ISA-AD Advanced Course: Chemometrics for Analyzers
Multivariate Analysis for Inferentials and Analyzers

A lot has been learned in the last decade about how best to optimize and maintain spectrometers and chromatographs in support of refinery and chemical plant process monitoring. This course examines a series of algorithmic approaches with the goal of streamlining multivariate model construction to make the analyzers significantly more robust when put into routine practice.

- Simple visualization techniques can greatly speed the development of inferentials and can also provide insight into processes that may not be evident using non-multivariate techniques;
- A simple approach can reduce the calibration requirements of gas chromatographs and optical spectrometers making these devices much closer to being truly plug-and-play;
- Even if calibrations were performed properly during initial installation, staffing changes and lack of training undermine subsequent recalibrations; and
- It is of benefit to minimize software maintenance frequency to control both expense and product giveaway.

Multivariate tools are commonly available but are often not properly applied; this must change.

Target audience:

This class will benefit those who want to better understand the tools available to build qualitative and quantitative inferentials for their process. It will also benefit technicians who perform both routine and irregular maintenance of chromatographic and spectroscopic instruments in both process and laboratory settings. Managing pressure, temperature, flow and level as an ensemble rather than as independent measurements to track will be highlighted. Attention will also be aimed at optical spectrometers, in particular near infrared and Raman. Chromatographic applications will be discussed with the purpose of simplifying maintenance.

Course objectives:

By the end of the course, attendees will have been instructed on chemometrics best practices and the practical application of new techniques, including:

1. How to get significantly more information from any source of data
2. Reducing the calibration requirements for both chromatographs and spectrometers
3. Optimizing calibration models using Robust statistics
4. Choosing appropriate preprocessing techniques and how that affects model quality
5. Understanding the trade-off between algorithmic technologies like Multiple Linear Regression, Partial Least Squares, Locally Weighted Regression, and others
6. Avoiding overfitting calibration models and observing how they can be used for longer periods
7. Applying transfer of calibration through augmentation, piecewise, or direct methods
8. Evaluating the trade-offs in deploying global models compared to optimizing every instrument separately

These topics are designed to cover the best practices of multivariate technology and will prepare participants for tackling a vast array of problems. This course is useful for any chemist or engineer who is concerned about optimizing their analytical methods to get the most out of their process operations. To sign up for the course go online to the ISA site and click on the register now link.