McMaster Advanced Control Consortium

McMASTER UNIVERSITY
Chemical Engineering Department
Hamilton, Ontario, Canada, L8S 4L7
Facsimile: (905) 521-1350

MULTIVARIATE PROCESS ANALYSIS RESEARCH GROUP

For Information Please Contact:

Prof. Theodora Kourti
Telephone: (905) 525-9140, ext. 27035
e_mail: kourtit@mcmaster.ca

Prof. John MacGregor
Telephone: (905) 525-9140, ext. 24951
e_mail:macgreg@mcmaster.ca

INDUSTRIAL INTERACTIONS

More than 60 Major Industrial Applications of Multivariate Statistical Analysis on production scale operations (on-line and/or off-line) in the following areas:

- Pharmaceuticals
- Semiconductor industry
- Film (Photography) industry
- Tire / Rubber
- Polymerization Processes
- Petrochemicals
- Mineral Processing
- Refineries
- Pulp and Paper
- Catalyst Conditioning
- Steel Industry
- Chemical Companies
- Polymer Latex Production
- Food Industry

PUBLICATIONS

Theory / Algorithms

Svensson, O., Kourti, T., MacGregor, J. F. (2002). A comparison of orthogonal signal correction algorithms and characteristics. J. Chemometrics, 16, pp.176-178.

Rujii Shi and John MacGregor (2001) A Fremework for Subspace Identification Methods. American control Conference.

Seongkyu Yoon and MacGregor John (2002). Incorporation of External Information into Multivariate PCA / PLS models. Submitted Journal of Chemometrics. Presented at 4th IFAC workshop on on-line Fault Detection and Supervision in the Chemical Process Industries, June 7-8, Chejudo, Korea

Seongkyu Yoon and MacGregor John (2001). Unifying PCA and Multiscale Approaches to Fault Detection and Isolation. 6th IFAC symposium on Dynamics and Control of Process Systems, June 4-6, Korea.

Burnham,A.J., MacGregor,J.F., Viveros,R. (2001). Interpretation of regression coefficients under a latent variable regression model. J. Chemometrics, **15**, 1-20

Burnham,A.J., Viveros, R., MacGregor,J.F. (1999). A statistical framework for Latent Variable Multivariate Regression methods based on Maximum Likelihood. J.Chemometrics, **13,** 49-65.

Burnham, A.J., Viveros, R., MacGregor, J.F. (1999). Latent Variable Multivariate Regression Modelling. Chemometrics and Intelligent Lab Systems. **48** / 2, 167-180.

Westerhuis,J.A.,Kourti,T., MacGregor, J.F. (1998). Analysis of Multiblock and Hierarchical PCA and PLS Models. *J. Chemometrics*, **12**, 301-321.

Dayal, B.S. and MacGregor, J.F. (1997). Improved PLS Algorithms. J. Chemometrics. 11, 73-85.

Burnham,A.J.,Viveros, R., MacGregor, J.F. (1996). Frameworks for Latent Variable Multivariate Regression. J. Chemometrics, 10, 31-45

Nelson, P.R.C., Taylor, P.A., MacGregor, J.F. (1996). Missing Data Methods in PCA and PLS: Score Calculations with Incomplete Observations. Chemometrics & Intelligent Laboratory Systems, 35, 45-65.

Process Analysis and Monitoring
- General Papers –

Kourti, T. (2003). Multivariate Dynamic Data Modelling for Analysis and Statistical Process Control of Batch Processes, Start – Ups and Grade Transitions. J. Chemometrics, 17, 93-109

Kourti, T. (2002). Process Analysis and Abnormal Situation Detection: From Theory to Practice. IEEE Control Systems, 22(5), 10-25.

Dushesne, C., Kourti, T., and MacGregor, F., (2002). Application of Multivariate Methods to Start-Up, Re-start and Grade Transition Problems. AICHE Journal, 48 (12), 2890-2901.

Yoon, S. and MacGregor, J.F. (2000) "Relationships between statistical and causal model based approaches to fault detection and isolation", Amer. Inst. Chem. Eng. J., **46**, 1813-1824, (Simplified version in ADCHEM 2000 proceedings. , Pisa, Italy, June, 2000)

Yoon, S. and MacGregor, J.F. (2000) Authors' reply to letter to the editor on above paper, Amer. Inst. Chem. Eng. J., 46, 1887-1889.

S. Yoon and J.F. MacGregor, J., "Fault diagnosis with multivariate statistical models, Part I: Using steady state fault signatures", J. of Process Control, in press, 2000

MacGregor, J. F., and Kourti, T. (1999). Multivariate Statistical Treatment of Historical Data for Productivity and Quality Improvements. AIChE Symposium Series No. 320, Volume 94, 3rd International Conference on *Foundations of Computer Aided Process Operations.* (Joseph F. Pekny, Gary E. Blau, Brice Carnahan Editors), CACHE and AICHE, pages 31-41.(ISBN 0-8169-0776-5)

MacGregor, J.F. (1997). Using On-Line Process Data to Improve Quality: Challenges for Statisticians. International Statistical Review, 65, 3, 309-323.

Kourti, T., and MacGregor, J.F. (1996). Recent Developments in Multivariate SPC Methods for Monitoring and Diagnosing Process and Product Performance. Journal Of Quality Technology, 28 (4), 409-428.

MacGregor, J.F. and Kourti, T. (1995). Statistical Process Control of Multivariate Processes. Control Engineering Practice, 3 (3) 403-414.

Kourti, T., and MacGregor, J.F. (1995). Process Analysis, Monitoring and Diagnosis Using Multivariate Projection Methods - A Tutorial. Chemometrics and Intelligent laboratory Systems, 28, 3-21.

Kresta, J., MacGregor, J.F and Marlin, T.E. (1991). Multivariate Statistical Monitoring of Process Operating Performance. Can. J. Chem. Eng. 69, pp. 35-47.

Kresta, J.V., Marlin, T.E., MacGregor, J.F. (1994). Development of Inferential Process Models using PLS. Computers Chem. Engng., 18, 597-611.

Process Analysis and Monitoring of Batch Processes

Duchesne, C. and J.F. MacGregor (2000), "Multivariate Analysis and Optimization of Process Variable Trajectories for Batch Processes", *Chemometrics and Intelligent Laboratory Systems*, 51, 125-137.

Yasuaki, Yabuki, Nagasawa Tooru and MacGregor John (2000). An Industrial Experience with Product Quality control in semi-batch processes. Computers & Chemical Engineering 24, 585-590.

Westerhuis, J.A., Kourti, T., and MacGregor, J.F. (1999). Comparing Alternative Approaches for Multivariate Statistical Analysis of Batch Process Data. *J. Chemometrics*. **13**, 397-413.

Rännar S., MacGregor, J.F., Wold., S. (1998). Adaptive Batch Monitoring using Hierarchical PCA. Chemometrics & Intelligent Laboratory Systems, **41** , pp.73-81

Neogi, D. and Schlags C.E., (1998). Multivariate Statistical Analysis of an Emulsion Batch Process. Ind. Eng. Chem. Res. 37, 3971-3979. – A*pplication by Air Products, MACC member company*.

Kourti, T., Lee, J. and MacGregor, J.F. (1996). Experiences with Industrial Applications of Projection Methods for Multivariate Statistical Process Control. Computers in Chemical Engineering, 20 Suppl. S745-S750.

Nomikos, P. (1996). Detection and Diagnosis of Abnormal Batch Operations Based on Multiway Principal Component Analysis. ISA Transactions, 35, 259-267.

Nomikos, P., and J.F. MacGregor. (1995). Multiway Partial Least squares in Monitoring Batch Processes. Chemometrics and Intelligent Laboratory Systems, 30 97-108.

Kourti, T., Nomikos, P. and MacGregor, J.F. (1995). Analysis, Monitoring and Fault Diagnosis of Batch Processes Using Multiblock and Multiway PLS. Journal of Process Control, 5, pp. 277-284.

Nomikos, P. and MacGregor, J.F. (1995). Multivariate SPC charts for Monitoring Batch Processes. Technometrics, 37(1) pp.41-59.

Nomikos, P. and MacGregor, J.F. (1994). Monitoring of Batch Processes using Multi-way Principal Component Analysis. AIChE Journal, 40 (8), pp. 1361-1375.

Applications of Projection Methods to Industrial Processes (publications by MACC and MACC members)

Champagne, M. and M. Dudzic (2002) Industrial Use of Multivariate Statistical Analysis For Process Monitoring and Control. American Control Conference, Anchorage, Alaska

Dudzic Michael and Shannon Quinn, (2002). Predictive Modeling Using Adaptive PLS Desulphurization Reagent Control System American Control Conference, Anchorage, Alaska.

Dudzic Michael And Ivan Miletic, (2002). Multivariate Statistical Monitoring Of A Continuous Steel Slab Caster. American Control Conference, Anchorage, Alaska**.**

M. Champagne and R. Monette (2002). Batch Multivariate SPC Monitoring of a Sulfite Pulp Digester. ACC , Anchorage , Alaska

M. Champagne and I . Ivavov" (2002) Multigrade modeling – Paperboard quality modeling. ACC , Anchorage , Alaska

I.Ivanov , S.Wold and N. Kettaneh-Wold (2002), Multivariate Modeling for a Multigrade Application, Control Systems 2002, June 3-5, 2002, Stockholm, Sweden

M. Champagne, N. Bendwell and R. Monette, The application of on-line statistical based soft sensor for process monitoring and control, Control Systems 2002, June 3-5, 2002, Stockholm, Sweden.

F. Yacoub and J.F. MacGregor (2002). Analysis and Optimization of an Industrial Polyurerhane reaction injection molding (RIM) process using projection methods.

Dudzic, M., Vaculik, V, Miletc, I,(2000) "On-line Applications of Multivariate Statistics at Dofasco", IFAC Workshop on Future Trends in Automation of the Mineral and Metal Processing Proceedings, Helsinki, Finland, Aug. 2000
Nancy Bendwell (2000) Les Techniques multivariables au service du controle des procedes;, Vecteur environnement - Volume 33, numero 2, mars 2000. A*pplication by Tembec, MACC member company*

Marc Champagne, S. Wold, N. Kettaneh-Wold. The use of OSC and Wavelets to improve NIR readings of Pulp Properties; To be published in Pulp and Paper Canada

Isabelle Ivanov (2000) Optimization of Paperboard Production and Prediction of End-Use Performance using multivariate Analysis. Control Systems 2000 Conference.A*pplication by Tembec, MACC member company*

Nancy Bendwell (2000) Monitoring of a Waste Water Treatment Plant with a Multivariate Model, Control Systems 2000 Conference. A*pplication by Tembec, MACC member company*

Rhondi Monette and Marc Champagne (2000) Multivariate SPC for Sulphite Batch Control. 2000 TAPPI Pulping Conference A*pplication by Tembec, MACC member company*

Vaculik, V, Miletic, I. (1999) "Applications of PCA and PLS at Dofasco", Proceedings of the International Symposium on Control and Optimization in Minerals, Metals and Materials Processing, 38th annual Conference of Metallurgists, Quebec City, Canada, Aug. 1999. A*pplication by Dofasco, MACC member company*

Schlags, C.E., and Anani, A.S. (1998). Waste Treatment Process Analysis using Multivariate Statistical methods. Presented at the AIChE annual meeting, Miami Beach, Florida. A*pplication by Air Products, MACC member company.*

Piovoso, M.J., Kosanovich, K. A., Dahl, K.S., MacGregor, J.F., and Nomikos, P., (1994). Multi-way PCA applied to an Industrial Batch Process. American Control Conference, IFAC, Baltimore, Maryland. (June 29 - July 1, 1994).

Dayal, B., J.F. MacGregor, P.A. Taylor, R. Kildaw, & S. Marcikic. (1994). Application of Feedforward Neural Networks and Partial Least Squares Regression for Modelling Kappa Number in a Continuous Kamyr Digester. Pulp and Paper Canada, 95 (1), pp. 26-32.

Vaculik, Vit (1994). Multivariate Data Analysis Using PCA/PLS with extensions to performance monitoring at Dofasco. Presented at the 3rd Advanced Modeling and Control Seminar by the Association of Iron and Steel Engineers, Cleveland, Ohio.// M. Eng. Thesis, McMaster University, Canada.

Hodouin,D., MacGregor, J.F., Hou, M., and Franklin, M. (1993). Multivariate Statistical Analysis of Mineral Processing Plant Data. CIM Bulletin, Mineral Processing, 86(975), pp. 23-34.

Skagerberg, B., MacGregor, J.F., Kiparissides, C. (1992). Multivariate Data Analysis Applied to Low Density Polyethylene Reactors. Chemometrics and Intelligent Laboratory Systems, 14, pp. 341-356.

Slama, C. F. (1991). Analysis of Industrial FCCU data using PCA and PLS. M.Eng. Thesis, McMaster University.

Multivariate Calibration

Gossen, P.D., MacGregor, J.F., Pelton, R.H. Composition and Particle Diameter for Styrene / Methyl Methacrylate Copolymer Latex using UV and NIR Spectroscopy. Applied Spectroscopy, 47(11), 1852-1870.

Multiblock PLS and Contribution Plots

MacGregor, J.F., Jaeckle, C., Kiparissides, C. and Koutoudi, M. (1994). "Process Monitoring and Diagnosis by Multi-Block PLS Methods". AIChE Journal, 40 (5), pp. 826-838.

Speech Recognition Methods for Fault Detection and Batch Alignment

Kassidas, A., Taylor, P.A., MacGregor, J.F.(1998). Off Line Diagnosis of Deterministic Faults Diagnosis in Continuous Dynamic Multivariate Processes Using Speech Recognition Methods. Journal of Process Control. 8, 381-393

Kassidas, A., MacGregor, J.F., Taylor, P.A. (1998). Synchronization of Batch Trajectories using Dynamic Time Warping. AIChE J., **44**, 864-875.

Dynamic Systems / Process Identification

Ruijie Shi and J. F. MacGregor (2001) A Framework for Subspace Identification methods. American Control Conference 2001.

Ruijie Shi and John F. MacGregor, Modeling of Dynamic Systems using Latent Variable and Subspace Methods, J. of Chemometrics, 14, 1-17, 2000.

M, Esmaili, A., MacGregor, J.F., and Taylor, P.A. "Direct and Two-Step Methods for Closed-Loop Identification: a Comparison of Asymptotic and Finite Data Set Performance", Journal of Process Control, 10(6), 525-537, 2000

Duchesne, C. and J.F. MacGregor, Jackknife and Bootstrap Methods in the Identification of Dynamic Models, to appear in *Journal of Process Control* (2000).

B.S. Dayal and J.F. MacGregor (1997). Recursive exponentially weighted PLS and its applications to adaptive control and prediction, J. Proc. Control. vol. 7(3) . pp. 169-179.

Dayal, B.S. and MacGregor, J.F. (1997). Multi - Output Process Identification. Journal of Process Control, 6,

Dayal, B.S. and MacGregor, J.F. (1996). Identification of Finite Impulse Response Models Methods and Robustness Issues. Ind Eng Chem Res, 35 4078-4090.

MacGregor, J.F., Kourti, T. and Kresta, J.V. (1991). "Multivariate Identification: A Study of Several Methods ", IFAC Intern. Symp. on Advanced Control of Chemical Processes Proceedings, K. Najim and J.P. Babary, eds., Toulouse, France, pp. 369-375.

Process Control

Flores-Cerrillo J. and and MacGregor, J.F (2002). Control of Particle Size Distributions in Emulsion Semi-Batch Polymerization Using Mid-Course Correction Policies *Ind. Eng. Chem. Res*. **41**, 1805-1814.

Flores-Cerrillo J. and and MacGregor, J.F (2002). Inferential – Learning Control of Quality Properties in Semi-batch Reactors. IFAC 15th World Congress, July 21-26, Barcelona, Spain.

Clarke-Pringle, T., and MacGregor, J.F. (1998). Product Quality Control in Reduced Dimensional Spaces. Ind. Eng. Chem. Res. 37, 3992-4002.

Clarke-Pringle, T., and MacGregor, J.F. (1998). Optimization of Molecular Weight Distribution Using Batch –to- Batch Adjustments. Ind. Chem. Res. 37, 3660-3669.

Dayal, B.S. and MacGregor, J.F. (1997). Recursive Exponentially Weighted PLS and its Applications to Adaptive Control and Prediction. Journal of Process Control, 7, 169-179.

Yabuki Yasuaki, and MacGregor, J.F. (1997). Product Quality Control in Semibatch Reactors Using Midcourse Correction Policies. Ind. Eng. Chem. Res. 36, 1268 - 1275.

Roffel, J.J., MacGregor, J.F., and Hoffman, T.W. (1989). The design and implementation of a multivariable internal model controller for a continuous polybutadiene polymerization train, IFAC DYCORD '89, Maastricht, The Netherlands (August 1989); Pergamon Press, New York.

Product Design / Model Inversion problems

Jaeckle, J.M., and MacGregor, J.F. (2000). Industrial \Applications of Product Design through the Inversion of Latent Variable Models. Chemometrics and Intelligent Laboratory Systems, 50, 199-210.

Jaeckle, J.M., and MacGregor, J.F. (2000). Product Transfer Between Plants Using Historical Process Data. Amer. Inst. Chem. Eng. J., 46, 1989-1997.

Jaeckle, J.M., and MacGregor, J.F. (1998). Product Design Through Multivariate Statistical Analysis of Process Data. AIChE Journal, 44, 1105-1118.

Multivariate Specifications

Duchesne C and MacGregor J. F. (2002). Establishing Multivariate Specification Regions for Incoming Materials. AICHE Journal .

DeSmet J. (1993). Development of Multivariate Specification Limits using Partial Least Squares Regression. M. Eng., McMaster University, Hamilton, Ont. Canada.

Image Analysis

Bharati, M., MacGregor, J.F. M.Champagne and M. Barrete (2002). Using NIR Multivariate Image Regression Techniques to predict Pulp Properties. Control Systems 2002, Stockholm, Sweden, June 3-5, 2002

Bharati, M. and MacGregor, J.F., "Texture Analysis of Images using Principal Component Analysis", Proc. SPIE - Process Imaging for Automatic Control, Boston, MA, Nov. 2000.

MacGregor, J.F., Bharati, M. and Yu, H., "Multivariate Image Analysis for Process Monitoring and Control", Proc. SPIE - Process Imaging for Automatic Control, Boston, MA, Nov. 2000.

Bharati, M. and MacGregor, J.F., (1998). Multivariate Image Analysis for Real Time Process Monitoring and Control. Ind. Eng. Chem. Res. 37, 4715-4724.