

Chemometrics Tools for Process Monitoring School Modena 6 – 9 February 2024

Program

Tuesday 6 February (optional)

AULA Informatica Uint 3 (piano -1)

8:30 Registration

9:00 – 10:30 Principal Component Analysis (PCA): basis, pre-treatments, nature of data, model dimensionality assessment, graphical representation of results, interpretation, validation. Orthogonal Rotations. (R. Leardi)

10.30 – 10.45 coffee break

10:45 – 13:00 Lab Exercises: PCA (L. Strani - R. Leardi – E. Farinini)

13:00 – 14:15 lunch

14.15 – 16.15 Partial Least Squares (PLS): basis, pre-treatments, nature of data, model dimensionality assessment, graphical representation of results, interpretation, validation. Multivariate Calibration (M. Cocchi)

16.15 – 16.30 coffee break

16.30 - 18.30 Lab Exercises: PLS (L. Strani - M. Cocchi)

Wednesday 7 February

8.30 Registration

9:00 – 10:30 Introduction to Process Monitoring – Univariate vs. Multivariate control charts T2, Q. Contribution plots. (M. Cocchi)

10:30 – 10:50 coffee break

10:50 – 12:45 Use of PCA models in the context of process monitoring (R. Leardi)

12:45 – 14:00 lunch

14:00 – 15:45 Practical Lab: Multivariate Control Chart Continuous Process (R. Leardi, M. Cocchi, E. Farinini, L. Strani)

15:45 – 16:00 coffee break

16:00 – 18:30 Handling model mismatch and dynamics (lagging) including Practical Lab (A. Ferrer)

20:30 Social Dinner

Thursday 8 February

9:30 – 11:00 Introduction to PLS model inversion for (restricted) process optimization (J. Borràs)

11:00 – 11:15 coffee break

11:15 – 12:30 Practical lab application (J. Borràs)

12:30–13:30 lunch

13:30 – 15:30 Practical issues in Batch MSPC: synchronization, preprocessing and modelling (A. Ferrer)

15.30–15.45 coffee break

15.45–18.15 Practical Lab application (A. Ferrer)

Friday 9 February

9:00 – 10:30 Data Fusion in MSPC context (M. Cocchi, L. Strani,)

10.30 – 10.45 coffee break

10:45 – 12:30 Case of Studies presentation from industrial practice

10:45 – 11:15 Controllo di Processo on-line con sensori NIR e sensori virtuali (F. Bonacini, Versalis SpA, MN)

11:20-11:50 From process chemometrics to process metaverse (P. Facco, University of Padova)

11:55-12:25 Process Modelling journey at J&J (M.C. Cerrato-Oliveros, Janssen Europe)

12.30 – 13:30 Question Time (Closure)