



Detailed Hydrocarbon Analysis Downstream Applications

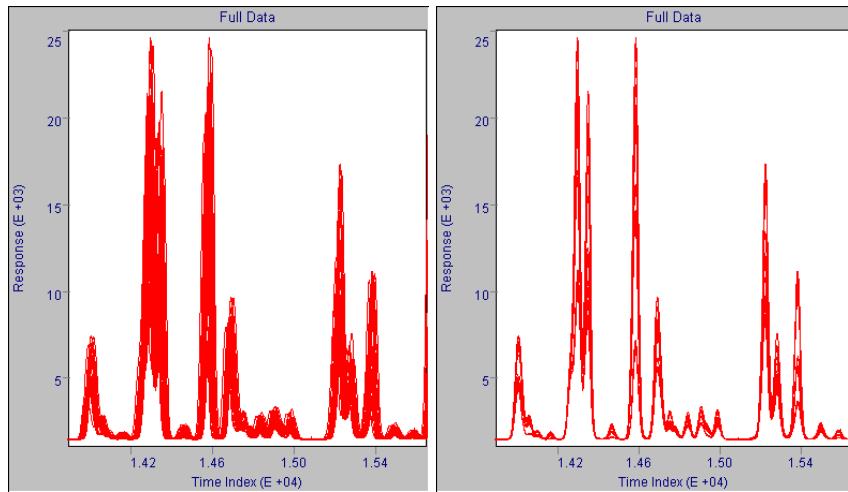
Gas chromatography in a refinery setting needs to analyze multiple fuel types each with hundreds or thousands of compounds. One common GC procedure is detailed hydrocarbon analysis (DHA). The procedure as it is typically performed in a refinery lab is diagrammed on the right.

Retention time variability causes misidentifications which, in turn, forces the processing of samples to be interrupted in the middle to create a preliminary report that is reviewed by at least one analyst. Corrections are made by adjusting the peak table *of the standard* and the report is rerun. In a process such as this, quality of the QC depends on the experience of the reviewer.

Working with the lab supervisor, we changed this hands-on analysis to a fully automated procedure, eliminating preliminary reports and automating the heretofore manual QC steps. The pattern recognition solution is:

- Cost-effective, automated, and does not require a change in the existing instrument hardware and software
- Aligns the chromatogram to remove retention changes and feeds the aligned chromatogram into the DHA reporting software
- Identifies the product and any system failures

The key problem turned out to be retention time instability. Using multivariate correlation adjusts for variation in column loading, column aging and changes in flow. The solution causes an improvement in reproducibility that can be seen below.



An overlay of 30 consecutive naphtha runs prior to alignment (left) and after alignment (right)

Business Model: An automated alignment technology has been integrated into routine DHA analysis. Applying the same tools to other laboratories for this analysis would result in immediate cost savings. Further, this process of alignment in combination with pattern recognition may eliminate the need to review chromatograms in most routine analyses. This development leads the way to performing reliable chromatography on-line. With alignment and objective, automated identification, efficient mining of a global chromatographic database is achievable.