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Mapping of compositional properties of coal using isometric log-ratio transformation and sequential Gaussian simulation – A comparative study for spatial ultimate analyses data

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ABSTRACT

Chemical properties of coal largely determine coal handling, processing, beneficiation methods, and design of coal-fired power plants. Furthermore, these properties impact coal strength, coal blending during mining, as well as coal's gas content, which is important for mining safety. In order for these processes and quantitative predictions to be successful, safer, and economically feasible, it is important to determine and map chemical properties of coals accurately in order to infer these properties prior to mining.

Ultimate analysis quantifies principal chemical elements in coal. These elements are C, H, N, S, O, and, depending on the basis, ash, and/or moisture. The basis for the data is determined by the condition of the sample at the time of analysis, with an "as-received" basis being the closest to sampling conditions and thus to the in-situ conditions of the coal. The parts determined or calculated as the result of ultimate analyses are compositions, reported in weight percent, and pose the challenges of statistical analyses of compositional data. The treatment of parts using proper compositional methods may be even more important in mapping them, as most mapping methods carry uncertainty due to partial sampling as well.

In this work, we map the ultimate analyses parts of the Springfield coal from an Indiana section of the Illinois basin, USA, using sequential Gaussian simulation of isometric log-ratio transformed compositions. We compare the results with those of direct simulations of compositional parts. We also compare the implications of these approaches in calculating other properties using correlations to identify the differences and consequences. Although the study here is for coal, the methods described in the paper are applicable to any situation involving compositional data and its mapping.

1. Introduction

Aside from being characterized as containing only organic and inorganic compounds, coal is a chemically, petrographically, and physically complex and heterogeneous natural material, which is not easy to fully characterize for all of its properties. Its organic part contains different macerals as the building blocks, whereas the inorganic part contains different clays, minerals, and various major and trace elements. These compositional properties of coal and how they may interact with air, for instance, can significantly influence how it should be mined, handled, processed, utilized, and even how coal-fired power plants should be designed to reduce emissions. Moreover, these properties affect coal strength, coal blending design, as well as coal's gas content, which is important for mining safety. In other words, coal's properties and composition impact all processes, from its safe mining to its utilization in different industries.

Two of the basic and most common analyses to describe properties of coal are proximate and ultimate analyses. Proximate analysis determines moisture, volatile matter, ash, and fixed carbon within the coal (ASTM D121, 2006). These properties are important for coal utilization, as moisture and ash affect heat absorption and thus calorific value of coal. Ultimate analysis, on the other hand, is more detailed and involves the determination of carbon, hydrogen, nitrogen, total sulfur, oxygen, and ash yield. Carbon and hydrogen contents are determined by analyzing the gaseous products of the complete combustion of the coal, oxygen by difference, and total sulfur, nitrogen, and ash yield are based on the coal material as a whole. After corrections for carbon, hydrogen, and sulfur derived from the inorganic material, and for ash to mineral matter, the ultimate analysis represents composition of the organic material in coal in terms of carbon, hydrogen, nitrogen, sulfur,

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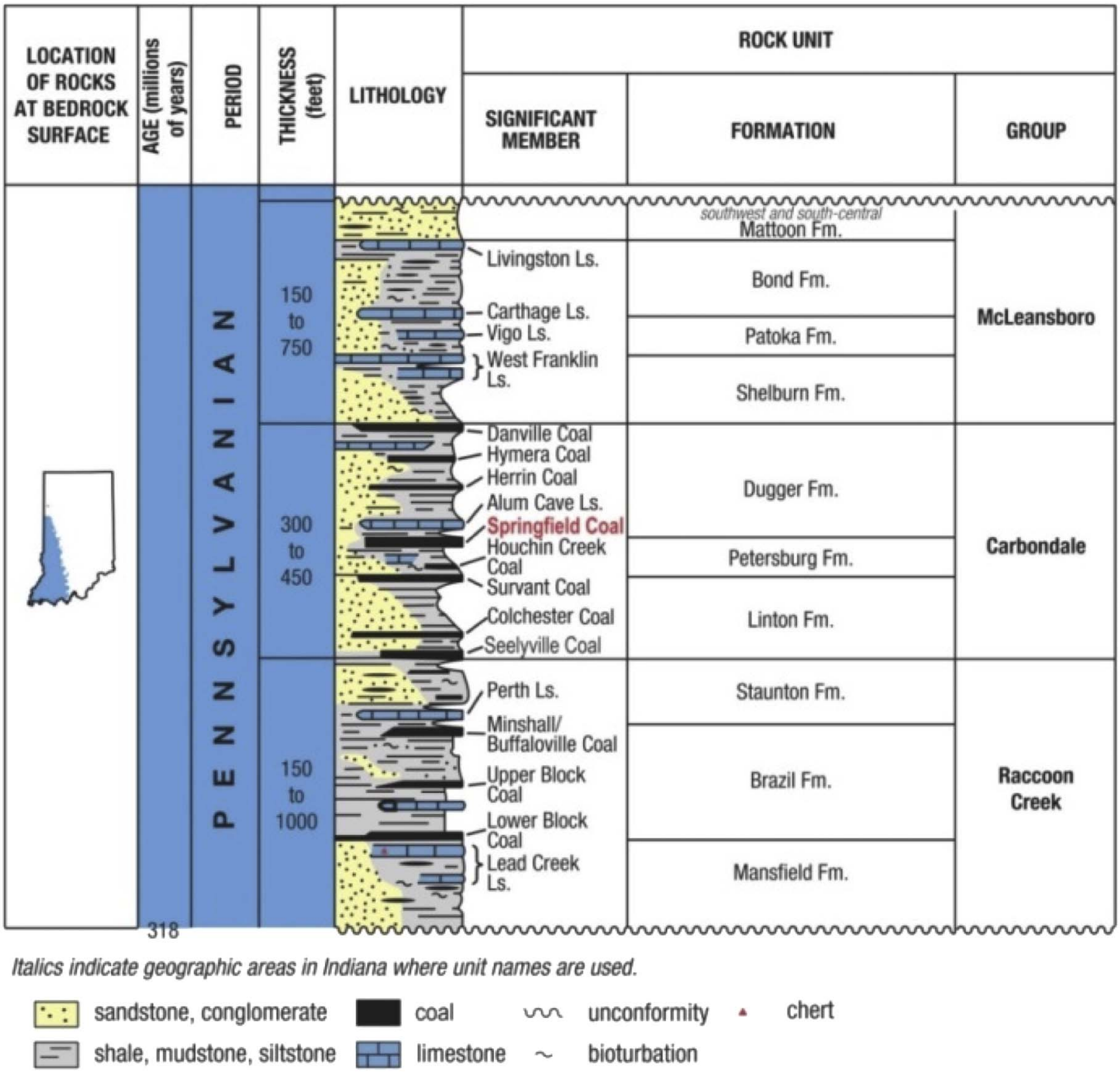

Fig. 1. General stratigraphy of Indiana's Pennsylvanian system of formations and coal members (after Thompson et al., 2013).

and oxygen (Riley, 2007).

The elemental composition of coal determined by ultimate analysis can be important for various purposes. For instance, it gives an idea about maturity of coal. Carbon, oxygen, and hydrogen are, to some degree, rank-dependent elements. The highest rank coals have the highest carbon contents and the lowest oxygen contents. High-volatile B and C bituminous coals, on the other hand, have the highest hydrogen contents, with decreasing amounts as rank increases. Therefore, ratios of these elements can indicate the rank of the coal and its coalification degree.

The results of ultimate analysis can also be used in different correlations to predict various properties of coal. Chelgani et al. (2008) investigated the effects of proximate and ultimate analysis, maceral content, and coal rank for a wide range of Kentucky coal samples on Hardgrove grindability index (HGI) using multivariable regression and artificial neural network (ANN) methods. One of the most comprehensive papers that cover correlations, such as density, the Hardgrove grindability index, the free swelling index, pyrolysis yields, direct liquefaction yields, and carbon dioxide yields, by using ultimate, proximate, and maceral analyses results, is published by Mathews et al. (2014). They reviewed 42 correlations found in the literature addressing multiple coal properties and compared against vitrinite-rich United States coals sampled from the Pennsylvania State University Coal Sample Bank and Database.

Mathews et al. (2014) concluded that while some correlations, such as calorific value predictions, are accurate over a wide range of coals, others are restricted in applicability to a select rank range. They interpret the limitation in applicability as a consequence of the creation intent of the correlations or to the complex nature of the coal. While these are true and valid arguments, all statistical analyses are done using compositional data (i.e. observations carrying relative information) such as ultimate, proximate, and maceral analyses. The outputs are used to correlate them to non-compositional data and, in some cases, to other compositional data. Therefore, the way that the data is handled and analyzed using classical statistics may make a difference as well in the predictive performance of correlations built on compositional data. Since ultimate analysis gives six partial components, as in the case of an "as received" basis to the whole—carbon (C), hydrogen (H), nitrogen (N), sulfur (S), oxygen (O) and ash—the results can be evaluated mathematically in the realm of compositional data analyses.

The ultimate analysis is a *D-part composition* of the whole, and its sampling space is the *D-part simplex* with a set of real vectors with positive components, which can be represented by a constant-sum constraint without loss of information (Otero et al., 2005). This constant value is 100% in the case of ultimate analysis on an "as received" basis. The compositional character of the vector, and thus its relative