

Letters to the Editor

Discussion of "The Use of k Values in the Interpretation of Glass Density and Refractive Index Data"

Dear Sir:

In a recent article in this journal (Vol. 34, No. 6, Nov. 1989, pp. 1323–1328), Thornton proposed improved interpretation of glass density and refractive index data using a k value, calculated by taking the ratio of dispersion to density. This approach is informative in that it takes a closer look at the processes controlling measured physical parameters than does the traditional approach of comparing ranges for each parameter independently. Thornton's article is timely because improved consistency in the physical and optical properties of glass, resulting from recent changes in sheet glass manufacturing processes, may make it more difficult to distinguish between similar glass fragments [1].

However, an important point omitted in Thornton's discussion is the influence of analytical precision on the calculated k values. As stated by Thornton, the k value should be constant across a sheet of glass of slightly varying composition, because dispersion and density vary concordantly. However, analytical precisions of the four measurements which go into the k value dictate a limit on the ability to distinguish between similar values of k . This point is illustrated by taking Thornton's data and placing uncertainty measures on each of the calculated values. For this calculation, assume all refractive indices are measured with a precision of 0.000 04, as stated by Thornton, and individual density measurements are made with a precision of 0.0003, the value given by Miller [2]. Thus, FBI Glass 222, used as an example by Thornton has the following properties:

$$n_c = 1.5137 \pm 0.000\ 04$$

$$n_D = 1.5162 \pm 0.000\ 04$$

$$n_F = 1.5223 \pm 0.000\ 04$$

$$D = 2.4870 \pm 0.0003$$

[Note: The analytical uncertainty in refractive indices implies a greater number of significant figures than generally reported.] Propagation of these uncertainties into calculation of Thornton's k value yields:

$$n_F - n_c = 0.0086 \pm 0.000\ 057$$

$$V = 60.0233 \pm 0.3948$$

$$k = 24.1348 \pm 0.1588$$

Using a 3σ comparison criterion, k values which differ by less than 0.5 are analytically indistinguishable. In comparison, Thornton suggested a 3σ value of 0.001 as a criterion to differentiate between within-source and across-source variation. In his discussion, Thornton compared k values for a glass with the values calculated after having the refractive index and density elevated or depressed, but within the "Miller criteria" for within-sheet variation. In the worst cases, the change in the value of k was 2000 times the 0.001 criterion. The large magnitude of this number implies a great sense of discrimination capability when using the k value approach. In comparison, the same worst-case change in k is only four times the 0.5 criterion derived from consideration of analytical precision.

Estimation of the effects of changing a discrimination criterion for k from 0.001 to 0.5 can be seen by applying both criteria to the seven examples in Thornton's Table 1. By either criterion, Cases 2 and 3 are indistinguishable from Case 1. Application of either

criterion results in classifying Cases 4, 5, and 6 as sources separate from Case 1. The only cases for which results using 0.001 and 0.5 as criteria differ are Cases 7 and 8. These cases, with k values of 0.019, are analytically indistinguishable from Case 1, but are differentiated as separate sources when using the 0.001 criterion. In these cases, which Thornton calls the severest test of the k value concept, all refractive indices are varied in the same manner, but opposite to the change in density.

Consideration of the individual contributors to the precision and discrimination capability of the k value is instructive. The most important term in the overall calculation of the precision of k is the $n_f - n_c$ term in the denominator of V . The random error associated with each refractive index term is 0.000 04, or about 0.006% of the value of the index. However, the precision of the difference is 0.000 057, or about 0.7% of the relatively small difference. This uncertainty dominates other precision terms (that is, n_D and D) in calculating the uncertainty associated with the k value. The importance of the difference term is seen in Thornton's Cases 4 and 5, for which n_c and n_f are varied by 0.0004 in opposite directions. The $n_f - n_c$ term then changes by 0.0008 and the highest k values are observed.

Several alternative approaches can be used to combine the positive aspects of the k value approach with the analytical precisions. For example, k'' , the ratio of n_D to D , can be used for comparison and a dispersion measure considered separately. The values of k'' and its associated precision using the preceding example are $0.609\ 65 \pm 0.000\ 075$. Thus, a 3σ within-source variation criterion for k'' is 0.0002, or about 0.03% of the k'' value. For dispersion, consider the following. If n_c and n_f each have a within-item variation of 0.0004 (or about 10 times the analytical uncertainty, which can thus be ignored), then their difference should have a within-item variation of 0.000 56 if they are independent and less if they act concordantly. The two examples of Thornton in which $n_f - n_c$ were changed by 0.0008 exceeded this expected maximum, although they fit within the Miller criteria if each value were to be considered independently. Using k'' and $n_f - n_c$ as comparison criteria results in better discrimination capability than using k with a cutoff of 0.5.

Another approach, which this author favors, is to determine the range of each of the individual refractive index, dispersion, and density measurements among fragments from the known-source exemplar in each case. Using these as criteria for determining within-source variation (both analytical precision and source heterogeneity combined) provides a more valid means of discriminating similar sources than applying fixed criteria, such as those of Miller or the k or k'' approaches. For many window glasses, particularly those of modern manufacture, the variation in refractive index is less than that in the Miller criteria. Use of within-source variations of refractive indices in the 0.0001 to 0.0002 range provides improved discrimination of similar sources in comparison with the fixed criteria and has the advantage of not relying upon assumptions based upon generalized studies of glass homogeneity. Variations in values of $n_f - n_c$ are also in the 0.0001 range, since true heterogeneity in the glass affects them in a concordant manner, and n_c and n_f rarely, if ever, change significantly in an opposite sense in comparing one fragment with another from the same source.

In summary, Thornton's approach is excellent in that it encourages a closer look at the data generated in glass comparisons and asks the glass examiner to consider the chemical processes which led to the observed values. However, it is important that one also consider both the analytical and within-source variations specific to each individual case in forming an opinion concerning glass comparisons.

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References

- [1] Koons, R. D. and Hall, B. W., "Elemental Analysis of Sheet Glass Fragments for Source Discrimination," paper presented at the American Chemical Society National Meeting, Washington, DC, August 1990.
- [2] Miller, E. T., "Forensic Glass Comparisons." *Forensic Science Handbook*, Vol. 1, R. Saferstein, Ed., Prentice-Hall, Englewood Cliffs, NJ, 1982.

Discussion of "The Biohazard Potential of Cyanide Poisoning During Postmortem Examination"

Dear Sir:

I was reading the article "The Biohazard Potential of Cyanide Poisoning During Post-mortem Examination" (Andrews, et al., *Journal of Forensic Sciences*, Vol. 34, No. 5, Sept. 1989, pp. 1280–1284), when I was struck by the following very curious phrase describing air movement: "exhaust fan (rated at 2683 m³/s (4560 ft³/min production)" (page 1281).

First—there is a parenthesis missing. Then, there are the mathematics: surely "m³/s" is cubic metres per second?

The *Handbook of Chemistry and Physics* indicates that there are 35.315 ft³ per cubic metre, and I have always heard that there were 60 s per minute, thus 2683 m³/s is 2683 × 35.315 × 60 = 5 685 008.7 ft³/min. This is truly an impressive fan!

Most curious the fact is that our figures disagree by 1246.7—or did I miss something somewhere?

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