State-of-the-art Analytical Techniques for a Changing Feed- and Products Landscape in Petrochemistry

M. Jennerwein*/**/***, U. Käfer*/**, M. Sarji****, D.Harrision*****, J. Wendt******, T. Wilharm**, R. Zimmermann*/**, T. Gröger*
*Comprehensive Molecular Analytics (CMA), Helmholtz-Zentrum München; **Chair for Analytical Chemistry, University of Rostock; ***ASG Analytik Service GmbH, ****Photonion GmbH, *****VUV Analytics; ******LECO European Application & Technology Centre

Abstract

Fossil feeds and the products derived therefrom are very challenging to analyze in a comprehensive way by a single analytical technique. Therefore, a wide range of analytical standard techniques have to be applied to ensure the comparability and quality of a product and/or the compatibility of a feedstock with a process. These aspects become even more difficult since the landscape of the feeds as well as the composition of the products are changing due to a shortage in resources but also because of legal and environmental regulations for the products.
Often, the standard techniques like ASTM could only be adapted to some extend to these new and changing matrices and therefore, the validity of the results may precarious. In such cases new more selective and more robust techniques have to be applied. On the one hand, these techniques have to be very advanced to handle a high variability in the composition of the matrix but on the other hand they have to be also applicable for process monitoring and standard lab environments.
The lecture will cover different state-of-the-art as well as novel approaches, where GC and GC×GC will be combined with very selective detection systems to become more robust regarding a changing composition of the matrices.
A fist example will focus on the addition of bio-contents to light and middle distillates to fulfill legal regulations but also to increase the performance of these fuels. We will demonstrate how GC×GC and/or a selective detection system like vacuum ultraviolet spectroscopy or photo ionization mass spectroscopy could be applied without a need for a special adaption to the specific compositions of the matric to gain more detailed qualitative but also quantitative information about the composition compared to a range of standard ASTM Methods.
The second part will focus more on the feedstock for the refining process. We will demonstrate how such techniques could be extended to higher boiling points to cover also very complex feedstocks like e.g. light crude oil and how to combine such approach with standard techniques like simulated distillation to gain unique qualitative information.
In a last part an outlook for the applicability of these techniques for qualitative and quantitative on-line process monitoring will be given.