Pearson Coal Petrography Research

Probability analysis of blended coking coals

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ABSTRACT

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Probability analysis of vitrinite-reflectance data and whole-coal reflectance data involves assigning a probability based on the standard deviation of each reflectance value measured, and displaying data in the form of probability graphs. These graphs, which plot cumulative probability versus reflectance, use a non-linear probability scale, that converts the sigmoid curve of the cumulative normal distribution into a straight line.

In probability graphs, vitrinite reflectance data from single coals plot as straight lines, the slopes of which depend upon the standard deviation of the readings. Blends are recognized by their distinctive patterns of curves and inflection points. Whole-coal reflectance probability plots also have distinctive patterns depending on rank, coal type, and number of coals involved.

The proportions of constituent coals in blends can be read directly from the probability scale of vitrinite reflectance probability plots, but these values must be corrected for the vitrinite-contents of the component coals. By contrast, the direct calculation of constituent coal proportions is possible from whole-coal reflectance data using probability analysis and iterative computer modelling.

INTRODUCTION

Vitrinite reflectance data from single-seam and blended samples, are usually tabulated in the form of frequency distributions, where the individual reflectance values are classified into groups of either 0.1O% reflectance (the V-types), or 0.05% reflectance (the Half V-types). In this format, V-type groups are used in some computations of predicted coke-strength, and may be plotted as vitrinite histograms (ICCP Handbook, 1971).

The proportions of coals in a blend are often checked using this vitrinite distribution, but because the amounts of the vitrinite maceral in the constituent coals may vary widely, and this is not recognized by the analysis procedure, these estimates are commonly in error. And, in those instances where considerable overlap of the constituent coal V-types occurs, it is even more difficult to establish proportions of the constituents.

Probability analysis of reflectance data is very rarely reported, perhaps because the analysis of vitrinite is often of a single population from a single coal, and it is only in cases where more than one population of vitrinite is present that this method of data analysis is useful. Probability analysis is therefore most commonly used in statistical analyses of geological data where mixing of populations is expected, and there are examples of interpretations of geochemical, geophysical and mineral exploration data (Sinclair, 1981).

PROBABILITY ANALYSIS OF REFLECTANCE DATA

Probability analysis of geological data involves the use of standard cumulative probability paper and the interpretation of probability graphs. Fortunately, many statistical software-packages for personal computers now include probability analysis, and the techniques involved in partitioning probability-graphs, and in their interpretation have been well explained (for example, Sinclair, 1981). Probability paper has an arithmetic scale (in this instance, vitrinite reflectance), and an unusual cumulative percentage (probability) scale, which is designed such that a cumulative normal distribution will plot as a straight line (Fig. 1). Although the scale is non-linear for cumulative percent, it is linear for numbers of standard deviations from the central reference value, or population mean. Figure 1 shows the relationship between the cumulative probability and standard deviations for a normally-distributed population. It can be appreciated from Fig. 1, that the more peaked a normal distribution is (greater kurtosis), the steeper will be the line joining the known cumulative percentages of the probability scale, and vice-versa.

To use vitrinite reflectance data in probability analysis, the mean of the series is computed, and a standard deviation calculated for each reflectance value. Reference is then made to statistical tables which give the probabilities associated with standard deviates.

There are two types of coal reflectance data which can usefully be examined by probability analysis:
(1) Vitrinite reflectance data.
(2) Whole-coal reflectance data.
The patterns displayed by single and mixed populations of these data types on probability graphs are different and are discussed separately below.

It is emphasized that probability analysis is a statistical technique for obtaining more information from reflectance data. With regard to precision and accuracy, (topics which were raised by reviewers of this article), these are terms that refer to reproducibility in the data-acquisition technique, and are analytical parameters that are not addressed in this paper.

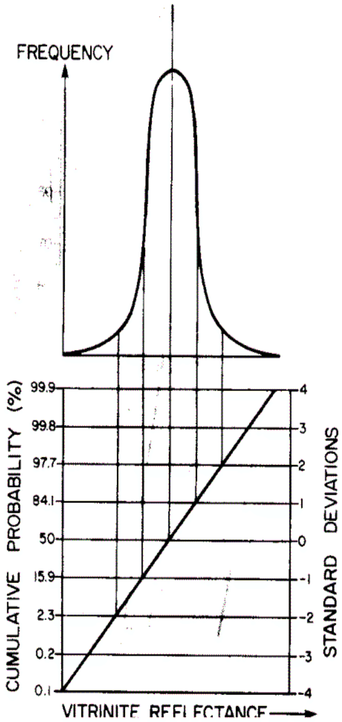

Figure 1.
Diagram showing the relationship between cumulative probability (%) and standard deviations for a vitrinite reflectance population from a single coal, showing a normal distribution. The upper diagram is a frequency histogram and the lower diagram is a probability plot of the same data.

PROBABILITY GRAPHS OF VITRINITE REFLECTANCE DATA

Single vitrinite populations

The patterns of single-seam coals, which possess single populations of vitrinite reflectance, are simple, and plot as straight lines on probability paper. As examples, four single-seam coals, A, B, C and D, with maximum vitrinite reflectance (R_{omax}) values of 0.85%, 1.01%, 1.09% and 1.35%, are shown in Fig. 2. The slope of these lines is governed by both the standard deviations of the distributions, which is a function of rank, and by the reflectance scale on the abscissa of the graph. The standard deviation of single coals with a R_{omax} reflectance of 0.50% is about 0.03; with R_{omax} = 1.00%, St.Dev. ~0.05; and with R_{omax} = 1. 5%, St.Dev. ~0.06. In probability graphs, the mean reflectance of a single population of vitrinite can be read from the cumulative probability scale at the 50% level, and the standard deviation can also be determined by reference to the 16% and 84% levels.

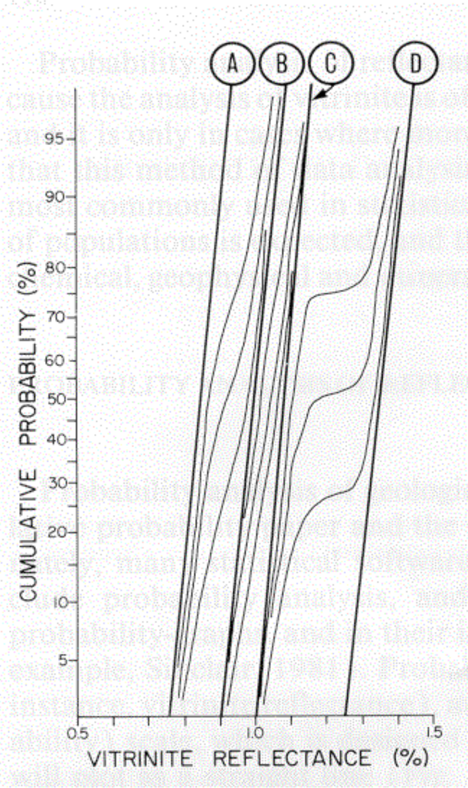

Figure 2.
Diagram showing straight-line probability plots of four single vitrinite populations, A, B, C and D and three vitrinite mixtures, A-B, B-C and C-D. The further apart the R_{omax} of the constituent vitrinites, the more pronounced the curves and inflexion points.

Binary vitrinite populations

Where two different coals are combined, two separate populations of vitrinite are mixed, and a probability plot of the blend generally will not have a straight-line distribution. If the separation between the Rornax values of the two coals is large enough, it is likely that the distribution will have a distinct stepped-shape, with a pronounced inflection point. Figure 2 shows computer-generated mixtures of three blends, A-B, B-C and C-D, in three different different percentages of mixing, 25:75, 50:50 and 75:25.

The proportions of vitrinite in a mixed population can be read directly from the probability scale. Thus, in the case of blend C-D, in Fig. 2, the proportions of the two parent vitrinite populations is chosen as the inflection point between the two directions of curvatures of the line. The location of the inflection point occurs precisely at the cumulative percentile that represents the proportion of that vitrinite population in the blend.

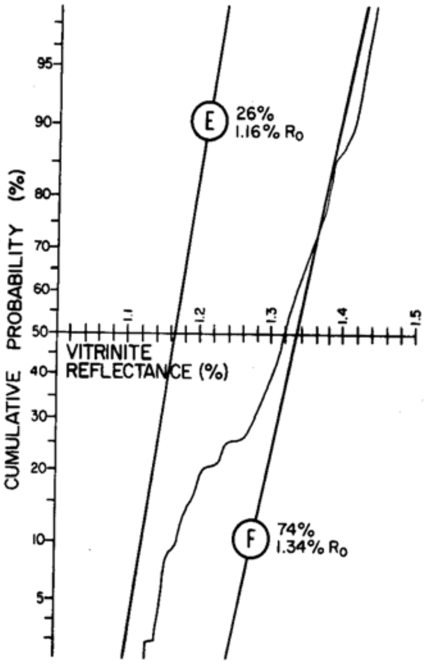

Figure 3.
Probability analysis of 100 vitrinite reflectance R_{omax} readings. The data have been partitioned into two populations of vitrinite, 26% from a coal with a R_{omax} of 1.16% and 74% from a coal with a R_{omax} of 1.34%.

In the case of blend C-D, where the R_{omax} separation between the coals is 0.26%, obvious partitions of the population can be made at 25%, 50% and 75% cumulative probability. However, there is only a 0. 1 6% difference in R_{omax} between coals A and B and the three examples of blend A-B display only a small inflection. This is more a function of the abscissa scale used, because an actual blend (E-F), with a similar R_{omax} separation of 0.18%, but with an expanded scale, displays the distinctive stepped-curve (Fig. 3).

In the third blend shown in Fig. 2, there is a R_{omax} difference of only 0.08% between coals B and C. The probability plot of this blend has a shallower slope than the two component coals, but the distinctive stepped-shape is absent. In such cases, the separation into component vitrinite populations is made by choosing a partition point so that the standard deviations of the populations are balanced on either side of the partition point.

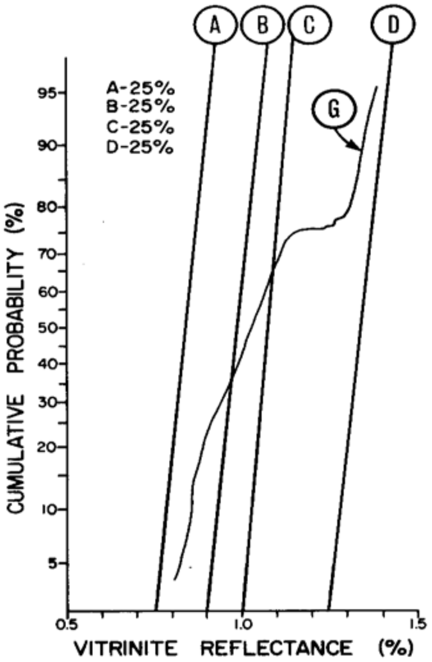

Figure 4.
Four single populations of vitrinite A, B, C and D (from Fig. 2), have been mixed in equal proportions to generate plot G, a theoretical 4-vitrinite blend.

Multiple vitrinite populations

Where more than two populations of vitrinite are mixed, as usually happens in the preparation of coal blends at coke plants, the resulting probability plot is not a straight line, but has a series of inflection points, or changes in curvature, depending on the number of the constituent coals, and also the difference between the reflectances. The partition of the graph and its interpretation however follows the same techniques described above. For example, a hypothetical four-coal vitrinite plot is shown in Fig. 4, where equal portions (25%) of coals A, B, C and D have been mixed in a computer simulation to make coal G. Obvious changes in the slope of the line occur at cumulative probabilities of 25% and 75%. The shallower slope of the central portion between these two inflection points indicates that these vitrinites are also from a blend.

CONSTITUENT-COAL PROPORTIONS FROM VITRINITE REFLECTANCE DATA

Vitrinite reflectance analysis is concerned with only one maceral component of coal and, consequently, the proportions of vitrinite populations determined by probability analysis are not the same as the proportions of coals in the blend. The probability analysis has assumed a vitrinite-only composition to the coals present in the blends and these have to be corrected for the vitrinite contents of the constituents obtained from maceral analysis using the following formulae.

TABLE 1

Calculation of blend composition

	Coal #1	Coal #2	Coal #3
Vitrinite populations from probability plot(%) (Obtained from reflectance analysis of blend)	26	54	20
Percent vitrinite (Obtained by maceral analysis of component coals)	90	62	70
Percentage of coal in blend	20	60	20

If the proportion of vitrinite in each of the constituent coals is known, then the actual proportions of the constituent coals in the blend can be computed, as follows.
Let the percentage of vitrinite population from probability plot analysis= P_1 Let percentage of vitrinite in the coal from maceral analysis= M_1

In a binary bend, (for example), $P_1 / M_1 = C_1$, and $P_2 / M_2 = C_2$, and $C_1 + C_2 = T$. The proportions of the constituent coals, B_1 and B_2, in the blend are given by $B_1 = C_1 / T * 100$ and $B_2 = C_2 / T * 100$. Table 1 shows a worked example from a ternary blend.

PROBABILITY GRAPHS OF WHOLE-COAL REFLECTANCE DATA

Whole-coal reflectance data, obtained by automated- or manual-scanning of coal samples by photometer-based, or video-image analysis techniques, can also be analysed effectively by probability analysis. Detailed histograms of reflectance and grey-levels from such systems provide a rapid visual means of comparison of similar coals, but further analysis quantifying the differences has been rare.

Single-coal populations

Two single whole-coal probability plots are shown in Fig. 5. Coal H, with a $R_{omax} = 1.07\%$, is a vitrinite-rich Pennsylvanian-age coal which contrasts with a western Canadian, inertinite-rich, single-coal J, with a $R_{omax} = 1.61\%$, of Cretaceous age. Although these coals are of quite different type (in the case of coal H, 12% of the coal is inertinite, whereas 33% of coal J is inertinite), coals similar to them cover the coking coal reflectance range (R_{omax} = 0. 60%-1.80%) and continuous variation exists between them.

The probability plots of coals H and J are distinctly different. The steeper, lower-reflectance part of each coal's probability plot is caused by the vitrinite,

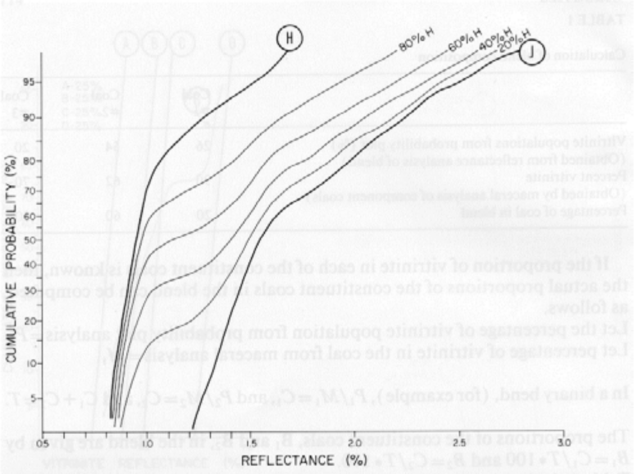

Figure 5.
An example of graphic blend design using probability analysis of whole reflectance data from two distinctly different coals, H and J. Coal H, is a typical high-volatile, vitrinite-rich coal. Coal J, is a typical inertinite-rich, low-volatile coal. The four blends show increasing percentages of H with J.

and the shallower, higher-reflectance portion is caused by inertinite. The older coal has about 77% vitrinite and the younger, 60% vitrinite. Vitrinite-rich coals have longer steep (vitrinite) slopes and shorter, inertinite tails, like coal H. In contrast, inertinite-rich coals, the typical Canadian and Australian coking coals, generally have shorter vitrinite slopes, and longer inertinite tails, like coal J.

The steep vitrinite slope and the shallower inertinite tail, is a shape superficially similar to that which would be generated by a mixture of two normally-distributed populations, one with a small distribution (vitrinite), and the other with a wide distribution (inertinites), described by Sinclair (1981) (Figs. IV-5 and IV-8). To examine this possibility, the actual distributions of inertinites from 58 1000-measurement whole-coal reflectograms of western Canadian coking-coals were compared with theoretical, similar, normal distributions, using the Kolmogorov-Smimov test. The results of this study showed that the inertinites of all 58 samples failed the test for normality, and the apparently normal distribution of inertinites is fortuitous (Pearson, 1986). Hence, only the vitrinite portion of whole-coal reflectance data is normally distributed. The inertinites do not follow a normal distribution.

PROBABILITY ANALYSIS OF BLENDED COKING COALS

Binary coal populations

Coals H and J, being of quite different rank and type, are shown in computer-generated mixtures of various proportions in Fig. 5. The proportions of mixing of the component coals H:J are 20:80, 40:60, 60:40 and 80:20, but the proporitions of H determined from the probability scale are 17.5%, 35%, 52% and 70% respectively. The proportion of normally distributed material in the blend determined by this technique is 87.5%, which suggests that some of the low-reflecting inertinite (the "reactive" semifusinite), also falls in this category.

The patterns displayed by binary coal mixtures are not always of the stepped-variety described above. Where the constituent coals in a binary blend are close in terms of reflectance, the resulting pattern is like that of a single coal, with a slope to the vitrinite portion of the curve intermediate between the two components.

Multiple coal populations

Where numerous coals are mixed, the vitrinites from one coal will have the same reflectance as inertinites from another. Because the probabilities are based on standard deviations from the mean value of the whole-coal reflectance data, the resulting pattern is a gently curved line, with no obvious in-flection points. In such cases, only if the reflectance characteristics of the individual component coals are known can iterative computation allow the blend recipe to be calculated and contaminants recognized, as described below.

CONSTITUENT-COAL PROPORTIONS FROM WHOLE COAL REFLECTANCE DATA

The biggest advantage of using probability analysis of whole-coal reflectance data is that a coal is represented by a single line, and the effects of blending can be more easily appreciated as changes to the line, rather than as modifications to the shape of a multi-celled, whole-coal reflectogram. For instance, computer modelling of coal blends using probability analysis allows both the desired recipe and actual samples to be compared. Such an example is displayed in Fig. 6, which shows a compute-modelled five-coal blend K, designed from three coal components, L, M and N, in the percentages 20:20:60. The coals L and M are single coals, but coal N is itself comprised of three coals (as may be deduced from its shallower vitrinite slope). A commercial sample of the blend P, is also shown in the diagram. By iterative computer modelling, the commercial sample was ascertained to have the coals L, M and N in the percentages 0:35:65 (Pearson and Wozek, 1991).

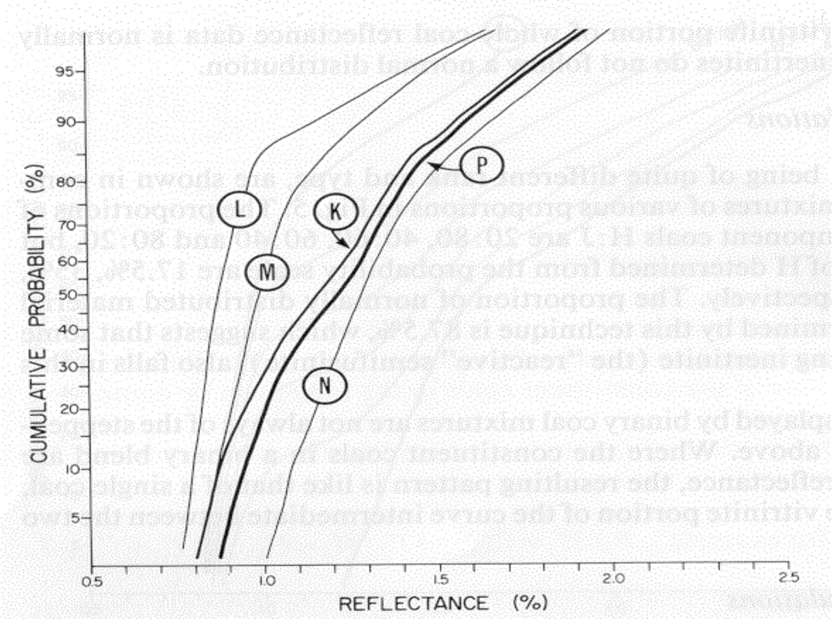

Figure 6.
An example of the commercial application of probability analysis in an investigation of product quality. The target blend recipe using the three coals, L, M and N, in proportions 20:20:60, would give the probability plot of coal K. Coal P, which is a commercial sample, shows a deficiency in the product of the component coal L, and has the composition 0:35:65.

CONCLUSIONS

Increasingly, statistical process control (SPC) will dictate that raw materials for manufacturing processes vary only within known boundaries. For blended coking coals, application of probability analysis to vitrinite reflectance data can be used to evaluate mixing-technology and to monitor blend consistency, for improved plant efficiencies.

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