

Principal of Chemometrics

On-Line Analyzers - Categories

Discrete Analyzers

Direct analyses of a physical property (*ASTM-based*) according to standardized methods, i.e. Density, Boiling Points, RVP, RON, MON...

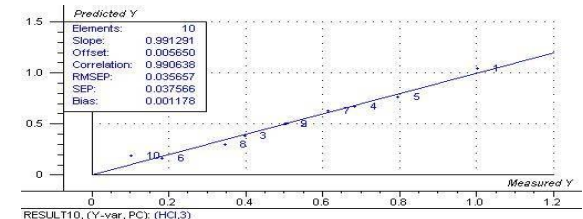
- Best correlation with the laboratory
- Response time is long
- Maintenance is expensive



Correlative Analyzers

Correlative analyzers are based on the correlation between spectral data and physical properties, i.e. NIR, RAMAN, IR and NMR spectrometry-based process analyzers. Physical properties are calculated by means of chemometrics

- Multi-property analysis
- Fast response time
- Minimal maintenance



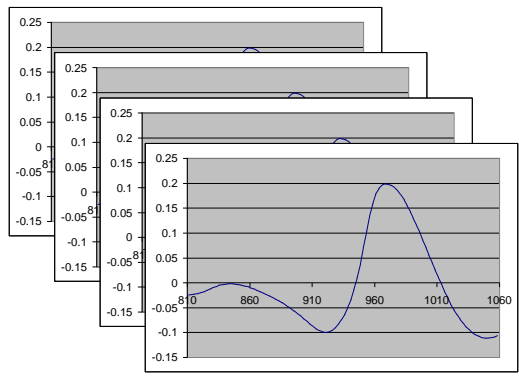
Principles of Chemometrics

Calibration Phase

Reference Spectra

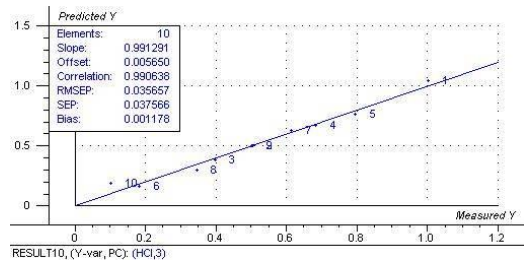
Reference Measurements

Calibration Model



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mix#	HCl	HF
0	0	0
1	1.178964	0.39912
2	0.790395	0.442637
3	1.090314	0.496751
4	1.06258	0.543865
5	0.852719	0.593886
6	0.99566	0.634382
7	0.873404	0.669103
8	0.988138	0.721126
9	0.849897	0.778561
10	1.000474	0.81478
11	1.102819	0.853354
12	1.135659	0.893109
13	0.799425	1.009638
14	0.950737	0.958367

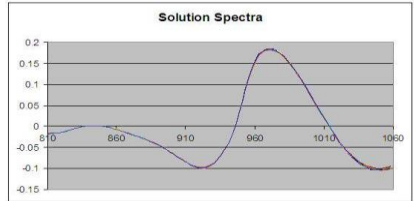


Measurement Phase

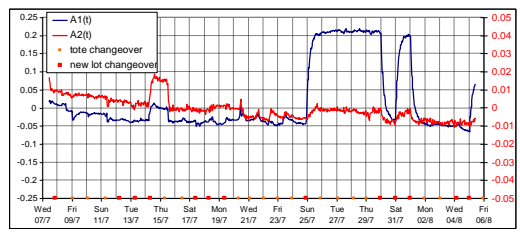
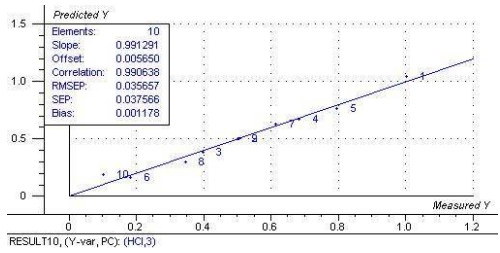
Unknown Spectra

Calibration Model

Predicted results

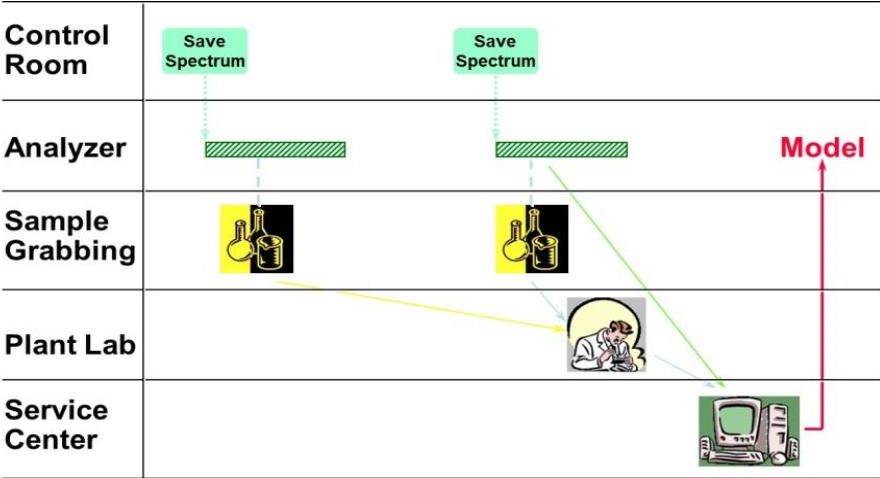


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Lab Sample Grabbing and Testing

It is imperative to keep the "Time Stamp" of the sample grabbing, since the chemometric model relies on the spectra taken at the exact same time.



The chemometric model depends on Lab Data! "Inferior Lab Data" will result in "Inferior NMR Results".

