Chemometrics

Application Note

Analysis of Petroleum Mixtures

Abstract

One challenge in petroleum analysis is to determine the proportion of different sources of oils in a mixed oil. Software tools exist for this purpose; this note describes a demonstration of the capability.

A series of mixtures of kerosene (Jet A) and diesel fuel were prepared in order to evaluate the use of Pirouette® to unmix the chromatograms. These mixtures ranged from pure kerosene to pure diesel in 10% steps. The chromatographic traces of all mixtures are shown in Figure 1.

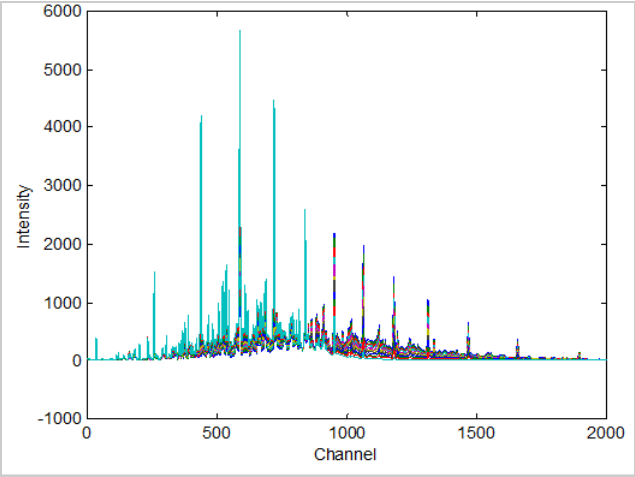

Figure 1. An overlay of 11 mixed chromatograms ranging from pure kerosene to pure diesel

Data were collected on an Agilent 6890 GC using EZChrom as the processing software, and the software method was directed to export an AIA file. Pirouette supports any system that saves AIA (netCDF) files, including Agilent, ChromPerfect, Beckman, Shimadzu, Waters, Thermo and PerkinElmer. LineUp was used to align the data files, removing inconsistencies in retention time.

In this test, we removed from the data set those samples containing pure kerosene and pure diesel, then ran the mixture analysis algorithm. Note that this algorithm was not supplied any of the original mixing proportions. The algorithm estimates the pure end member profiles and determines the proportion of each end member in every mixture. The analysis requires only a few seconds.

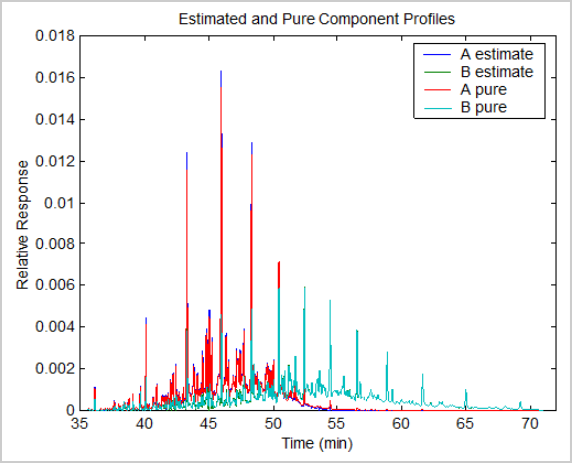

Figure 2: Comparison of the estimated pure kerosene and pure diesel to actual (A = kerosene, B = diesel)

Figure 2 shows the estimates of the pures along with the actual pure chromatograms for both kerosene and diesel.

The correspondence between the estimated and the actual profiles is very high: the traces are almost perfectly superimposable. There is also little variability even if the peaks in the chromatogram are considered one-at-a-time. This can be seen by zooming in on a portion of the chromatogram, as in Figure 3.

Mixture #	Measured % Diesel	Inferred % Diesel
2	10	10.4
3	20	20.3
4	30	28.2
5	40	41.0
6	50	49.4
7	60	60.4
8	70	68.4
9	80	79.9
10	90	88.2

The results for the prepared samples can be compared to the nominal concentrations in the following table.

If we use only the pure kerosene and the pure diesel chromatograms, we can build a mixture analysis model which can then be used to estimate the concentrations of diesel and kerosene in any future sample.

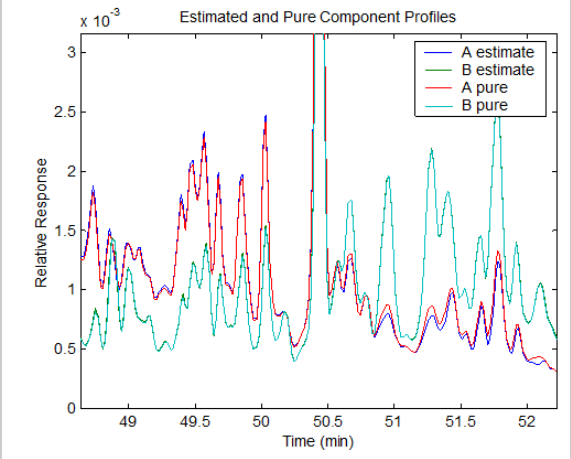

Figure 3: Comparison of the estimated pures to actual chromatograms (zoomed portion around 50 minutes)

This Pirouette technique works well, but the kerosene and diesel chromatograms have unique regions (where one has peaks and the other does not). We have demonstrated that this unique region is not needed, although it does help improve the accuracy of the estimates.