



# Calorific value and compositional ultimate analysis with a case study of a Texas lignite



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## ABSTRACT

Measurements to determine coal quality as fuel include proximate analysis, ultimate analysis and calorific value. The latter is an attribute taking non-negative real values, so a simple transformation is sufficient for its spatial modeling applying geostatistics. The analyses, however, involve proportions that follow the properties of compositional data, thus requiring special preprocessing for an adequate modeling already described in a previous publication for the case of proximate analysis data.<sup>1</sup> Here we model the results of calorific value and ultimate analysis. We propose to use two different binary partitions, one per analysis, map the corresponding isometric logratio transformations, and backtransform the results. The methodology is illustrated using the same coal bed in the previous paper modeling proximate analysis data. Results are summarized using probability maps that, in the case of this deposit, show a prominent channel crossing the deposit and separating the best quality coal from that of lower quality.

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## 1. Introduction

Proximate analysis provides the weight percentages of the four components in which coal is customarily subdivided: ash, fixed coal, moisture and volatile matter (ASTM, 2013). These four parts include 100% of all chemical components of a coal. At least two other reports also provide measurements of coal quality. Ultimate analysis includes selected concentrations of elements primarily for the purpose of calculating the amount of air required for the complete combustion of a coal: hydrogen, nitrogen, oxygen, and sulfur (ASTM, 2015). The other typical laboratory measurement is the calorific value, a fundamental attribute when coal is intended to be used as fuel.

In the common situation when a proximate analysis is followed by an ultimate analysis of the same coal specimen, all elements in the latter analysis are counted twice. However, given an element, say, sulfur, it is unknown how such an element is dispersed among the proximate components of ash, fixed coal, moisture and volatile matter. In a previous paper, Olea and Luppens (2015) have reported a way to model the

proximate analysis parts according to the latest mathematical developments both in compositional data analysis (Pawlowsky-Glahn et al., 2015) and two-point geostatistics (Caers, 2011; Pycz and Deutsch, 2014). Here, we complete the coal quality modeling by mapping calorific values and the results of ultimate analysis.

## 2. Methodology

The calorific value can be considered a ratio scale attribute. For example, an increase by a factor of 2 in the calorific value will allow increasing to the same temperature a volume of water twice as large. The calorific value of coals can approach a value of zero, but it cannot be negative. Hence it cannot take all real values from  $-\infty$  to  $\infty$ , yet a transformation, as simple as a logarithmic transformation, is ordinarily sufficient for the adequate application of statistical and geostatistical methods. On the contrary, the information from proximate and ultimate analyses is compositional, thus requiring the application of logratio transformations.

Proximate and ultimate analyses offer the mathematical peculiarity of partitioning twice the same whole in two different ways. In addition, proximate analysis provides data for all four parts, while ultimate analysis provides concentrations for only a few of all possible elements in the periodic table. We postulate here that the data from these two coal quality analyses should be modeled using one binary partition for each analysis,

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<sup>1</sup> Olea, R.A., Luppens, J.A., 2015. Mapping of coal quality using stochastic simulation and isometric logratio transformation with an application to a Texas lignite. International Journal of Coal Geology, 152, 80–93.

followed by geostatistical modeling of the logratios. If the structural analyses reveal that the proximate analysis logratios are spatially correlated to those of ultimate analysis, then there should be a joint geostatistical modeling of both families of logratios using methods such as sequential Gaussian co-simulation (Verly, 1993). The benefits, however, will be marginal because at all sampling locations all attributes will be collocated. If there is no spatial correlation in the logratios, the mapping of ultimate analysis concentrations can proceed separately. A paper by Olea and Luppens (2015) explains in detail how to conduct the modeling using the isometric logratio transformation (ilr), which we advocate here as well: preparation of the binary partition matrix, calculation of logratios, generation of realizations and backtransformation to the original units.

### 3. Mapping case study

Fig. 1 displays the drill-core data for the two coal quality attributes not considered in the first part of the modeling of a Texas lignite (Olea and Luppens, 2015). Note that in this case ultimate analysis reduces to the bare minimum of one element: sulfur. The sulfur distribution has a severe positive skewness, while the distribution for calorific values is more mildly skewed in the opposite direction.

#### 3.1. Modeling of sulfur

First step is the preparation of the ilr transformation, which is trivial when only one part in the system has been measured: it involves the ratio of the measured element to the sum of all other components without measurements. In the case of sulfur,  $S$ :

$$ilr_1 = \sqrt{\frac{1}{2}} \ln \frac{S}{100-S}. \quad (1)$$

Dropping the constant, which is irrelevant for the modeling, the expression turns simply into the logratio of the part over its complement

$$\text{logit}(S) = \ln \frac{S}{100-S}, \quad (2)$$

which is known as the logit function or simply logit (e.g., Pardo-Igúzquiza and Heredia, 2011). Fig. 2 shows the transformed data.

The second step is the structural analysis, which did not find significant anisotropies. Differently from the case of the balances of

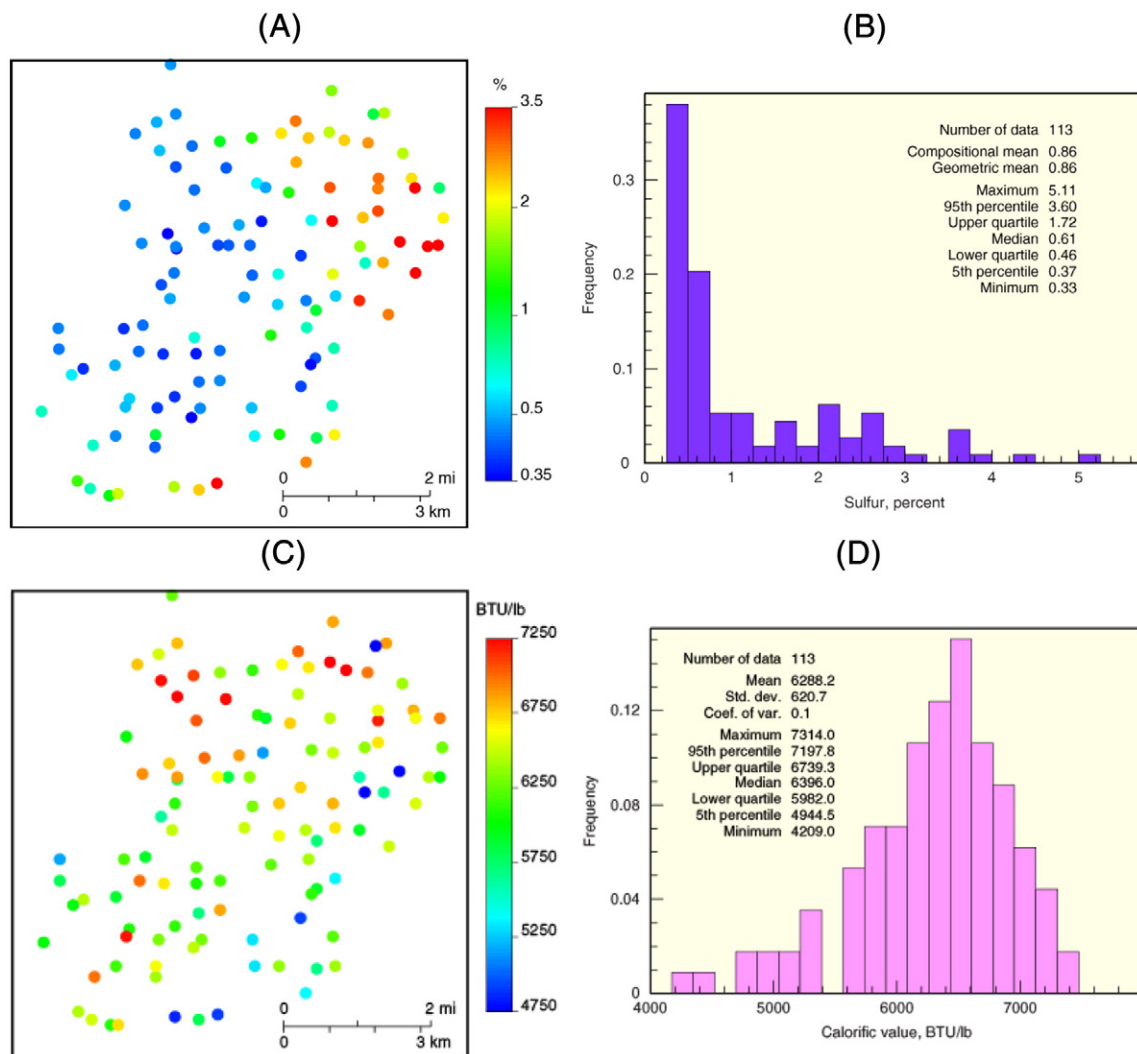


Fig. 1. Drill-hole data: (A) posting of sulfur concentrations in logarithmic scale; (B) sulfur histogram and listing of a few statistics; (C) posting of calorific values; (D) histogram and statistics of calorific values.

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