

## Volunteer-led training course: Advanced Course on Chemometrics

54<sup>th</sup> Analysis Division Symposium

Sunday, 19 April 2009

### Course Description –

Sensors and instruments are installed in process lines as a means of measuring parameters that govern our ability to control the process. Unfortunately, there is no single sensor that informs us the process is running in an optimal way, so we use a collection of measurements to navigate our control world. Process data, therefore, involves many measurements made on many samples. Such multivariate data has traditionally been analyzed using one or two variables at a time. However, this approach misses the point; to work efficiently and reliably, we must process all of the data simultaneously. Enter chemometrics. Chemometrics is the field of extracting information from multivariate chemical data using tools of statistics and mathematics. Chemometrics is typically used for one or more of three primary purposes:

- Process understanding – to explore patterns of association in data;
- Continuous quality assessment – to track properties of materials; and
- Discrete quality assessment (recognizing good versus bad) – to prepare and use multivariate classification models.

The 2009 ISA AD Advanced Course will be divided into four segments:

1. Chemometrics overview – The first section of the course will cover the basic principles of chemometrics, and seeks to provide the attendees with a practical understanding of the field without focusing on the underlying mathematics. We will discuss principal component analysis, regression analysis and classification modeling.
2. Dealing with sensor data – Applying a multivariate (chemometric) approach to general process data, rather than the traditional univariate approach, will be discussed. Examples of multivariate statistical process control and inferential modeling will be presented.
3. Spectroscopy – Infrared and near-infrared spectroscopy offer the ability to evaluate compositional or property values in real time. Data from these instruments are really a series of highly-correlated sensor results that require chemometric approaches to extract information.
4. Chromatography – Application of chemometrics to online GCs and HPLCs as a calibration technique to predict chemical or physical properties will be reviewed and demonstrated in real time.

### Instructor Bio –



Brian Rohrback is the President of Infometrix and has managed the company since 1985. In these 20+ years, he has steered Infometrix into position as a dominant independent supplier of chemometrics technology for laboratory and process analyzers. His experience prior to Infometrix was in the petroleum business where he managed a chromatography group for Cities Service Oil Company, now Occidental Petroleum, and performed support work for upstream activities. He was also involved in a specialized process instrument company (Rohrback Cosasco Systems: corrosion monitoring), since sold.

Rohrback holds a B.S. in chemistry (Harvey Mudd College), a Ph.D. in organic geochemistry (UCLA) and an MBA (University of Washington). Dr. Rohrback chairs the Chemometrics for On-line Process Analytics (COPA) initiative which meshes the process user community with both software and instrument suppliers. He is also a Sponsor and the industry liaison for the Process GC Initiative at the Center for Process Analytical Chemistry (CPAC), located at the University of Washington.