



## Development of multivariate and multiresolution statistical techniques for industrial applications

- Successful applications of multivariate statistical methods to different industrial applications:
1. realtime monitoring of industrial manufacturing of resins and coatings:
    - online estimation of the product quality
    - batch length prediction
    - automatic adaptation to changes
  2. defect detection/localization in the manufacturing of integrated circuits:
    - image analysis of semiconductors
  3. characterization in nanofiber membrane fabrication:
    - artificial vision system for the measurement and the estimation of chemical and physical attributes
  4. standardization of near-infrared instrumentation:
    - estimation of the quality of forages for bovine feeding

## Multivariate and multiresolution statistical methods

- Multivariate statistical methods:**
- deal with data collinearity, correlation and noise
  - principal component analysis, PCA [1]
  - projection on latent structures, PLS [2]
- Multiresolution approach (frequency domain):**
- decomposes signals in different resolution scales with no loss of spatial/temporal information
  - wavelet convolution [3]

**Challenge:** dealing with data space/time evolution

**PCA**

$$X = \sum_{a=1}^A t_a p_a^T + E \quad \text{with } A \leq J$$

**PLS**

$$\begin{cases} X = TP^T + E \\ Y = UQ^T + F \end{cases}$$

**wavelet convolution**

$$T(a, b) = \int_{-\infty}^{+\infty} x(t) \psi_{a,b}^*(t) dt$$

## Quality monitoring in fine chemicals manufacturing

Challenges:

1. the plant is almost fully manually driven
2. midcourse correction of the recipe
3. different initial state of the pieces of equipment, of the utilities and of the raw materials

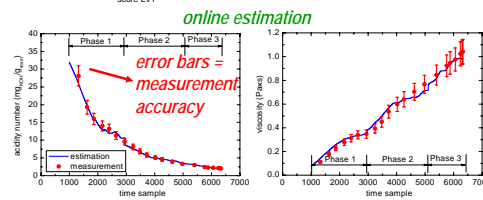
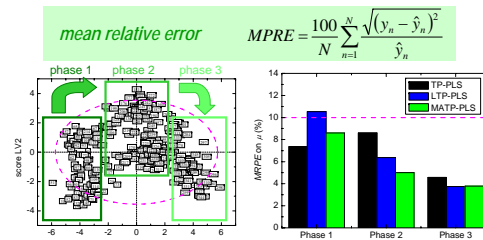
Issues:

1. scarce number of delayed quality lab analysis
2. unpredictable batch length

## Soft sensor for the estimation of quality

Adaptive multiphase moving-average PLS soft sensor:

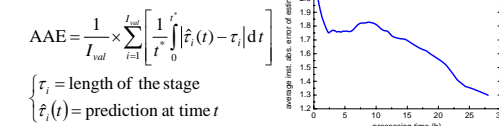
- multiphase structure compensates non-linearity
- moving average gives memory to the estimator [4,6]
- frequent estimations with high accuracy (10-12%)



## Batch length prediction

Time evolving PLS models [5] to predict the production stages length:

- prediction accuracy increases with time
- few hours after batch start the prediction accuracy is very high (1-3h)

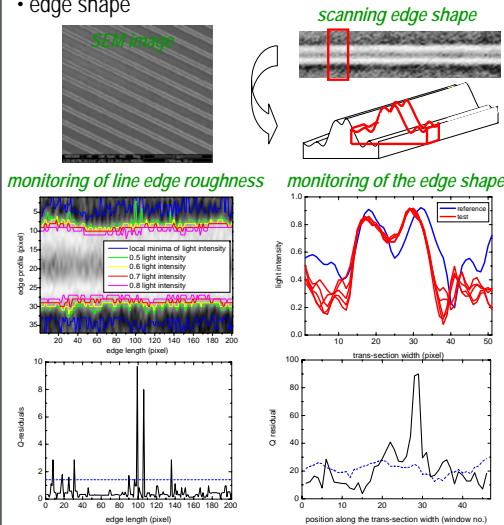


## Artificial vision systems for the characterization of nanomaterials

### Semiconductor fabrication

Effective defect detection and localization from multivariate image analysis [7]:

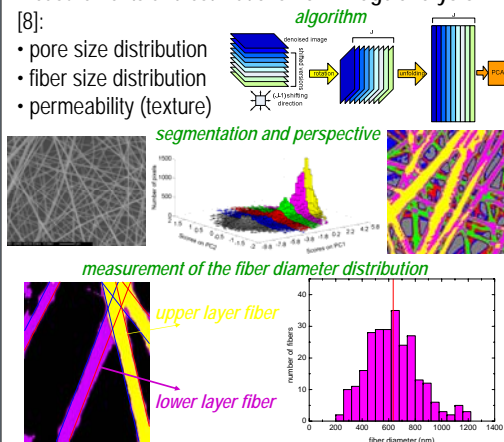
- roughness of the line edge
- edge shape



### Nanofiber membranes

Measurements and estimations from image analysis [8]:

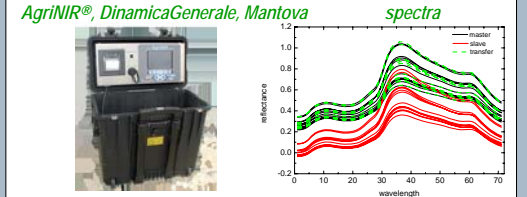
- pore size distribution
- fiber size distribution
- permeability (texture)



## Standardization of NIR spectrometers for the estimation of forage quality

Objectives:

- even responses in diverse NIRS
- limited calibration effort through PLS
- reduced number of calibration samples
- accurate prediction of the quality of bovine foodstuff



## Conclusions and future perspectives

Multiresolution and multivariate statistical techniques demonstrate to be highly beneficial in the industrial application of quality control paradigms. Great benefits are expected in the processing of pharmaceuticals, foodstuff, wood, textiles, etc...

## References

- [1] Jackson, J. E. (1991). A user's guide to principal components. John Wiley & Sons Inc., New York (U.S.A.).
- [2] Geladi, P. and R. Kowalski (1986). Partial least squares regression: a tutorial. *Anal. Chim. Acta*, 185, 1-17.
- [3] Addison, P. S. (2002). *The illustrated wavelet transform handbook*. IOP Publishing, London (U.K.).
- [4] Facco, P., F. Doplicher, F. Bezzo and M. Barolo (2009). Moving-average PLS soft sensor for online product quality estimation in an industrial batch polymerization process. *J. Process Control*, 19, 520-529.
- [5] Faggian, A., P. Facco, F. Bezzo and M. Barolo (2009). Multivariate statistical real-time monitoring of an industrial fed-batch process for the production of specialty chemical. *Chem. Eng. Res. Des.*, 87, 325-334.
- [6] Facco, P., F. Bezzo, and M. Barolo (2010). Nearest neighbor method for the automatic maintenance of multivariate statistical soft sensor in batch processing. *Ind. Eng. Chem. Res.*, 49, 2336-2347.
- [7] Facco, P., R. Mukherjee, F. Bezzo, M. Barolo and J. A. Romagnoli (2009). Monitoring roughness and edge shape on semiconductors through multiresolution and multivariate image analysis. *AIChE J.*, 55, 1147-1160.
- [8] Tomba, E., P. Facco, M. Rosso, M. Modesti, F. Bezzo, and M. Barolo (2010). Artificial vision system for the automatic measurement of inter-pore characteristics and fiber diameter distribution in nanofiber assemblies. *Ind. Eng. Chem. Res.*, 49, 2957-2968.