theory of contact between different phases [1]. Here we discuss the kinetics of evaporation of water drop of deionized water. In the course of evaporation of the drop, as the drop's contact angle changes, we measure the frequency of appearance of such angles within prescribed angle intervals.

2. Physical Data

The experimental data consist of the collection of measured contact angles ϑ of an evaporating water drop. We register the frequencies f of occurrence of these contact angles contained in a given set of adjusted angle intervals. One can name these frequencies of contact angles as the "state spectrum" of the evaporating drop. The measurement is performed at equidistant time intervals (5 minutes). We use data from several drops measured simultaneously to have a statistical ensemble for calculating mean values and standard deviations. The measurement of the contact (wetting) angle is carried out by an optical microscope method due to Antonov [2]. In more details, (Fig. 1) a light refraction pattern in the form of a dark ring occurs when a light beam 1 crosses the drop 2, placed on a non wetting folio 3 (hostaphan), near its boundary. Under the folio there is a glass plate 4 with a thickness d and a refraction index n. One measures the width a of the dark ring thus produced. According to the laws of geometric optics one can calculate the tangens of contact angle as a function of the above cited parameters as follows: here N is the water refraction index and the segment denoted by δ on Fig. 1 can be neglected since $\delta \ll a$. We give below a graphs on which the frequencies f are shown versus the collection of measured contact angles. We present one type of such curves that corresponds to the water treated by the gamma rays of a source of Co-60 (65 krad/h) for a time of 2 minutes (Figure 2-circles).

$$\operatorname{tg}\vartheta = n/\left[\left(N^2\Delta - n^2\right)^{12} - \Delta\right]^{1/2}; \quad \delta = 1 + d^2(a-\delta)^2,$$

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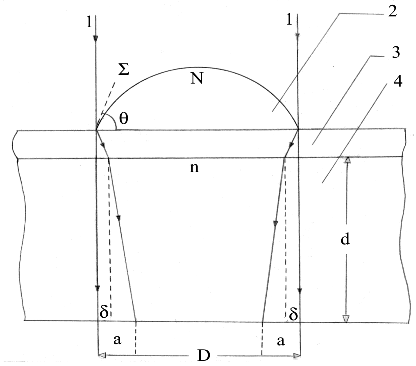

Figure 1. **Experimental setup**

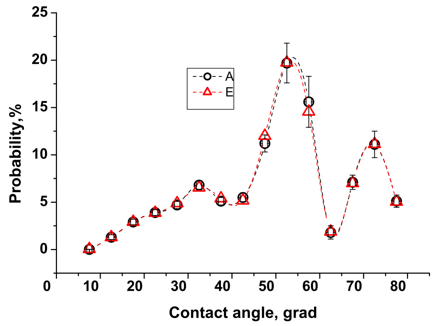

Figure 2. **OPEM approximation by 11-th degree orthonormal polynomials (triangles) of deionized treated water data(circles)**

3. Mathematical Algorithm

Define by $\{\vartheta_i, f_i\}$ arbitrary pairs of monitoring data $\vartheta = \vartheta_i$ and $f = f_i$, $i = 1, \ldots, M$, introduced in section 2. We have also the experimental errors in both variables — σ_{f_i} and σ_{ϑ_i}. Consider the square of total uncertainty (total variance) $S(\vartheta, f)$, associated with (ϑ, f)

$$S_i^2 = {\sigma_{f_i}}^2 + \left(\frac{\partial f_i}{\partial \vartheta_i}\right)^2 {\sigma_{\vartheta_i}}^2, \tag{1}$$

according the ideas of Bevington (1977) [3], where his proposal is to combine the errors in both variables and assign them to dependent variable. One defines the errors corridor $C(\vartheta, f)$, which is the set of all intervals

$$\left[f(\vartheta) - S(\vartheta, f), f(\vartheta) + S(\vartheta, f)\right], \tag{2}$$

associated which each pair (ϑ, f). The first criterion to be satisfied is, that the fitting curve should pass within the errors corridor $C(\vartheta, f)$. In the cases of errors only in f, (i.e. $\sigma(\vartheta) = 0, \sigma(f) \neq (0)$) the errors corridor $C(\vartheta, f)$ reduces to the set of intervals

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

for any f. The second criterion for the fitting curve $f^{\mathrm{appr}}(\vartheta)$ is, that the expression

$$\chi^2 = \sum_{i=1}^{M} w_i \left[f^{\mathrm{appr}}(\vartheta_i) - f(\vartheta_i)\right]^2 / S^2\left(\vartheta_i, f_i\right) \tag{3}$$

should be minimal. Some details of our calculation procedure are presented in our papers [4–6].

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

$$f^{(m)}(\vartheta) = \sum_{k=0}^{L} a_k P_k^{(m)}(\vartheta) = \sum_{k=0}^{L} c_k \vartheta^k.$$

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

$$a_i = \sum_{k=1}^{M} f_k w_k P_k^{(m)}(\vartheta_k).$$

Our recurrence relation for generating orthonormal polynomials and their derivatives $(m = 1, 2, \ldots)$ is carried out by:

$$P_{i+1}^{(m)}(\vartheta) = \gamma_{i+1}\left[(\vartheta - \mu_{i+1})\, P_i^{(m)}(\vartheta) - (1-\delta_{i0})\,\nu_i P_{i-1}^{(m)}(\vartheta) + mP_i^{(m-1)}(\vartheta)\right],$$

where μ_i and ν_i are recurrence coefficients, and γ_i is a normalizing coefficient, defined by scalar products of given data. One can generate $P_i^m(\vartheta)$ recursively. The polynomials satisfy the following orthogonality relations:

$$\sum_{i=1}^{M} w_i P_k^{(0)}(\vartheta_i)\, P_l^{(0)}(\vartheta_i) = \delta_{k,l}$$

over the discrete point set $\{\vartheta_i, i = 1, 2, \ldots\}$, where $w_i = 1/S^2(\vartheta_i, f_i)$ are the corresponding weights. The inherited errors in usual coefficients are given by the inherited errors in orthogonal coefficients:

$$\Delta c_i = \left(\sum_{k=1}^{L} \left(c_i^k\right)^2\right)^{1/2} \Delta a_i,$$

where coefficients c_i^k are defined explicitly in [6] and

$$\Delta a_i = \left(\sum_{k=1}^{M} P_i^2(\vartheta_k)\, w_k \left(f_k - f_k^{\mathrm{appr}}\right)^2\right)^{1/2}.$$

All the calculations for the sake of uniformity are carried out for ϑ in $[-1, 1]$, i.e. after the input interval is transformed to the unit interval. We remark some advantages of OPEM: It uses unchanged the coefficients of the lower-order polynomials; it avoids the procedure of inversion of the coefficient matrix to obtain the solution. The preference is given to the first criterion and when it is satisfied, the search for the minimal chi-squared stops. All these features shorten the computing time and assure the optimal solution (by the criteria (2), and (3)). The procedure is iterative because of the evaluation of derivatives on every iteration step and the result of the consequent k^{it}-th iteration is called below the k^{it}-the approximation. The similar algorithm is given as “effective variance method” from Jones [7] and the solution is discussed in the other papers, [8] Lybanon.

4. Approximation Results. Treated Deionized Water Data

The numerical experiment is carried out for $M = 15$ points data of water, treated by γ rays and containing measurement errors in both variables. We approximated them with the polynomial curve of optimal degree $L = 11$, chosen between 2 to 14 with chi-squared= 0.64011. The iteration step is $k^{\mathrm{it}} = 4$. If $k^{\mathrm{it}} = 1$, chi-squared is 0.82612, if $k^{\mathrm{it}} = 2$, chi-squared is 0.64942, if $k^{\mathrm{it}} = 3$, chi-squared is 0.64014. On the Fig. 2 we present the given data (circles) with their errors and the approximated data by orthonormal polynomials (triangles). Here two types of data are enough close.

In the Table 1 the given and approximated data by orthonormal and usual expansions with 10-th degree of polynomials are presented. In the last column the deviation

$$\Delta\,(f_a^{\mathrm{ap}} - f_c^{\mathrm{ap}}) = f_a^{\mathrm{appr},10} - f_c^{\mathrm{appr},10}$$

is given. In the most points the two approximations are close till 3-rd meaningful digit.

Table 1

OPEM approximation of contact water angle data

No.	ϑ	f	σ_ϑ	σ_f	$f_a^{\mathrm{appr},10}$	$f_c^{\mathrm{appr},10}$	$\Delta(f_a^{\mathrm{ap}} - f_c^{\mathrm{ap}})$
1	7.5	0.01	0.6	0.001	1.15489	1.15349	0.01400
2	12.5	1.30	0.6	0.25	0.76497	0.76102	0.00395
3	17.5	2.90	0.6	0.30	3.13892	3.12845	0.01047
4	22.5	3.90	0.6	0.30	3.22969	3.20843	0.02126
5	27.5	4.70	0.6	0.38	5.84499	5.80593	0.03906
6	32.5	6.80	0.6	0.45	6.36952	6.29145	0.07807
7	37.5	5.10	0.6	0.40	4.79228	4.68782	0.10447
8	42.5	5.50	0.6	0.48	6.33505	6.16855	0.16650
9	47.5	11.20	0.6	0.90	12.03489	11.88760	0.14729
10	52.5	19.70	0.6	2.10	15.21490	15.19192	0.02298
11	57.5	15.60	0.6	2.70	10.17058	9.77367	0.39692
12	62.5	1.80	0.6	0.70	2.89065	2.57517	0.31548
13	67.5	7.10	0.6	0.75	5.50987	6.65696	-1.14709
14	72.5	11.10	0.6	1.40	11.74320	12.53682	-0.79362
15	77.5	5.10	0.6	0.66	5.06331	6.50434	-1.44104

In conclusion, the approximating results with optimal degrees of OPEM orthonormal polynomials for contact (wetting) angle found by orthogonal and usual coefficients show good accuracy, demonstrated from Fig. 2 and Table 1. The approximating curves are chosen at $4-th$ approximation step to satisfy the proposed criteria. The results show that the orthonormal and usual expansions are close to given one in the whole interval. We have received good descriptions of the angle variations useful for further investigations.

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Применение метода полиномиальной аппроксимации к испарению капли воды

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В данной работе наш метод построения ортонормированных полиномов — метод расширения ортонормированных полиномов [OPEM] — применяется к изменениям краевого угла смачивания. Для этой цели развиты некоторые особенности данного метода. Демонстрируется метод полной дисперсии, чтобы включить ошибки как в зависимые, так и в независимые переменные. Два расширения полинома представлены для аппроксимирующей функции: ортонормированное и «обычное».

Ключевые слова: аппроксимация ортонормированными и обычными полиномами, испарение капли воды.