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Statistical analysis of vitrinite reflectance data—a new approach

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Abstract

The reflectance of vitrinite (collotelinite) particles is a widely used parameter as a geothermometer for the estimation of the thermal maturity of organic matter enclosed in rocks. However, several problems have occurred during the last decades, which can be traced back to basically three causes: human mistakes, technical problems, and problems associated with the structural and compositional inhomogeneity of organic matter. Whilst in most cases the first two types of uncertainties can be handled by standardization, the third can cause significant problems during interpretation due to its generally inestimable character. The suppression of vitrinite reflectance and statistical problems originated from small sample size, and outliers belong to this latter type.

International standards, such as the ASTM and the ISO, define the vitrinite reflectance parameter as a statistical average of measured data, disregarding the fact that the average is an unresisting and unrobust statistical parameter. In other words, the average is very sensitive to outliers and distribution.

The aim of this research was to find and test a better, more resistant, and robust statistical parameter used by traditional parametric and nonparametric statistics, which can be applied in practice instead of the average. Three categories of statistical problems were studied on coal and disperse organic matter (DOM) samples: the distribution of measured values, the effect of data number, and the effect of outliers on statistical parameters. The statistical experiments carried out on numerous original and generated sample sets show that the median (med) and the most frequent value (Mn), a special weighted average, are better parameters to estimate the thermal maturity of organic matter especially above 1% reflectance value.

Keywords: Vitrinite reflectance; Statistical analysis; Gaussian distribution; Median; MAD

1. Introduction

The best possible establishment of the level of organic matter alteration—maturity —is one of the basic concerns both in coal and in petroleum research. One of the most frequently used maturity parameters is the so-called vitrinite (in case of coal samples, collotelinite) reflectance parameter (ICCP, 1998), which is based on the change of reflection properties of synsedimentary organic matter of terrestrial origin (type III) by structural and molecular alteration (ordering) as a function of mainly temperature and, subordinately, time and pressure (Philippi, 1965; Dow, 1977; Mukhopadhyay and Dow, 1994; Hunt, 1995). Basically, three types of uncertainties arise in the value of collotelinite reflectance during sampling, sample prep-

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Table 1
The factors that influence the value of the parameter R_o (modified after Fedor and Hámor-Vidó, 2000)

	References	Can it be avoided?	Estimated type of the error	Influence on R_o
1. Measurement of the reflectance of another matter mistakable with collotelinite				
1.1. Inclusions inside collotelinite	[1,2]			
1.1.1. Pyrite		Yes	R	+
1.1.2. Bitumen filling up the intergranural space		Yes	R	−
1.1.3. Macerals belonging to other maceral groups		Yes	R	+, −
1.1.4. Other macerals belonging to the vitrinite maceral group		Yes	R	−, +
1.2. Measurement of the reflectance of other macerals mistakable with collotelinite	[1,2]			
1.2.1. Semifusinite		Yes, no	R	+
1.2.2. Pseudovitrinite		Yes	R	+
1.3. Measurement of the reflectance of bitumen	[2]	Yes	R	−
2. Measurement of the reflectance of not "fresh" collotelinite				
2.1. Measurement of the reflectance of allochtonous collotelinite	[2,3]			
2.1.1. Matured allochtonous collotelinites come from erosion of sediments		Yes	R	+
2.1.2. Collotelinite of near-autochthonous resedimented organic matter		Yes	R	+, −
2.1.3. Collotelinite of organic matter fallen back into the well during drilling	[4]	Yes	R	−, +
2.1.4. Collotelinite from additives of drilling mud	[4,5]	Yes	S	+
2.2. Properties of collotelinite change by chemical or physical processes				
2.2.1. Oxidation of collotelinite	[1]			
2.2.1.1. Oxidation due to application of turbo drilling technique (air blowing)	[6]	Yes	S	+
2.2.1.2. Oxidation due to drying sample rapidly	[6]	Yes	S	+
2.2.1.3. Oxidation of allochtonous collotelinite		Yes	R	+
2.2.1.4. Oxidation of collotelinite near the erosion surface	[1,2]	Yes, no	S	+
2.2.1.5. Oxidation of collotelinite by the influence of aggressive acids during preparation		Yes	S	+
2.2.2. Weathering of collotelinite				
2.2.2.1. Weathering of collotelinite near the erosion surface	[2]	Yes	S	−
2.2.2.2. Weathering of allochtonous collotelinite		Yes	R	−
2.2.2.3. Weathering by the influence of meteoric waters[a]	[2]	Yes	S	−
2.2.2.4. Weathering by the influence of mineral waters	[2]	Yes	S	−
2.2.2.5. Weathering by the influence of drilling mud		Yes	S	−
2.2.2.6. Weathering of collotelinite by the influence of aggressive acids during preparation		Yes	S	−
2.2.3. Reflectance of fractured collotelinite				
2.2.3.1. Fractures due to chemical and physical processes in "fresh" collotelinite		Yes	R	−
2.2.3.2. Secondary fractures by the influence of drilling (it depends on the type of bit)		Yes	S	−
2.2.3.3. Fractures from preparation of DOM by jaw crusher		Yes	S	−
3. Uncertainties during measurement of "fresh" collotelinite				
3.1. Suppression of the reflectance of collotelinite	[5,6]			−
3.1.1. Compounds built in the molecular structure of the collotelinite or absorbed				
3.1.1.1. H-rich collotelinite can be found in types I and II kerogen (H-rich vitrinite)		No	R	−
3.1.1.2. Bitumen generated "in situ" during the maturation is absorbed in the surface or built in the molecular structure of the collotelinite		No	R	−
3.1.1.3. Bitumen generated during the maturation of organic matter of other bands is migrated and absorbed in the surface or built in the molecular structure of the collotelinite		No	R	−
3.1.1.4. Compounds absorbed or built in the molecular structure of the collotelinite during preparation, or the influence of treatment by aggressive acids		Yes	S	−
3.1.1.5. Bitumen derived from oil-based muds is absorbed in the surface or built in the molecular structure of the collotelinite		Yes	S	−

Table 1 (*continued*)

	References	Can it be avoided?	Estimated type of the error	Influence on R_o
3.1.2. Fluid film on the surface of the collotelinite derived from high volatile content coals	[7]	Yes	S	–
3.1.3. Influences of the particles that surround collotelinite		Yes	R	+, –
3.1.3.1. Influence of corpogelinite reflectance to R_o [b]		Yes	R	+
3.2. H-poor vitrinite	[8]	No	R	+
3.3. Rough mistakes derived from human inattention				
3.3.1. Possible ordering during bedding to resin (?)		?	S	?
3.3.2. Roughly polished surface of the sample	[6]	Yes	R	–
3.3.3. Pass over a step of polishing (waved surface of the sample)		Yes	R	–
3.4. Corrigible "inaccuracies" of the technical equipment				
3.4.1. Alteration of immersion oil during time	[7]	Yes	S	
3.4.2. Parasite reflectance	[7]	Yes	S	+, –
3.4.3. Unconformity of standards	[9]	Yes, no	S	+, –
3.5. Casual inaccuracies could not be corrected generally				
3.5.1. Random optical orientation of collotelinite particles in thin section	[10]	No	R	?
3.5.2. Size of collotelinite particles is too small		No	R	+, –
3.5.3. Statistical problems				
3.5.3.1. Sample size (the number of measured particles)	[7,11,12]	Yes, no	R	+, –
3.5.3.2. Distribution of measured values	[12]	Yes	–	
3.5.3.3. Choice of good statistics	[12]	Yes	S	+, –
3.5.4. Effect of heterogeneity of vegetation (molecular heterogeneity) [c]	[13]	No	R	+, –
3.5.5. Effect of tectonic stress (uniaxial or biaxial character) [c]	[1,14]	No	S	+

(+) The value of R_o increases; (–) the value of R_o decreases; (R) random; (S) systematic.

[1] Dow (1977); [2] Hunt (1995); [3] Lo (1992); [4] Feazel and Aram (1990); [5] Price and Barker (1985); [6] Buiskool Toxopeus (1983); [7] Taylor et al. (1998); [8] Fang and Jianyu (1992); [9] Dembicki (1984); [10] Kilby (1991); [11] Barker and Pawlewicz (1993); [12] Fedor and Hámor-Vidó (2000); [13] Wild et al. (2000); [14] Hower et al. (1994).

[a] Difference between the reflectance of collotelinite is weathered and reburied previously (2.2.1.4), or weathering now.

[b] Difference between macerals of vitrinite A (used in coal petrography) and vitrinite 1 (used in hydrocarbon research).

[c] Part of statistical problems originated from molecular and structural heterogeneity.

aration, measurements, and interpretation: human problems, for example, measurements other than collotelinite reflectance (Dow, 1977; Taylor et al., 1998) or postsedimentary collotelinite (Dow, 1977; Buiskool Toxopeus, 1983); technical problems (e.g., parasite reflectance or alteration of immersion oil) (Taylor et al., 1998); and uncertainties originating from the molecular and structural inhomogeneity of organic matter (Price and Barker, 1985; Barker and Pawlewicz, 1993; Fedor and Hámor-Vidó, 2000). The degree of molecular and structural inhomogeneity depends on the vegetation diversity (Wild et al., 2000), the circumstances of the burial, and the tectonic events. The summary of possible types of uncertainties is presented in Table 1.

Whilst in most cases the first two types of uncertainties can be handled by standardization (ASTM, 1994; ISO, 1994; ICCP, 1998), the third, due to its generally inestimable character, can cause significant problems during interpretation. The suppression of vitrinite reflectance (Price and Barker, 1985) and statistical problems originating from small sample size and outliers (Barker and Pawlewicz, 1993; Fedor and Hámor-Vidó, 2000; Fedor et al., 2001) belong to this latter type. The handling of the problem of suppression has been partly solved (Lewan, 1993; Lo et al., 1997; Wilkins et al., 2002), but the statistical basis of parameter estimation, in spite of the directives of parameter calculation included in international standards, is not clearly defined.

2. Preliminary studies

In the beginning of the application of vitrinite reflectance measurements, the Gaussian distribution (normal distribution, "bell-shaped" curve) was supposed to be the basis of the "Central Limit Theorem." Taylor et al. (1998) suggested 200 measurements, but especially in the case of disperse organic matter (DOM), this often is not possible because of the limited number of particles. In the early 1990s, Barker and Pawlewicz (1993) tried to determine a minimum number of measurements needed to estimate the mean random vitrinite reflectance of DOM. They supposed Gaussian distribution and studied the change of mean, standard deviation, skewness, and kurtosis. Their conclusions are, in a statistical point of view, that the minimum number necessary for good estimation is 20–30 particles. In case of elements less than 20, they suggested the usr of variance to decide on the reliability of calculated parameters. Disadvantages of this technique are the "presumed" Gaussian distribution, the decimal order precision, and the uncertainty of

Table 2
Location parameters, related scale parameters, and other parameters generally used in statistics

Location parameter	Formula	Related scale parameter	Formula
Location and scale parameters			
Median [med]	$\mathrm{med}_n = x_{(n+1)/2}$, if n is odd; $\mathrm{med}_n = \frac{[x_{n/2} + x_{(n/2)+1}]}{2}$, if n is even	Average median deviation [d]	$d_{\mathrm{emp}} = \frac{1}{n}\sum_{i=1}^{n} \lvert x_i - \mathrm{med}_n \rvert$
		Median absolute deviation [MAD]	$\mathrm{MAD} = \mathrm{med}(\lvert x_i - \mathrm{med}_n \rvert)$
Mean [m]	$m = \frac{1}{n}\sum_{i=1}^{n} x_i$	Standard deviation [σ]	$\sigma_{\mathrm{emp}} = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(x_i - m)^2}$
		Average deviation	$m_{\mathrm{d}} = \frac{1}{n}\sum_{i=1}^{n} \lvert x - m \rvert$
Most frequent value [Mn][a] (Steiner, 1988)	$M_n = \dfrac{\sum_{i=1}^{n} \frac{x_i}{(\varepsilon_{n-1}^2) + (x_i - M_{n-1})^2}}{\sum_{i=1}^{n} \frac{1}{(\varepsilon_{n-1}^2) + (x_i - M_{n-1})^2}}$	Dihesion [ε][a] (Steiner, 1988)	$\varepsilon_n^2 = \dfrac{3\sum_{i=1}^{n} \frac{(x_i - M_n)^2}{\left[\varepsilon_{n-1}^2 + (x_i - M_{n-1})^2\right]^2}}{\sum_{i=1}^{n} \frac{1}{\left[\varepsilon_{n-1}^2 + (x_i - M_{n-1})^2\right]^2}}$
Other parameters			
Upper quartile (q_{U}) and lower quartile (q_{L})	The upper and lower quartiles (the 0.25 and 0.75 quantiles) are the 25th and 75th percentiles of the distribution, respectively. The 25th percentile of a variable is such a value that 25% of the values of the variable fall below that value.	Half quartile range	$q = (q_{\mathrm{U}} - q_{\mathrm{L}})/2$
Kurtosis	Kurtosis measures the "peakedness" of a distribution. If the kurtosis is clearly different from zero, the distribution is either flatter or more peaked than normal; the kurtosis of the normal distribution is zero.	$\left(\frac{n(n+1)}{(n-1)(n-2)(n-3)}\sum_{i=1}^{n}\left(\frac{x_i - m}{\sigma}\right)^4\right) - \frac{3(n-1)^2}{(n-2)(n-3)}$	
Skewness	Skewness measures the deviation of the distribution from symmetry. If the skewness is clearly different from zero, that distribution is asymmetrical.	$\frac{n}{(n-1)(n-2)}\sum_{i=1}^{n}\left(\frac{x_i - m}{\sigma}\right)^3$	

[a] The most frequent value is the result of iteration, where ε is the fixed or calculated dihesion (Steiner, 1988). The starting points of iteration are: $M_1 = m$ and $\varepsilon_1 = \sqrt{3}/2\ [\max(x_i) - \min(x_i)]$.

variance at higher maturity level, especially at small sample size.

Observations of Hower et al. (1994) were similar, but they found that "in the case of high mineral matter coals or samples, where the volume of sample available for petrographic examination is severely limited, the reproducibility of reflectance readings implies that confidence can be placed in a limited number of readings provided the population approximates a normal distribution."

Following Barker and Pawlewicz (1993), international standards prescribe the calculation of vitrinite reflectance as an average value of a minimum of 50 reflectances measured under precisely defined circumstances.

On the other hand, Houseknecht and Weesner (1997) offered a new technique, the rotational reflectance measurements. The principle of this measurement is that 200 data are collected at 1.8° intervals during the simultaneous rotation of the polarizer in a 2-mm-diameter circular area of each vitrinite particle. The advantage is that it gives better knowledge of reflection properties from each particle. The measurements carried on one particle, however, are not independent and statistically cannot be interpreted. Furthermore, possible outliers have the same weight statistically in the results.

3. Methods

The measurements were carried out at the Geological Institute of Hungary, performed by a trained operator following ISO (1994). Reflectance is measured using vertical illumination on a Larica DMRX fitted with a microphotometric system, which was calibrated by different ISO glass standards.

The samples came from different ages and maturity levels, either from coal-type or DOM-type organic matter. Ten coal samples and 51 DOM samples were analysed. There are six coal samples (ICCP accreditation samples: M1–M6) with 100 particles, two coal samples with 150 particles, a coal sample with 200 particles, and another with 250 particles measured. Coal samples with different ranks were selected. Vitrinite reflectance ranged between 0.48% and 4.05%. On the other hand, 51 samples with different sizes ranging from 10 to 50 elements from

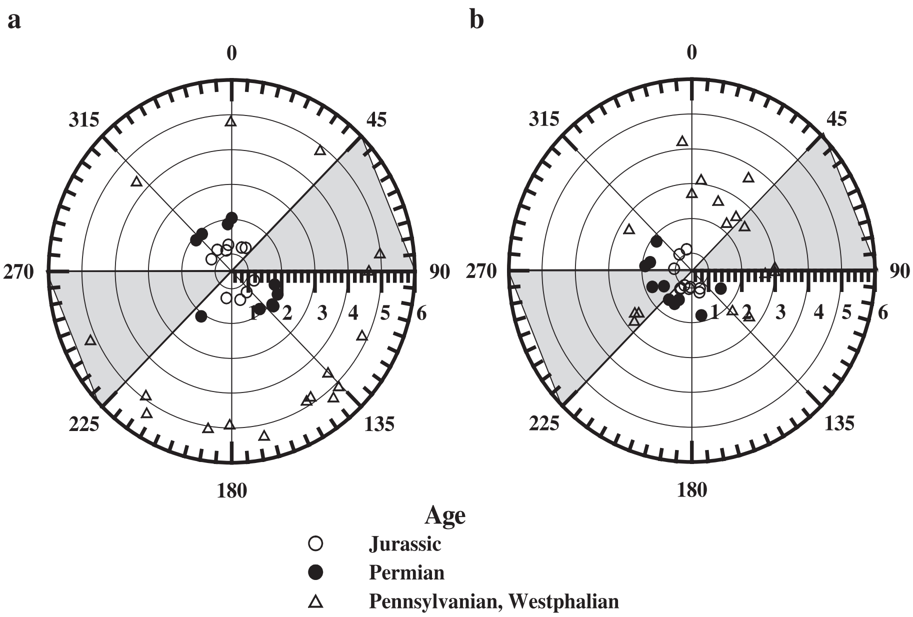

Fig. 1. The maximum reflectance (R_{max}) (a) and minimum reflectance (R_{min}) (b) vs. the angle from random reflectance (R_o) in a polar plot in case of three core samples with R_o>1.

Table 3
Statistical parameters and results of normality test of coal samples

Sample ID	Cretaceous	M1	M2	M3	M4	Jurassic	M5	M6	Permian	Pennsylvanian
Sample size (N)	250	100	100	100	100	150	100	100	150	200
Mean (X)	**0.485**	**0.496**	**0.564**	**0.774**	**1.132**	**1.232**	**1.303**	**1.775**	**1.785**	**4.050**
S.D. (X)	0.032	0.037	0.047	0.058	0.057	0.045	0.055	0.086	0.084	0.370
Average deviation	0.026	0.031	0.037	0.050	0.045	0.035	0.045	0.073	0.069	0.299
Med (X)	0.484	0.497	0.561	0.777	1.131	1.232	1.301	1.761	1.779	4.053
MAD	0.022	0.029	0.031	0.045	0.033	0.029	0.042	0.067	0.060	0.257
d_{emp}	0.026	0.031	0.037	0.050	0.045	0.035	0.045	0.072	0.069	0.299
Mn (X)	0.483	0.495	0.558	0.776	1.128	1.231	1.298	1.766	1.777	4.056
ε	0.005	0.042	0.036	0.069	0.049	0.038	0.058	0.097	0.086	0.348
Maximum	0.563	0.581	0.691	0.889	1.276	1.333	1.452	1.973	1.993	4.863
Minimum	0.429	0.440	0.503	0.680	1.039	1.158	1.226	1.654	1.664	3.368
Upper quartile	0.508	0.525	0.591	0.821	1.166	1.259	1.336	1.856	1.850	4.303
Lower quartile	0.462	0.467	0.530	0.732	1.100	1.197	1.259	1.705	1.724	3.786
q	0.023	0.029	0.031	0.045	0.033	0.031	0.039	0.076	0.063	0.258
Variance	0.001	0.001	0.002	0.003	0.003	0.002	0.003	0.007	0.007	0.137
Kurtosis	− 0.437	− 0.791	− 0.191	− 0.820	− 0.095	− 0.338	− 0.232	− 0.768	− 0.493	− 0.438
Skewness	0.235	0.130	0.315	− 0.167	0.282	0.159	0.479	0.090	0.395	− 0.082
MAD/med	0.045	0.058	0.055	0.057	0.029	0.023	0.032	0.038	0.034	0.064
Abs (med − mean)	0.0014	0.0001	0.0028	0.0026	0.0017	0.0005	0.0026	0.0138	0.0064	0.0039
Abs (med − Mn)	0.0011	0.0011	0.0031	0.0000	0.0021	0.0015	0.0025	0.0052	0.0025	0.0023
Results of normality tests										
D	0.07348	0.06921	0.12622	0.08360	0.06685	0.07517	0.08418	0.15809	0.09401	0.09400
Significance level of Lillefors	Reject at $a = 0.01$	$p > 0.2$	Reject at $a = 0.01$	$p < 0.05$	$p > 0.2$	$p < 0.01$	$p < 0.05$	Reject at $a = 0.01$	Reject at $a = 0.01$	Reject at $a = 0.01$
Correlation coefficient	0.995	0.992	0.988	0.98957	0.991	0.995	0.986	0.986	0.988	0.997
Equation of regression	$Y = 31.31x - 15.19$	$Y = 26.82x - 13.31$	$Y = 21.22x - 11.97$	$Y = 17.2x - 13.31$	$Y = 17.46x - 19.76$	$Y = 22.31x - 27.48$	$Y = 18.06x - 23.53$	$Y = 11.62x - 20.62$	$Y = 11.97x - 21.37$	$Y = 2.7x - 10.94$

Mean (X) value (in bold) is used by ISO 7404-5 standard as vitrinite reflectance.

the DOM-type organic matter were used. Thirty-one DOM samples ranged between 0.61% and 2.62% vitrinite reflectance. In the case of 20 DOM samples, vitrinite (huminite) reflectance was lower than 0.45% R_o.

The statistical experiments were performed in two ways. First, the originally measured reflectance values were analysed. This database was considered to be a ‘‘clean’’ sample set. Second, the samples with different sample sizes were generated from original samples by a random generator. ‘‘Clean’’ samples with different sample numbers ranging from 10 to 50 were generated. Each of these sample generations was repeated 50 times. After this, all the generated samples were contaminated by the maximum reflectance value of the original sample in different quantity ranges, from 2 to 24 percentages, known as a linear contamination.

Data processing was performed by Microsoft Excel®, Grapher®, Statistica 5.5®, and self-designed computer programs.

4. The importance of correct parameter choice

In most cases, a given property of either a sample set or a sample can be numerically defined. One of the most general approaches of definition is the parametrical evaluation. In this case, location parameters,

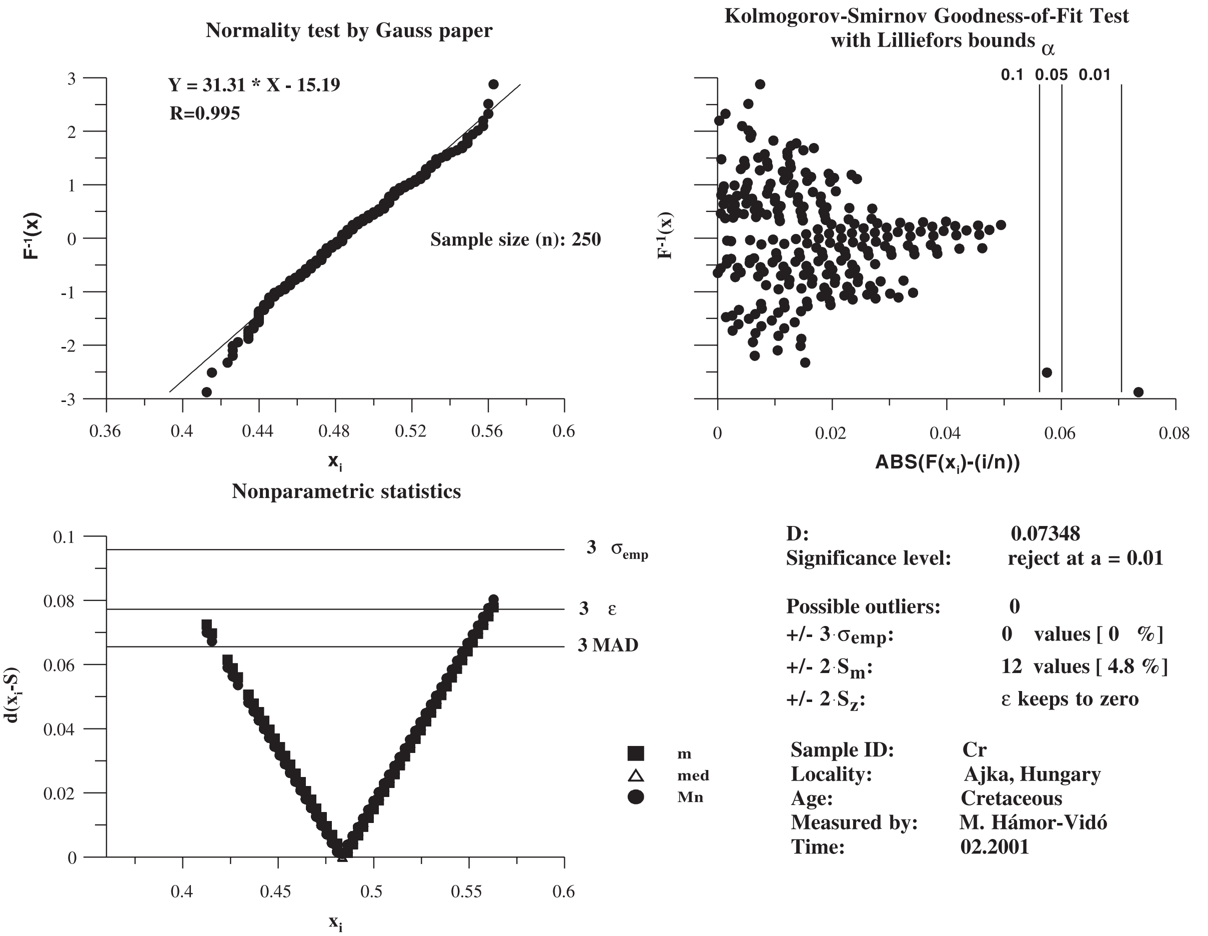

Fig. 2. Graphical statistical analysis of Cretaceous samples ($R_o = 0.48$) [S_m and S_z are statistical limits, $S_m = \mathrm{MAD}/\Phi_G^{-1}(0.75)$, $S_z = \varepsilon_n/\Phi_G^{-1}(0.75)$, where $\Phi_G^{-1}(0.75)$ is the value of inverse Gaussian distribution function in 0.75 probability].

such as mean (m), median (med), or the most frequent value (Mn) (Steiner, 1988, 1997) characterize a property of the examined sample and scale parameters, such as standard deviation (σ), median absolute deviation (MAD), or dihesion (ε) (Steiner, 1988, 1997), define the uncertainty of the location parameter (Table 2). These parameters have basic roles in applied research, either in economic projecting or theoretical aspects. However, the process of parameter selection is often accomplished automatically and the reliability of the parameter is not, or only superficially, examined. The danger of unlucky parameter selection can appear, to a greater extent, in the area of applied research, where only a limited or small sample size ($n < 50$) is available. Samples sometimes contain outliers originating for different reasons (Table 1) and, in most cases, experiments cannot be replicated because of time, financial, and technical limitations.

This is the reason why the reliability of parameters should be examined. This reliability depends on the conditions of sampling, sample preparation, measurement, and interpretation. Statistical analysis, such as the test of independence, goodness-of-fit tests, and, especially at small sample sizes, nonparametric statistics can help to define the reliability of the choice of the best parameter in a given situation.

5. Analysis of data

According to the statistical analysis suggested by Fedor et al. (2001), analysis consists of three steps. As

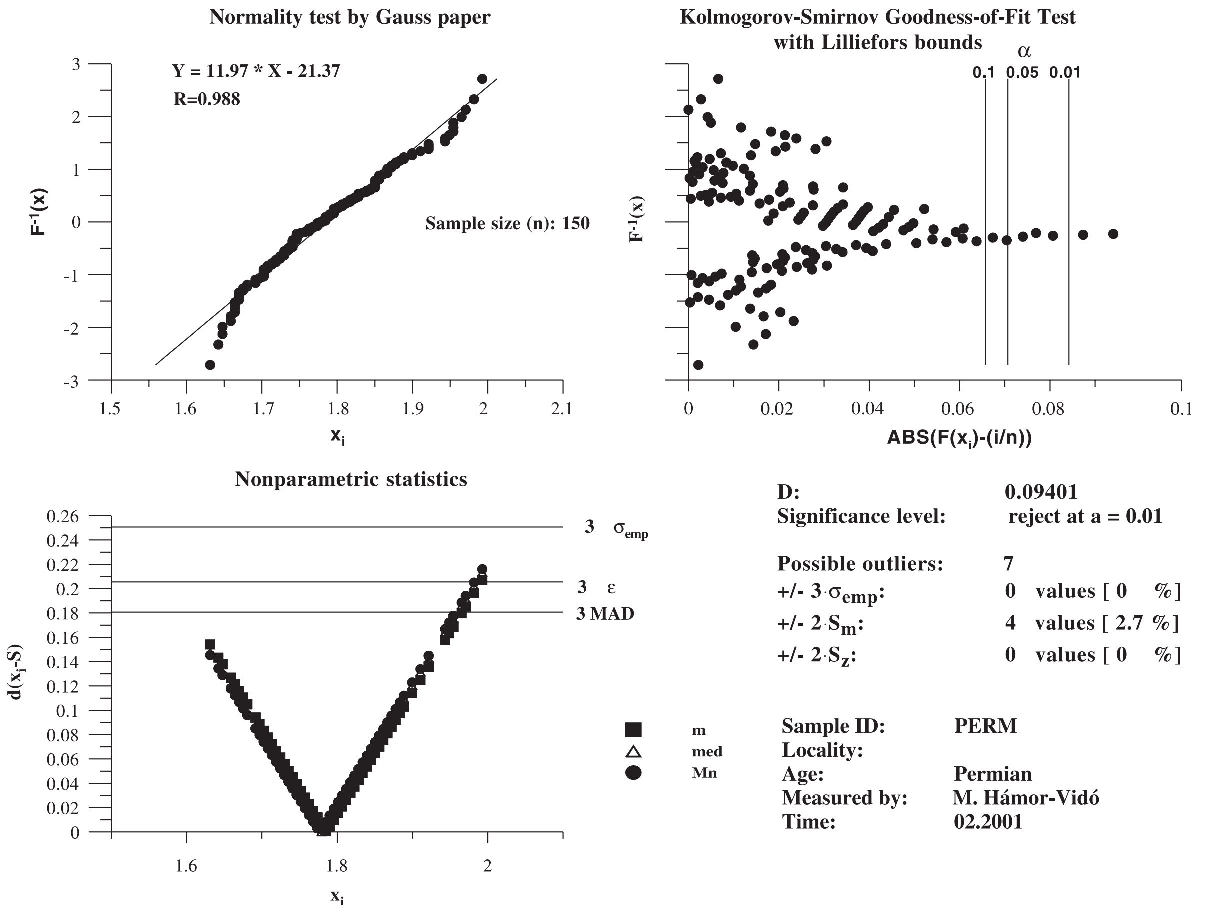

Fig. 3. Graphical statistical analysis of Permian samples ($R_o = 1.79$).

a first step, the dependence of variables (measured reflectance values) should be examined. As a second step, the statistical distribution of measured values should be estimated, and, finally, the adequate parameter to characterize a given property should be selected and tested by nonparametric statistics in the third step.

There were three steps during the analysis of reflectance data. The analysis of coal samples with different maturity (range 0.48–4.05%, vitrinite reflectance) gave general information about the statistical distribution of reflectance data (i.e., the reliability of basic concept of distribution). On the basis of these analyses, Gaussian or near-Gaussian distributions are generally observed. In the second step, the artificially generated samples were examined to determine the effect of contamination and sample size on location and scale parameters. In the third step, DOM samples were analysed to control the theoretical concepts in practice.

5.1. The independence of sample elements

In most cases in applied research, the statistical approach of independence is too rigorous because of the uncertainties of sample handling. In practice, the critical question is the reproduction of measurement, which postulates the independence of measured values at a given level of uncertainty. Although many uncertainties can occur during handling of the sample (Table 1), as a result of standardization, most technical and human problems can be avoided.

Standards give a basis of theoretical supposition of the independence of observed reflectance values. However, a possible ordering during the bedding of powdered particles in resin can be recognized in the case of maximum reflectance values from Jurassic and Permian coal samples vitrinites, as it can be seen in Fig. 1. This diagram represents the position of the maximum value of the collotelinite of the ground coal particles embedded in resin and polished in the traditional way. As it can be seen in Fig. 1a, possible ordering can be observed in Jurassic and Permian samples. The maximum vitrinite reflectance was 1.16 and 1.72, respectively. The minimum reflectance positions do not show a similar character (Fig 1b). A possible reason for the differentiation of the character of maximum and minimum values is that the real maximum and only apparent minimum values were measured. This problem will be studied in more detail in the future.

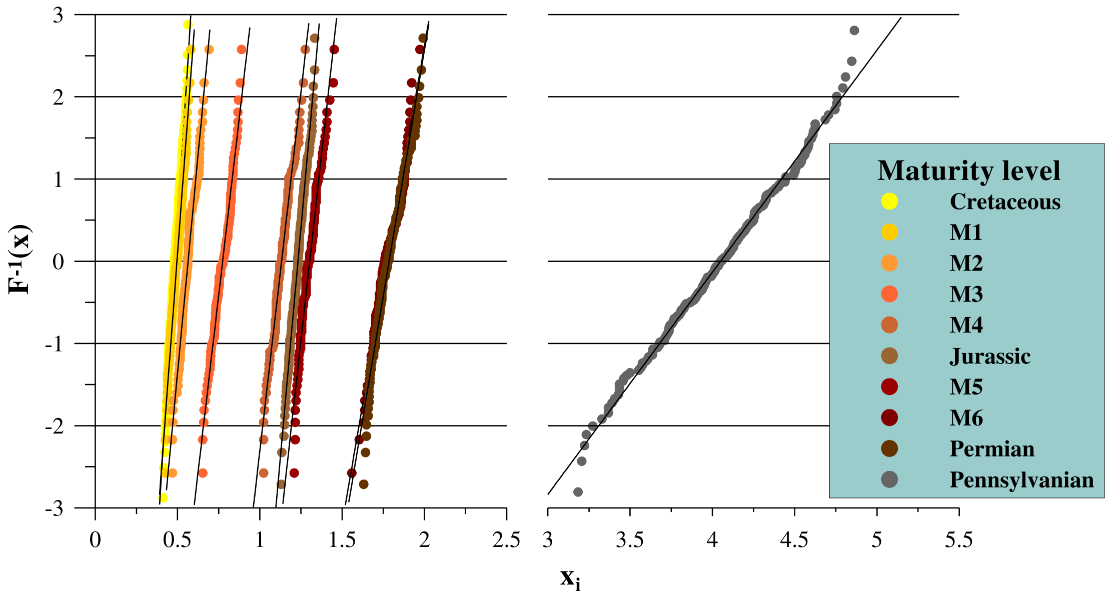

Fig. 4. Results of graphical normality test with increasing maturity in case of coal samples.

Table 4
Statistical parameters of DOM samples (*R* means rejection at all significance levels in column Lillefors significance level p_L)

Sample ID	N	m (X)	σ (X)	m_d	med (X)	MAD	d_{emp}	Mn (X)	ε	Max	Min	q	σ^2	K	Sk	|med − mean|	|med − Mn|	D	p_L	r	Equation of regression
AD1	30	**0.262**	0.023	0.018	0.265	0.015	0.018	0.265	0.010	0.302	0.240	0.014	0.001	− 0.537	− 0.129	0.0022	0.0007	0.0922	$p>0.2$	0.987	$Y=43x-11.28$
Eb1	18	**0.274**	0.041	0.030	0.270	0.020	0.029	0.270	0.000	0.350	0.270	0.019	0.002	− 0.274	0.176	0.0039	0.0000	0.1632	$p>0.2$	0.973	$Y=24.28x-6.65$
AD2	20	**0.282**	0.025	0.021	0.285	0.020	0.020	0.281	0.030	0.343	0.262	0.019	0.001	0.028	0.592	0.0028	0.0042	0.1562	$p>0.2$	0.964	$Y=39.83x-11.23$
AD5	30	**0.295**	0.033	0.024	0.294	0.016	0.024	0.291	0.025	0.382	0.269	0.018	0.001	1.214	1.027	0.0001	0.0037	0.1620	$p<0.01$	0.954	$Y=30.18x-8.89$
Eb2	18	**0.326**	0.043	0.037	0.320	0.030	0.037	0.326	0.056	0.390	0.310	0.034	0.002	− 1.263	0.011	0.0061	0.0055	0.1461	$p>0.2$	0.975	$Y=23.26x-7.58$
AD3	30	**0.332**	0.032	0.025	0.334	0.019	0.024	0.334	0.024	0.416	0.302	0.022	0.001	0.713	0.134	0.0013	0.0002	0.1189	$p>0.2$	0.988	$Y=30.86x-10.25$
Hsz1	20	**0.353**	0.060	0.046	0.355	0.035	0.046	0.359	0.054	0.460	0.330	0.033	0.004	0.957	− 0.652	0.0020	0.0036	0.2168	$p<0.01$	0.982	$Y=16.66x-5.88$
Hsz2	31	**0.354**	0.101	0.052	0.340	0.030	0.049	0.334	0.041	0.850	0.310	0.030	0.010	20.688	4.181	0.0135	0.0056	0.2353	*R*	0.731	$Y=9.92x-3.5$
AD4	30	**0.362**	0.034	0.026	0.355	0.020	0.025	0.355	0.022	0.450	0.339	0.019	0.001	0.433	0.700	0.0071	0.0003	0.1230	$p>0.2$	0.981	$Y=29.44x-10.65$
AD4 (2)	30	**0.363**	0.040	0.032	0.363	0.029	0.032	0.361	0.034	0.432	0.323	0.028	0.002	− 0.888	0.105	0.0002	0.0016	0.0970	$p>0.2$	0.986	$Y=25.07x-9.1$
Tip1	25	**0.401**	0.069	0.051	0.410	0.040	0.051	0.400	0.044	0.540	0.360	0.030	0.005	0.337	0.075	0.0092	0.0104	0.1508	$p<0.15$	0.981	$Y=14.43x-5.79$
Algyő1	30	**0.409**	0.045	0.032	0.415	0.021	0.032	0.413	0.023	0.544	0.376	0.017	0.002	1.882	0.506	0.0066	0.0020	0.1558	$p<0.05$	0.967	$Y=22.45x-9.18$
Hsz6	13	**0.417**	0.062	0.052	0.410	0.060	0.052	0.409	0.072	0.520	0.410	0.055	0.004	− 1.224	0.303	0.0069	0.0010	0.1286	$p>0.2$	0.976	$Y=16.03x-6.68$
Hsz5	19	**0.419**	0.042	0.034	0.410	0.030	0.033	0.412	0.041	0.500	0.390	0.033	0.002	− 0.500	0.549	0.0089	0.0024	0.1232	$p>0.2$	0.973	$Y=23.8x-9.97$
Hsz3	15	**0.422**	0.210	0.162	0.320	0.070	0.154	0.333	0.138	0.980	0.290	0.133	0.044	2.229	1.495	0.1020	0.0126	0.2195	$p<0.05$	0.902	$Y=4.75x-2.01$
Hsz7	15	**0.423**	0.073	0.058	0.420	0.050	0.057	0.413	0.071	0.580	0.390	0.043	0.005	0.064	0.590	0.0027	0.0070	0.1398	$p>0.2$	0.984	$Y=13.73x-5.8$
Eb6	21	**0.430**	0.106	0.063	0.410	0.050	0.058	0.409	0.027	0.840	0.390	0.035	0.011	11.561	3.015	0.0200	0.0012	0.2240	$p<0.01$	0.813	$Y=9.39x-4.04$
Tip2	25	**0.440**	0.047	0.037	0.450	0.030	0.036	0.450	0.037	0.540	0.410	0.030	0.002	− 0.028	− 0.310	0.0100	0.0002	0.1164	$p>0.2$	0.979	$Y=21.36x-9.4$
Tip3	25	**0.442**	0.044	0.034	0.440	0.030	0.034	0.441	0.038	0.540	0.410	0.025	0.002	0.116	0.093	0.0024	0.0006	0.1039	$p>0.2$	0.988	$Y=22.83x-10.1$
Hsz4	24	**0.445**	0.102	0.089	0.465	0.085	0.088	0.452	0.133	0.590	0.370	0.078	0.010	− 1.178	− 0.243	0.0204	0.0126	0.1022	$p>0.2$	0.976	$Y=9.85x-4.38$
Tip6	10	**0.614**	0.104	0.067	0.590	0.040	0.062	0.589	0.043	0.880	0.620	0.035	0.011	5.337	2.081	0.0240	0.0008	0.2389	$p<0.1$	0.878	$Y=9.61x-5.9$
Algyő2	50	**0.651**	0.060	0.048	0.643	0.035	0.047	0.641	0.054	0.793	0.594	0.033	0.004	− 0.044	0.561	0.0085	0.0017	0.0962	*R*	0.983	$Y=16.65x-10.84$
Algyő3	30	**0.651**	0.067	0.055	0.630	0.039	0.052	0.633	0.056	0.809	0.594	0.049	0.005	− 0.116	0.727	0.0212	0.0033	0.1669	$p<0.01$	0.972	$Y=14.98x-9.76$
Algyő4	13	**0.656**	0.044	0.034	0.651	0.027	0.034	0.645	0.039	0.745	0.651	0.023	0.002	− 0.115	0.823	0.0050	0.0055	0.1683	$p>0.2$	0.965	$Y=22.86x-14.99$

Algyő5	27	**0.676**	0.057	0.044	0.680	0.041	0.044	0.680	0.045	0.787	0.634	0.039	0.003	− 0.034	− 0.171	0.0039	0.0002	0.1090	$p>0.2$	0.995	$Y=17.53x-11.86$
Tip5	25	**0.682**	0.048	0.038	0.680	0.020	0.038	0.680	0.042	0.770	0.660	0.025	0.002	− 0.421	0.168	0.0016	0.0001	0.0852	$p>0.2$	0.983	$Y=20.98x-14.3$
Algyő6	30	**0.684**	0.056	0.046	0.674	0.046	0.045	0.674	0.044	0.785	0.629	0.045	0.003	− 0.849	0.258	0.0108	0.0007	0.1333	$p<0.15$	0.982	$Y=17.83x-12.2$
Algyő7	34	**0.722**	0.073	0.062	0.710	0.061	0.061	0.711	0.084	0.868	0.645	0.059	0.005	− 1.126	0.355	0.0119	0.0010	0.1129	$p<0.01$	0.972	$Y=13.78x-9.95$
Algyő8	30	**0.770**	0.051	0.042	0.770	0.040	0.042	0.771	0.054	0.877	0.719	0.039	0.003	− 0.834	0.065	0.0004	0.0002	0.0762	$p>0.2$	0.989	$Y=19.45x-14.98$
Hsz-9	13	**0.931**	0.073	0.053	0.920	0.030	0.052	0.916	0.052	1.100	0.920	0.030	0.005	1.308	1.099	0.0108	0.0037	0.1647	$p>0.2$	0.959	$Y=13.79x-12.84$
Algyő9	40	**0.931**	0.055	0.044	0.938	0.045	0.043	0.943	0.033	1.040	0.875	0.041	0.003	− 0.367	− 0.324	0.0066	0.0052	0.1178	*R*	0.988	$Y=18.16x-16.91$
Hsz8	20	**0.951**	0.069	0.057	0.945	0.055	0.057	0.942	0.073	1.070	0.890	0.058	0.005	− 1.066	0.318	0.0055	0.0029	0.1599	$p>0.2$	0.976	$Y=14.47x-13.76$
Eb5	22	**1.009**	0.115	0.083	0.995	0.060	0.082	0.987	0.060	1.280	0.960	0.054	0.013	0.807	1.061	0.0141	0.0076	0.1787	$p<0.05$	0.949	$Y=8.67x-8.75$
Algyő10	19	**1.035**	0.093	0.073	1.003	0.040	0.065	1.000	0.006	1.202	0.998	0.041	0.009	− 0.347	0.940	0.0321	0.0030	0.2450	*R*	0.920	$Y=10.75x-11.13$
Algyő11	10	**1.051**	0.111	0.082	1.039	0.055	0.081	1.035	0.018	1.222	1.079	0.044	0.012	− 0.380	0.058	0.0120	0.0040	0.1239	$p>0.2$	0.974	$Y=9.03x-9.49$
Tip4	12	**1.184**	0.195	0.156	1.215	0.135	0.156	1.209	0.179	1.530	1.260	0.131	0.038	− 0.573	− 0.081	0.0308	0.0060	0.1370	$p>0.2$	0.984	$Y=5.12x-6.06$
Eb4	29	**1.194**	0.179	0.140	1.210	0.130	0.138	1.217	0.116	1.560	1.050	0.120	0.032	− 0.429	− 0.072	0.0155	0.0075	0.1048	$p>0.2$	0.986	$Y=5.58x-6.67$
Eb3	45	**1.483**	0.148	0.114	1.470	0.090	0.112	1.470	0.097	1.820	1.340	0.095	0.022	− 0.158	0.351	0.0133	0.0001	0.0916	$p>0.2$	0.988	$Y=6.78x-10.06$
Eb7	22	**1.600**	0.161	0.127	1.640	0.105	0.125	1.638	0.141	1.810	1.540	0.103	0.026	0.294	− 0.926	0.0400	0.0024	0.1389	$p>0.2$	0.960	$Y=6.22x-9.95$
Tn3	30	**2.048**	0.123	0.105	2.035	0.110	0.105	2.051	0.153	2.230	1.950	0.098	0.015	− 1.007	− 0.209	0.0130	0.0164	0.0898	$p>0.2$	0.980	$Y=8.11x-16.61$
Tn1	30	**2.066**	0.111	0.083	2.070	0.070	0.082	2.070	0.031	2.280	1.990	0.061	0.012	− 0.292	0.064	0.0043	0.0001	0.1118	$p>0.2$	0.986	$Y=9.02x-18.62$
Tn2	30	**2.102**	0.145	0.119	2.080	0.100	0.116	2.093	0.139	2.370	2.020	0.094	0.021	− 0.806	0.026	0.0220	0.0129	0.1270	$p>0.2$	0.985	$Y=6.9x-14.51$
Tn6	30	**2.106**	0.115	0.088	2.105	0.075	0.088	2.108	0.107	2.340	2.030	0.071	0.013	1.392	− 0.528	0.0013	0.0031	0.5109	*R*	0.980	$Y=8.74x-18.4$
Tn5	30	**2.108**	0.125	0.099	2.080	0.080	0.097	2.097	0.102	2.360	2.010	0.086	0.016	− 0.173	0.079	0.0277	0.0166	0.1210	$p>0.2$	0.992	$Y=8.01x-16.88$
Tn9	30	**2.160**	0.141	0.110	2.145	0.075	0.109	2.155	0.108	2.430	2.080	0.074	0.020	− 0.322	0.041	0.0150	0.0096	0.0765	$p>0.2$	0.989	$Y=7.09x-15.32$
Tn4	30	**2.186**	0.141	0.112	2.215	0.085	0.110	2.202	0.122	2.460	2.070	0.089	0.020	− 0.131	− 0.224	0.0293	0.0133	0.0752	$p>0.2$	0.989	$Y=7.11x-15.54$
Tn7	30	**2.204**	0.150	0.107	2.210	0.055	0.106	2.212	0.067	2.570	2.100	0.056	0.022	0.972	− 0.118	0.0063	0.0018	0.1287	$p>0.2$	0.980	$Y=6.69x-14.73$
Tn8	30	**2.226**	0.131	0.107	2.250	0.095	0.104	2.244	0.120	2.470	2.100	0.099	0.017	− 0.585	− 0.228	0.0243	0.0059	0.0790	$p>0.2$	0.989	$Y=7.65x-17.02$
Tn11	30	**2.245**	0.183	0.142	2.225	0.105	0.141	2.233	0.153	2.660	2.120	0.118	0.033	0.160	0.101	0.0200	0.0083	0.1040	$p>0.2$	0.995	$Y=5.48x-12.3$
Tn10	30	**2.264**	0.194	0.153	2.275	0.110	0.153	2.271	0.176	2.670	2.110	0.106	0.038	0.010	− 0.115	0.0107	0.0041	0.0792	$p>0.2$	0.995	$Y=5.16x-11.69$
Teng1	18	**2.614**	0.190	0.147	2.605	0.110	0.147	2.582	0.152	2.970	2.500	0.114	0.036	− 0.508	0.269	0.0094	0.0235	0.1274	$p>0.2$	0.987	$Y=5.27x-13.77$

Mean (X) value (in bold) is used by ISO 7404-5 standard as vitrinite reflectance.

5.2. Goodness-of-fit tests

Goodness-of-fit tests indicate whether it is reasonable to assume that a random sample comes from a specific distribution. It is simpler to test whether the observations originated from the Gaussian distribution or not. Several goodness-of-fit tests exist, such as chi-square test, Kolmogorov–Smirnov test (Miller, 1956) and variants (e.g., Lilliefors, 1967), Anderson–Darling test, and Shapiro–Wilk test; as well as graphical tests such as probability plot, and others (e.g., D'Agostino and Stephens, 1986; Steiner, 1990; Lukács, 1996). The most common, and often automatically applied, test in geological practice is the chi-square test. However, this test is not recommended in case of small sample sizes because it does not give reliable information for elements under 100. On the other hand, the value of the test statistics depends on how the data are bound (Sachs, 1984, pp. 330–332). It is better to apply the Kolmogorov–Smirnov test with Lilliefors bounds in case of Gaussian distribution (Lilliefors, 1967), or combine it with the probability plot (Fedor et al., 2001).

The results of the Kolmogorov–Smirnov test in the case of medium and large (n>100) sample sizes are not unambiguous, as can be seen in Table 3 (the descriptive statistics of coal samples). The hypothesis regarding the distributional form is rejected for a given significance level (α) if the test statistic D is greater than the critical value. The possible reason for the rejected Gaussian distribution in case of Cretaceous, Jurassic, M6, and Pennsylvanian (Westphalian) samples is the outliers (e.g., Fig. 2). These outliers can also be observed in nonparametric statistics (e.g., Figs. 2 and 3). In case of M2 standard and Permian samples (Fig. 3), the Gaussian distribution can be rejected and only near-Gaussian distribution can be stated. However, the graphical normality tests show good agreement with hypothetical Gaussian distribution in all cases, as shown in Fig. 4. The correlation coefficients range from $R=0.986$ to $R=0.997$. They have good agreement with Houseknecht and Weesner (1997), who did not observe any bimodality on the results of rotational reflectance (R_{rot}) measurement. Furthermore, Hower et al. (1994) stated that the random reflectance (R_{random}) is half of the mean of R_{max} and R_{min}. Therefore, if the measurement were random, the effect of anisotropy could be neglected on the value of R_o, and it has an influence only on the value of scale parameters, such as standard deviation (σ).

To sum it up, it may be established that the previously stated Gaussian or observed near-Gaussian distribution is acceptable independent of maturity and anisotropy.

In case of DOM samples (Table 4), on the basis of Kolmogorov–Smirnov statistics and graphical goodness-of-fit tests, the Gaussian distribution can also be accepted. However, in some cases, an unreliable value caused by outliers randomly occurs, independent of maturity and sample size.

On the other hand, it is generally observed that the steepness of regression line increases with higher rank because of the increasing anisotropy, as seen in Fig. 4. An exponential relation of steepness vs. maturity can be observed in Fig. 5.

5.3. Goodness of parameter choice

During parameter choice, the robust and resistant character of a given parameter should be

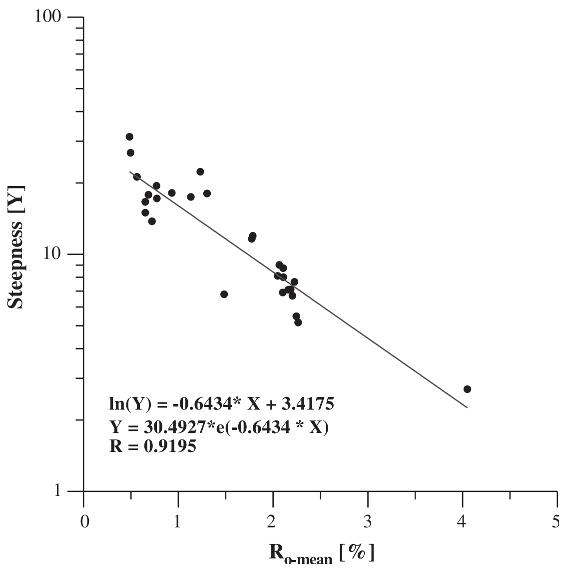

Fig. 5. The steepness (Y) of regression lines vs. maturity.

examined. "Robust" means the reliability of the parameter on a wide range of statistical distributions, and "resistant" means the sensitivity of the parameter to sample size and outliers. The best parameters of Gaussian distribution are mean (m) and standard deviation (σ), and they can be accepted in case of "clean" coal samples. However, because of the semisubjective character of the measurement, the sample contains outliers. The frequency of human mistakes depends on the experience of the operator. It practically means that some outliers that have higher reflectance than collotelinite, such as semifusinite, would be measured as it can be seen either in the graphical normality test and related Kolmogorov–Smirnov test, or in nonparametric statistics (Figs. 2 and 3). In addition, particularly in the case of dispersed organic matter, 50 reflectances usually cannot be measured because of the lack of collotelinite particles. Generally, only 10–30 measurements can be accomplished. Because of the unrobust and unresistant character of the mean, it is sensitive to outliers—and this sensitivity increases with the decrease in sample size and increase in maturity. This is the reason for the need to examine the applicability of more robust and more resistant parameters (e.g., median or most frequent value).

In Table 3, the descriptive statistics of coal samples are summarized. There are no significant differences between the values of the mean, maximum, and most frequent value, but the absolute difference of the median and the mean is, in some cases, greater than the absolute difference of the median and the most frequent value. The following relations can be observed:

- All the scale parameter values increase with increasing maturity.
- The value of MAD is the least and the value of standard deviation is the greatest from the scale parameters. The value of MAD is about half of the

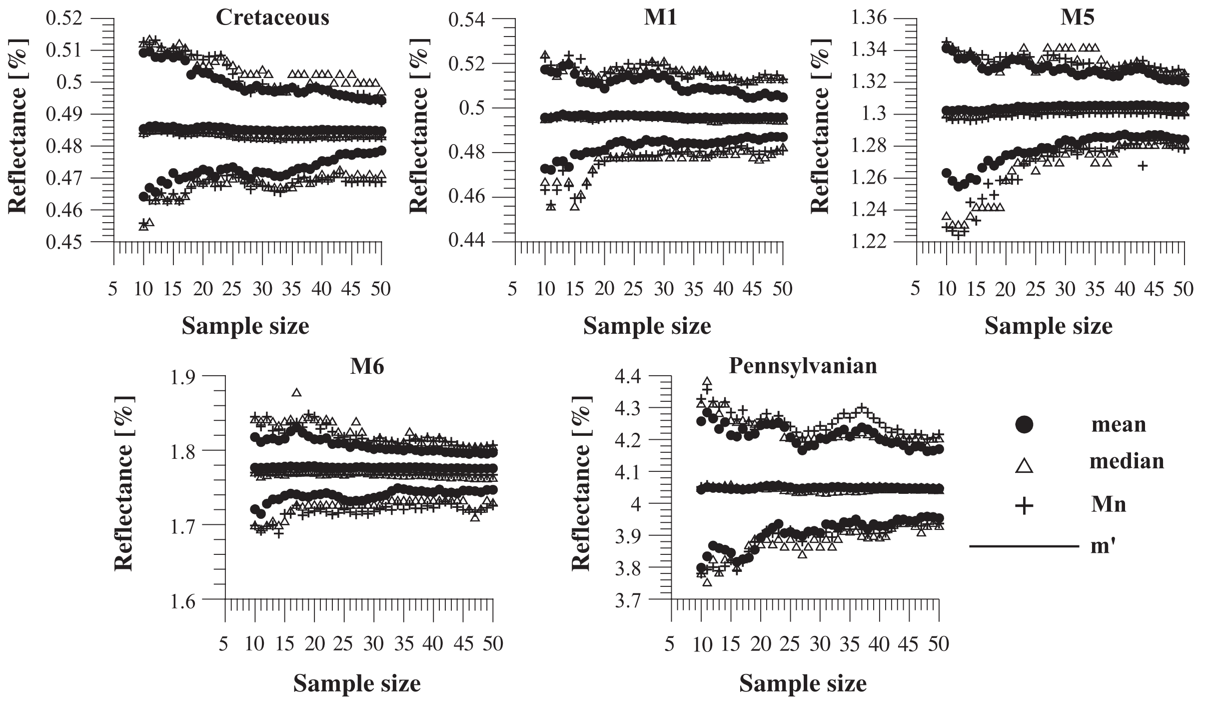

Fig. 6. Change of basic location parameters and its minimum and maximum values as a function of increasing sample size at different levels of maturity in case of artificial sample sets.

standard deviation. In case of Cretaceous samples, the value of ε is unreliable.

- The absolute difference between *m* and med increases with maturity and, in the case of matured samples (R_o>1.3), the absolute difference is greater than between med and Mn.
- The value of variance is low and increases with maturity.
- The kurtosis and the skewness are near zero, implying Gaussian or near-Gaussian distribution and symmetrical character of distributions, respectively.

This observation is correct either in the case of contaminated samples generated artificially, or samples with small sample size, as presented later.

To demonstrate the effect of sample size and quantity of contamination on statistical parameters, random sample generation was carried out from original coal sample data, as noted above. The contamination was carried out with different quantities of maximum reflectance values as a possible outlier of the original samples.

In Fig. 6, the change of maximum and minimum values, and the average of five generated sample sets can be seen with increasing sample size. Location parameters show no significant difference at a given sample size. The range of the difference between the minimum and maximum values of sample sets decreases with increasing sample size. Furthermore, the higher the maturity, the larger the difference for a small sample size. If the sample sets are contaminated with outliers by different rates ranging from 2% to 24%, it can be observed that the higher the quantity of the outliers, the less reflectance values fall into the range of the acceptable ± 1.5% tolerance level (see Fig. 7). The percent rate of different location parameters inside the ± 1.5% tolerance level can be seen in Fig. 8. These latter trends are summarized by values in Table 5. With greater contamination, the more significant difference is observed

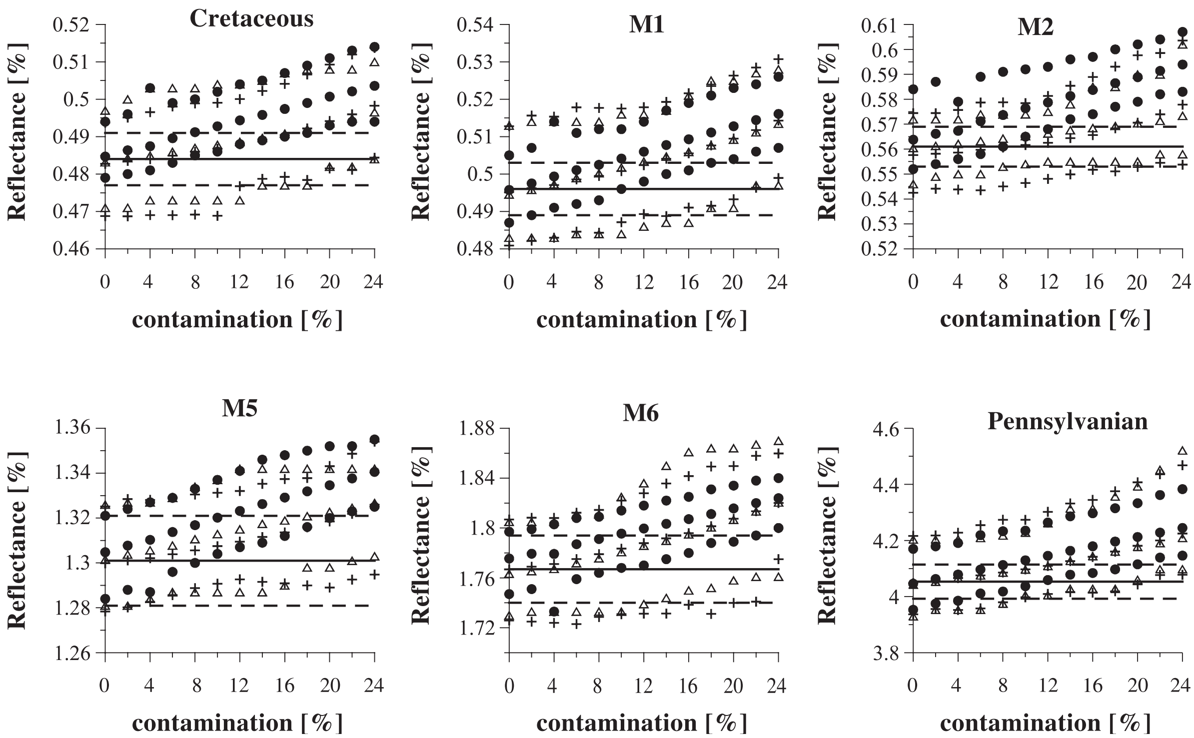

Fig. 7. Change of basic location parameters and its minimum and maximum values as a function of increasing quantity of outliers at different levels of maturity in case of artifical sample sets (lines mean the ± 1.5% tolerance limits).

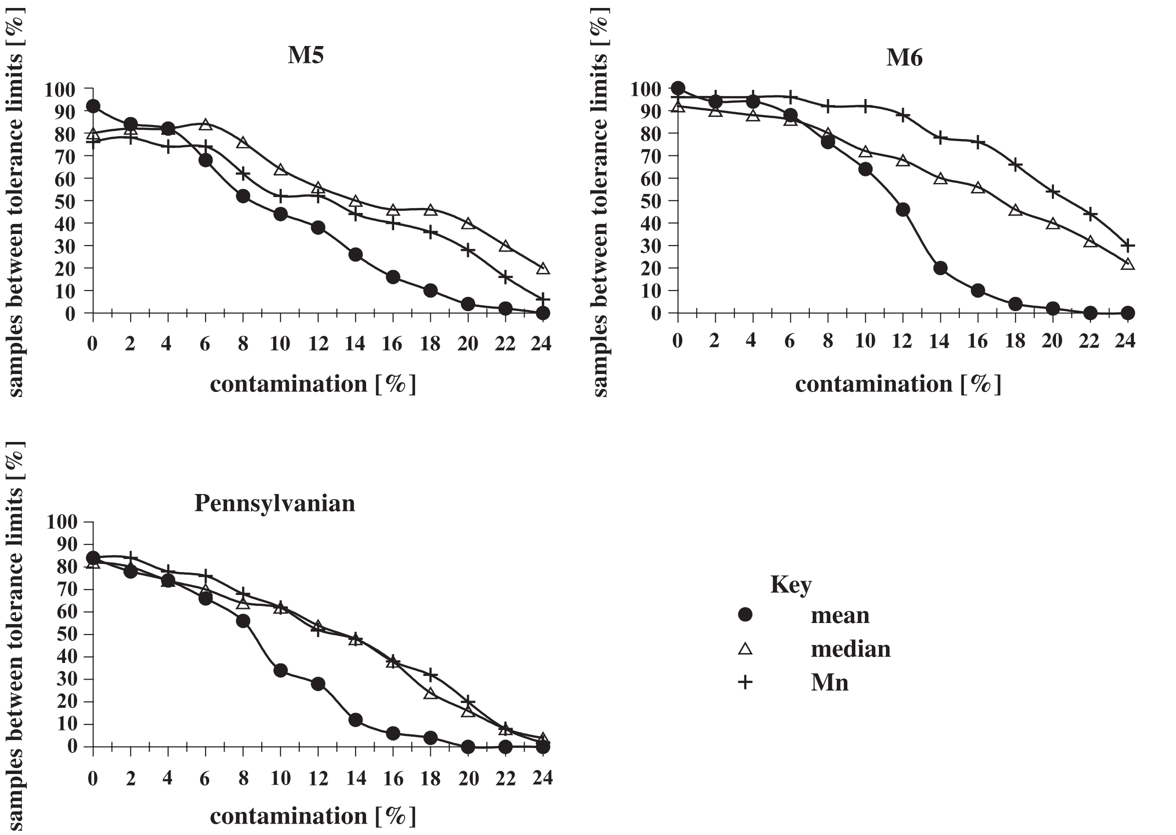

Fig. 8. Percent rate of different location parameters inside the ± 1.5% tolerance level plotted against the quantity of outliers in case of artifical sample sets generated from highly matured coal samples.

from the original parameter in the same sample set. The reliability of the mean value decreases faster than the other two parameter values because of the unresistant behaviour of the mean.

5.4. Analysis of DOM samples

To control the results of statistical analyses, DOM samples were examined. The summary of

Table 5
Percent rate of different location parameters inside ± 1.5% tolerance shown in Fig. 8

Contamination [%]	0	2	4	6	8	10	12	14	16	18	20	22	24
M5 – *m*	100	94	94	88	76	64	46	20	10	4	2	0	0
M5 – med	92	90	88	86	80	72	68	60	56	46	40	32	22
M5 – Mn	96	96	96	96	92	92	88	78	76	66	54	44	30
M6 – *m*	92	84	82	68	52	44	38	26	16	10	4	2	0
M6 – med	80	82	82	84	76	64	56	50	46	46	40	30	20
M6 – Mn	76	78	74	74	62	52	52	44	40	36	28	16	6
Pennsylvanian – *m*	84	78	74	66	56	34	28	12	6	4	0	0	0
Pennsylvanian – med	82	80	74	70	64	62	54	48	38	24	16	8	4
Pennsylvanian – Mn	84	84	78	76	68	62	52	48	38	32	20	8	2

descriptive statistics of these samples is given in Table 4. There are two possible ways of examination: with increasing sample size and with increasing maturity. As it can be observed in Table 4, in some cases, unreliable values occur randomly, independent of maturity and sample size. The following observations can be made from the data in Table 4:

1. The trend of correlation coefficients increases with increasing sample size.
2. The trend of MAD values increases less than the trend of the standard deviation values.
3. The trend of the sample range $[\max(x_i)-\min(x_i)]$ increases by one order of magnitude with increasing maturity.
4. The standard deviation is higher than 0.1 in 23 samples and, in all cases, the variance is lower than 0.1, despite the unreliable reflectance values.

In most cases, at small sample size (42 of 51 at small sample sizes and 5 of 10 at large sample sizes), the absolute difference between median and mean is greater than the median and is the most frequent value (Mn). Theoretically, in case of symmetrical unimodal distributions, such as Gaussian distribution, all of these location parameters should be equal. Whilst the median and Mn are robust and resistant parameters, the lower the difference between them, the greater is the authenticity. Although both of them are good location parameters, a significant difference can be observed in the uncertainty of related scale parameters (MAD and d in case of median and ε in case of Mn) because, in some cases, the result of the Mn$-\varepsilon$ iteration is equal to zero, as it can be seen in the Cretaceous sample or in two small samples (Eb1 and Algyő10). Because of these reasons, the median and related scale parameters seem to be the best for characterizing the maturity of the DOM in case of small sample size.

6. Conclusions

1) The goodness-of-fit tests (Kolmogorov–Smirnov test with Lilliefors bounds, and graphical test) show that the Gaussian distribution or near-Gaussian distribution is generally acceptable in the case of vitrinite reflectance, independently on the sample size. It means that the average, as a location parameter, and the standard deviation, as a scale parameter, provide good estimation in the case of samples that do not contain outliers.
2) Generally, the measurements contain varying numbers of outliers depending on the experience of operator. It is presumed that samples without outliers cannot be measured because of the semi-subjective nature of measurements. The quantity of outliers in the case of a trained operator is less than 10% of all observations.
3) The higher the reflectance of vitrinite, the greater the distance between the trend of the value of unrobust and unresistant mean (m) and the robust and resistant parameters, such as the median (med) and the most frequent value (Mn). This difference is a few per hundredths in the case of less mature samples and increases to a few tenths with increasing maturity.
4) In the case of small sample sizes, the median and related scale parameters—median absolute deviation and median average deviation (d)—are more reliable parameters than the mean and standard deviation because of their robust and resistant character, especially in case of outliers. The most frequent value is a reliable parameter, but the related scale parameter (dihesion) is not, because in some cases the result of the Mn$-\varepsilon$ iteration equals zero.
5) There are some problems because of the binomial character of distribution of measured values in case of higher-maturity samples. This binomiality results from the anisotropic character of vitrinite higher than 1% R_o. One of the possible reasons of this binomiality might be the ordering of vitrinite particles during sample preparation. This problem will be studied in more detail in the future.

In relation to these observations, older data should be studied in more detail from the point of view of the possibilities of reevaluation of reflectance data in the future. Moreover, the usability of other methods like bootstrap statistics (e.g., Efron and Tibshirani, 1993) and fuzzy numbers (e.g., Bárdossy et al., 2000) may be studied as possible ways to solve the problem originating from small sample size.

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