

Numerical Modeling of Reflectance of Coking Coals

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ABSTRACT

Quantitative image analysis has been used to obtain reflectance data on Vitrinite and Inertinite, because most coals are mixtures of these two macerals. The distribution of vitrinite reflectance follows a gaussian distribution, whereas the reflectance distribution of inertinite follows a gamma distribution. By changing the seven parameters that define these distributions, a replicated reflectance profile is modeled. Using this technique, the reflectance characteristics of any coal can be modeled numerically with precision, and to date, several hundred natural coals with vitrinite contents from 23% to 100%, inertinite contents of 0% to 77%, and vitrinite reflectances from 0.5% to 1.7%, have been examined. By using this technique, accurate information on vitrinite reflectance (rank), group maceral composition (type), and blend design can be rapidly obtained, without reference to traditional methods of petrographic analysis, or terminology.

1. INTRODUCTION

The optical analysis of coal using automated or semi-automated equipment is not new. With older systems, reflectance measurements were made on binder, mineral-matter, and coal, because discrimination between valid data and contaminants was not possible. More recently, analyses of video images have eliminated measurements made on binder, mineral matter and grain edges, and provide "clean" data. The apparatus used in this study consists of a petrographic microscope with a CCD digital camera, a 200Hz scanning stage, an autofocus device, and a 486i-based computer with 8-bit image-capture board. The system as described is capable of collecting 2 million readings per minute [1]. With such large amounts of data, smooth histograms and probability plots can be created, which then form the basis of numerical modeling experiments.

Regardless of the data-capture system used, reflectance data still require interpretation. Historically, this has taken the form of a reflectance histogram (reflectogram). Interpretation of such graphs may have included an estimate of the random reflectance of the vitrinite based on the location of a peak, and perhaps an estimate of the amount of vitrinite. But where coals have been mixed to form a blend, the interpretation of the reflectance histogram may have been difficult, with accurate determinations of proportions of blended coals, probably impossible.

The purpose of this paper is therefore to describe apparatus and data analysis techniques that allow the capture and interpretation of "clean" reflectance data.

2.MATHEMATICAL MODELING

The distribution of coal reflectivity follows a general pattern, in which the vitrinite population, at the front of the histogram forms a peak that follows a normal distribution. The Inertinites form the tail of the graph, with a portion of the inertinites overlapping the vitrinites. All single coals have this pattern, with the peak and the tail varying in size and location. Similarly, probability plots of single coals always follow a pattern. The steeper forward part of the curve is the vitrinite, whereas the shallower upper part of the curve is the inertinite. The amount of vitrinite relative to the inertinite determines the length of the steep curve and the amount of the flatter curve [2].

Modeling can be done on the reflectance curve or the probability plot, and involves the replication of the reflectance profile of the coal by iterative manipulation of the model. The replicated profile generated is as close as possible to that of the sample, so that the sum of the squared differences between the model and the coal for each of the 0.01% reflectance cells is the minimum achievable. This is quantified as the square root of the mean squares error (RMS). Because the characteristics of the replicated model are known, the petrography of the underlying coal sample can be inferred.

The normal distribution function is used to describe the vitrinite component of a single coal as a normal curve with a four sigma radius. It is modeled using the three parameters:-

1. Mean of the vitrinite reflectance,
2. Standard deviation of vitrinite reflectance,
3. Percentage vitrinite present.

The Inertinite component is modeled using a modified gamma distribution defined by the four parameters:-

1. Percentage of Inertinite present,
2. Starting reflectance value for the curve,
3. Alpha function, and
4. Beta function.

3.RESULTS & DISCUSSIONS

Single-coal populations are distinguished from blends by standard deviations of the vitrinite population of <0.09 . However, two other factors must be considered when evaluating the size of the standard deviation. A single-seam coking coal with 90% vitrinite will have a smaller vitrinite standard deviation (~ 0.06) than a coal of the same rank but with only 30% vitrinite (~ 0.085). Similarly, coals with vitrinite reflectances of $R_o > 1.5\%$ have larger vitrinite

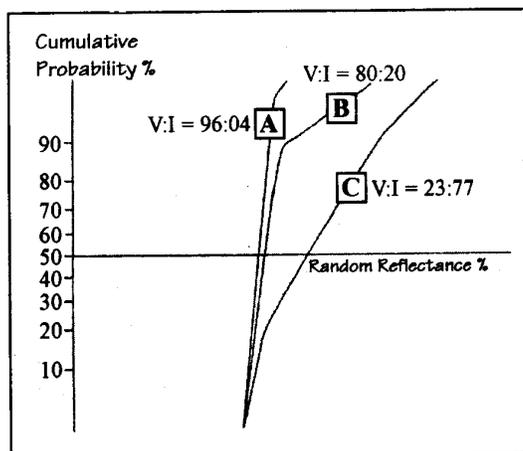


Figure 1.

Changes of model profiles of single seam coals caused by variation of the Vitrinite : Inertinite ratio.

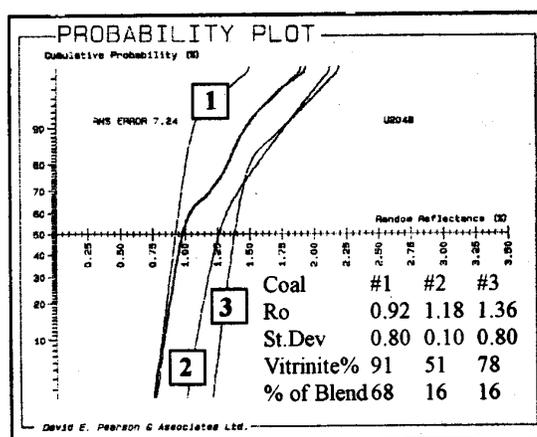


Figure 2.

An example of the modeling process. The component coals 1, 2 & 3 were mixed to generate a blend with the sigmoidal profile. This profile was replicated using the model.

standard deviations than say, coals with $Ro \sim 0.8\%$, because the spread of reflectance is greater at higher ranks. The slope of the vitrinite curve on probability plots is controlled by the standard deviation of the vitrinite population, so probability profile-changes in response to changes in the proportions of vitrinite and inertinite are easily identified. In Figure 1, modelled probability curves for three distinctly different single coals are shown, each with a different ratio of vitrinite and inertinite, but with the same vitrinite reflectance (rank).

Blends of coal can be mixtures of similar rank, or mixtures of dissimilar-rank coals. When the vitrinite reflectance of mixed coals are separated by more than 0.15% reflectance, a sigmoidal flexure occurs in the probability profile [2]. Figure 2 is a probability plot and a replicated model showing this sigmoidal curve, in which Coal #1 is lower in reflectance and dissimilar rank from Coal #2 & Coal #3. The three modeled component coals are also shown. One of the coals is actually a two-coal blend of similar rank (with $Ro=1.18\%$ $St.Dev=0.100$); whereas the other two coals are single seam coals (with $Ro=0.92\%$ $St.Dev=0.080$, & $Ro=1.36\%$ $St.Dev=0.80$).

The ability of this numerical modeling method to determine blend proportions is also demonstrated in Figure 2. The replicated curve using the three component coals, showed a best-

fit at a blending ratio of 68:16:16. This was the blending ratio used and later revealed by the laboratory that prepared the samples for the test.

4.CONCLUSIONS

Reflectance data from automated digital petrography have been interpreted by numerical modelling involving the replication of a reflectance profile. Because of their superior reproducibility and speed of acquisition, such analyses will eventually be preferred over manual analyses. The acceptance of replicated numerical models as digital "fingerprints" of coals, together with the recognition that coals are numerically definable, will lead to new classifications of coking coal, in which single coals and mixed coals will be identified and quantified. Numerically definable coals will become geomarkers in coal quality assurance, and quality monitoring.

REFERENCES

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