Online Batch Process Monitoring and Quality Prediction – Enhancements by Preserving Variable Direction and Charting Contributions

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Outline

- Introduction
  - Batch data challenges and solutions
  - Multi-way Partial Least Squares (MPLS) techniques
  - Multivariate Statistical Process Monitoring (MSPM) framework
- Enhanced Multivariate (MV) Monitoring Charts
- Case Studies: Fed-batch Penicillin Fermentation

Batch Data Challenges

- Unequal batch run (data) lengths
- Unsynchronized batch trajectories
- Missing values

Data Equalization and Alignment

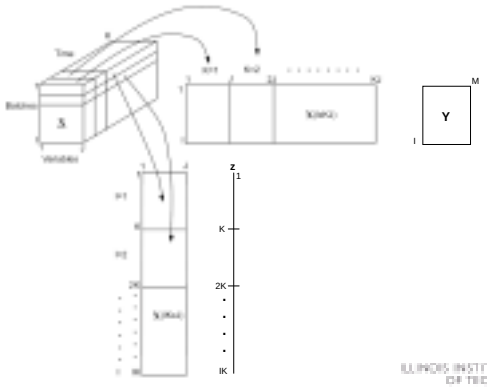
- Dynamic Time Warping (DTW)
- Curve Registration (CR)
- Indicator Variable (IV)
  - Easier to implement
  - Appropriate IV is needed
  - Process variables are re-sampled with respect to percent completion of IV

Indicator Variable Selection

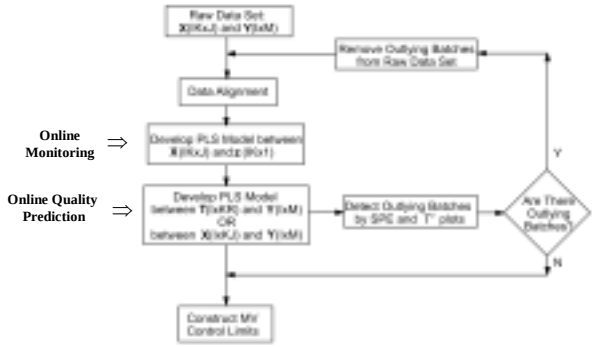
IV shows maturity of the evolving batch

- Smooth
- Monotonically increasing or decreasing
- Span the operation range for all the variables

Alternatives of Unfolding a Batch Data Array



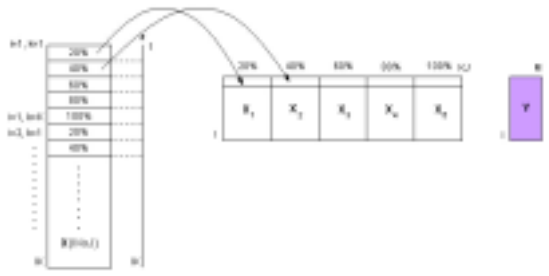
MSPM Framework Development



MSPM Charts

- Scores
  - Nonlinear dynamic behavior of score matrix **T** is removed
  - Student's *t*-distribution (normality assumption)
- T^2
  - Mean-centered score matrix is used
- Squared Prediction Error (SPE)
  - Large variations and deviations from NO
- Variable Contributions
  - SPE
  - T^2
  - Scores

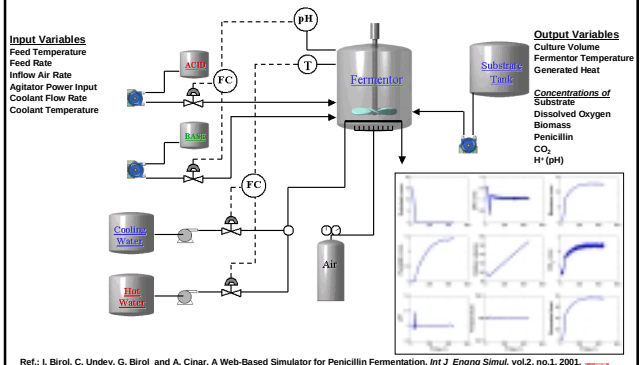
Online Quality Prediction



Case Studies

- Fed-batch penicillin fermentation
- I = 39, J = 14, M=5, R=5
- Two phases: Batch / Fed-batch
- Data alignment: IV technique
  - IV1: Volume decrease
  - IV2: % Amount substrate added
- Case 1: Step decrease in agitator power of magnitude 25%
- Case 2: Drift of magnitude 0.065% h^{-1} into substrate feed rate

Fed-batch Penicillin Process Flow Sheet

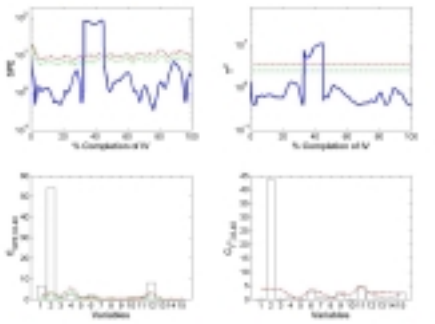


Ref.: I. Birol, C. Undey, G. Birol and A. Cinar, A Web-Based Simulator for Penicillin Fermentation, *Int J Engng Simul*, vol.2, no.1, 2001. http//www.intjes.co.uk/vol2num1/vol2num1.html; http://www.chee.iit.edu/~controlsoftware.html

Case 1: Fault Detection Times

Type	% Completed IV	Time, h
SPE	33.2	200
T^2	33.2	200
Linear Score LV 4	33.2	200
Linear Score LV 5	33.2	200
Nonlinear Score LV 4	33.2	200
Nonlinear Score LV 5	33.2	200

Case 1: SPE, T^2 and Contributions



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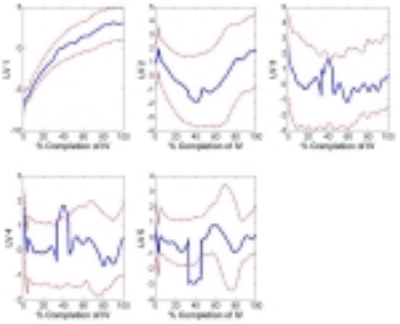
Case 1: Nonlinear Scores



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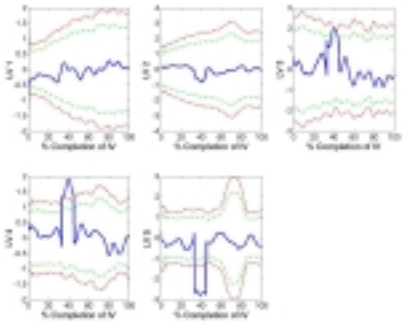
Case 1: Linear Scores



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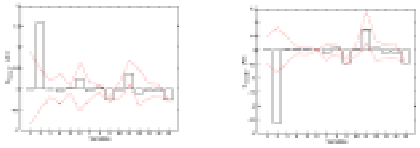
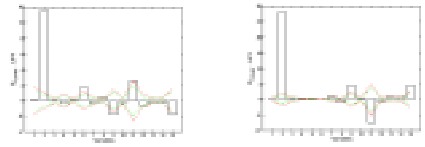
Case 1: Contributions to Scores

- Nonlinear Scores



- Linear Scores



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Case 2: Fault Detection Times

Type	% Completed IV	Time, h
T^2	44.8	246
Linear Score LV 5	46.2	251
Nonlinear Score LV 5	46.4	252
Linear Score LV 4	51	272
Linear Score LV 2	51.2	273
Nonlinear Score LV 4	52	277
Nonlinear Score LV 2	52.4	279
Linear Score LV 3	66	341
Nonlinear Score LV 3	68.4	352
SPE	82	419
Linear Score LV 1	91.2	467
Nonlinear Score LV 1	92.4	473

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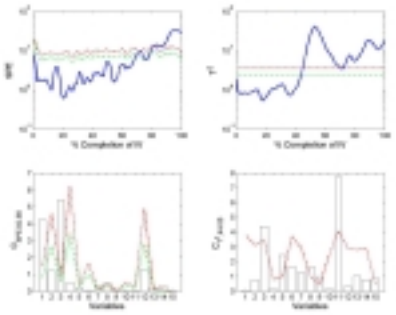
Case 2: SPE, T^2 and Contributions



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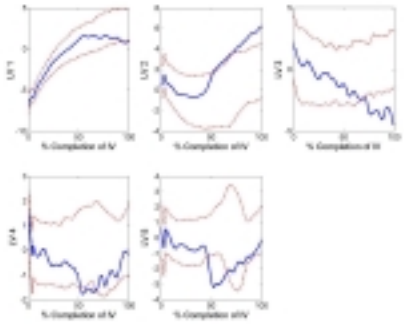
Case 2: Nonlinear Scores



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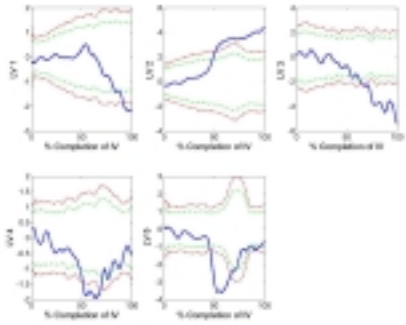
Case 2: Linear Scores



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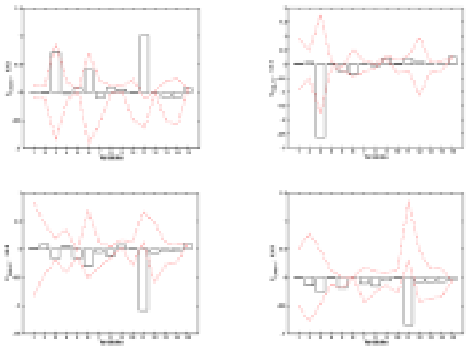
Case 2: Contributions to Nonlinear Scores



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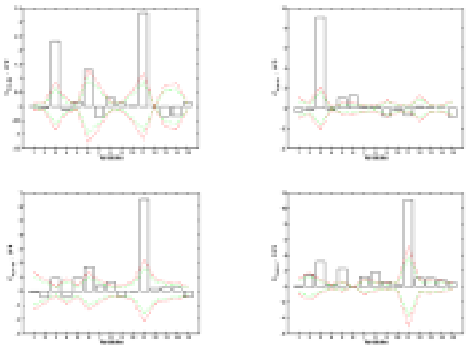
Case 2: Contributions to Linear Scores



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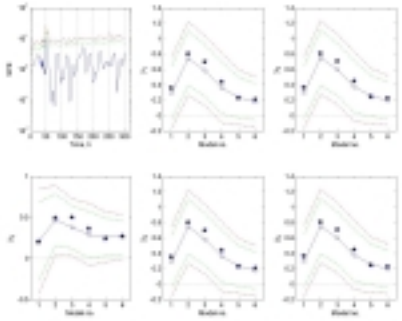
Intermediate Quality Prediction (NOC)



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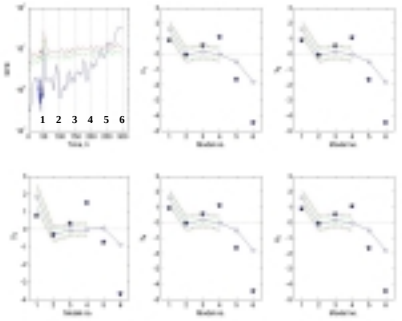
Intermediate Quality Prediction (Case 2)



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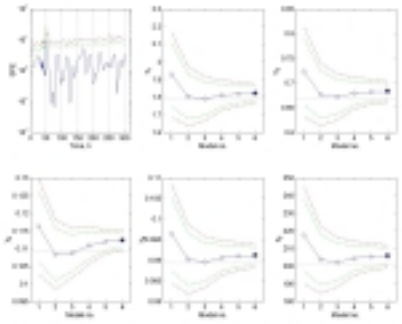
Local Modeling (NOC)



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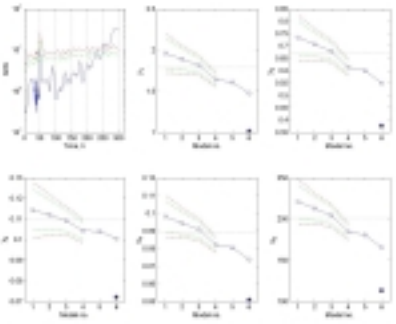
Local Modeling (Case2)



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Conclusions

- Earlier fault detection by modified MV charts
- Efficient fault diagnosis with contribution plots
- Intermediate quality prediction gives an early assessment about the product quality during the batch

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