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Review

# Multivariate statistical assessment of coal properties

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ABSTRACT

A set of 42 coal samples consisting of coal blends prepared for coking (subset A-blends) and lump coal from coal seams (subset B-single coals) was subjected to multicomponent statistical analysis. For these samples, the study determined their structural properties (total intrusion volume *TIV*, total pore area *TPA*, bulk density *BD*, average pore diameter *APD*, and porosity *PS*), proximate characteristics (moisture $W^a$, ash content $A^d$ and volatile matter $V^{daf}$), ultimate characteristics (total sulfur content $S^d$ and carbon content $C^d$), coal maceral characteristics (reflectance of vitrinite $R_r$, vitrinite *Vitr*, inertinite *Inert* and liptinite *Lipt*) and coking properties (contraction *a*, dilation *b* and swelling index *SI*). Using factor analysis (FA), 3 factors were separated. These include the most important coal characteristics with significant mutual correlations. The distribution of the entire set of 42 samples was performed by principal components analysis (PCA) and hierarchical clustering (HC). The coal samples were divided into two clusters, numbered I and II. Cluster I completely matched the samples included in subset A (blends), while cluster II matched the samples in subset B (single coals). A basic statistical evaluation of the investigated properties in both clusters I and II was performed, including correlation and regression analyses. Based on the results of FA, the reduced number of 9 relevant characteristics was selected. These were then gradually reduced from 9 to 3; HC separations were calculated for each of them. It was found that almost the same differentiation of 42 samples into clusters I and II (corresponding to blends and single coals, respectively) can be calculated using only 7 instead of the original 16 properties. These properties are *TPA*, $A^d$, $V^{daf}$, $R_r$, *Vitr*, *Lipt* and *b*.


**Contents**



## 1. Introduction

Coal is a combustible sedimentary rock formed of organic plant remains that have undergone a remarkable transformation while still preserving some of their original features. The main factors of coalification process are the pressure of overlying strata and temperature, which initiated physical and chemical changes of bituminous coals during the course of geological history [1,2]. The specific character of different coals depends

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**Table 1**
The factor loadings after Varimax rotation.

| Parameter | Factor 1 | Factor 2 | Factor 3 |
|---|---|---|---|
| TPA | −0.216 | 0.527 | −0.011 |
| BD | −0.066 | −0.061 | 0.665 |
| APD | −0.556 | −0.207 | −0.722 |
| PS | −0.673 | 0.072 | −0.633 |
| $W^a$ | 0.446 | −0.102 | 0.499 |
| $A^d$ | −0.709 | 0.236 | −0.094 |
| $V^{daf}$ | −0.322 | 0.894 | −0.012 |
| $R_r$ | 0.105 | −0.914 | −0.071 |
| Vitr | −0.925 | −0.010 | 0.106 |
| Inert | 0.910 | −0.128 | −0.086 |
| Lipt | 0.106 | 0.822 | −0.107 |
| $S^d$ | −0.612 | −0.082 | −0.409 |
| $C^d$ | 0.665 | −0.513 | 0.005 |
| a | −0.034 | −0.009 | 0.693 |
| b | −0.662 | 0.208 | −0.228 |
| SI | −0.771 | 0.322 | −0.177 |

**Table 2**
Assignment of coal characteristics by factor analysis.

| Factors | Group 1 | Group 2 |
|---|---|---|
| F1 | **Inert**, ($C^d$, $W^a$) | **Vitr**, **SI**, $\boldsymbol{A^d}$, **b**, (PS, $S^d$, APD) |
| F2 | $\boldsymbol{V^{daf}}$, **Lipt**, **TPA** | $\boldsymbol{R_r}$, ($C^d$) |
| F3 | **a**, **BD** ($W^a$) | (APD, PS, $S^d$) |

primarily on coal rank and maceral group compositions but also on content and composition of the mineral phases and coal microporosity [3,4].

Minerals are present in the inorganic matter of fossil fuel coal (especially the major elements—Si, Al, Fe, etc.) and to a lesser extent in its organic matter (especially the trace elements—Hg, Se, Ni, Co, etc. [5]). The affinity of elements to the inorganic and/or organic matter of coal is considered to control element mobility [6]. It is supposed that elements with an affinity to organic matter and to sulfides are more easily volatilized (e.g., during the combustion process) than those elements with an affinity to silicate minerals [6]. Moreover, it is also supposed that inorganic matter to some extent catalyzes and influences various coal processing technologies [7–9].

The organic matter of coal is formed by three maceral groups: vitrinite, liptinite and inertinite. Macerals are microscopically recognizable individual constituents of coal with characteristic reflectance, colour, shape and relief. To a certain degree, they also differ from each other in terms of their chemical composition. To exclude any ambiguity in definitions of the different macerals, the ICCP has established a standard rule for their determination via petrographic microscopy [10–13]. The ability of macerals to reflect light from a polished coal surface is one of the most noticeable physical properties of coal. With increasing coal rank, the macerals vary, displaying changes in their chemical, physical and technological properties [14]. Changes in the optical properties of vitrinite during coalification, contrary to other macerals, have a continuous character [15]. At present, vitrinite reflectance and volatile matter characteristics have proved to be the most precise way of determining coal rank [13,14].

The following properties are usually used for the characterization of coal: moisture ($W^a$), ash content ($A^d$), volatile matter ($V^{daf}$), calorific value ($Q$), reflectance of vitrinite ($R_r$), vitrinite content (*Vitr*), inertinite content (*Inert*) and liptinite content (*Lipt*), content of $C^d$, $H^d$, $O^d$, $N^d$ and $S^d$ [16]; furthermore, for the selection of coal for coking, the contraction *a*, dilation *b* and swelling index *SI* are also determined [14]. For special purposes (e.g., for adsorption of gases on coal), structural properties such as total intrusion volume (*TIV*), bulk density (*BD*), porosity (*PS*), specific surface area (*SA*), etc., are also determined [17].

Coal of different ranks shows different characteristics (proximate, ultimate, etc.); however, only some of these characteristics change significantly when coal is exposed to different conditions (pressure, temperature, oxidizing or reducing atmospheres). This means that the difference between coal with various degrees of coalification can be characterized, or changes in the properties of coal subjected to different conditions can be monitored, by means of a reduced number of characteristics. For example, the regression between vitrinite reflectance and volatile matter is very often used for comparison of various coal ranks [14]. Further examples include the very simple regression between maximum ($R_{max}$) and random ($R_r$) reflectance of vitrinite for coal samples from the Upper Silesian Coal Basin [18]. Somewhat more complicated regressions have been obtained between technological properties and contents of *H*, *C* and *O* [3]. Other regressions studied include the regression of vitrinite reflectance $R_o$ with carbon (*C*) and hydrogen (*H*) [19] and/or the regression $R_{max}$ with chemical and/or

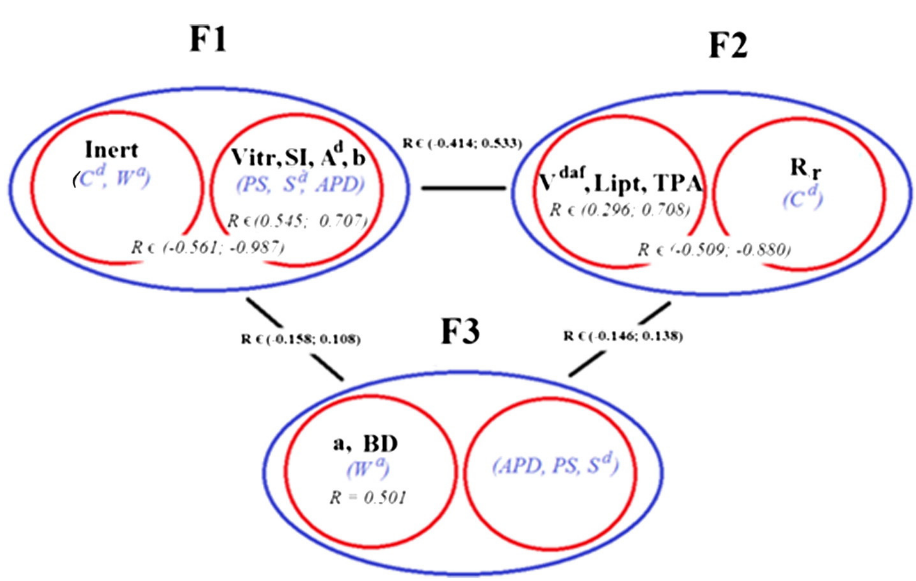


**Fig. 1.** Scheme of the calculated factors F1, F2 and F3 and mutual correlations among coal characteristics. (For interpretation of the references to colour in this figure, the reader is referred to the web version of this article.)