On-line monitoring of batch processes: Does the modelling structure matter?

CAC 2008

José Camacho
Jesús Picó
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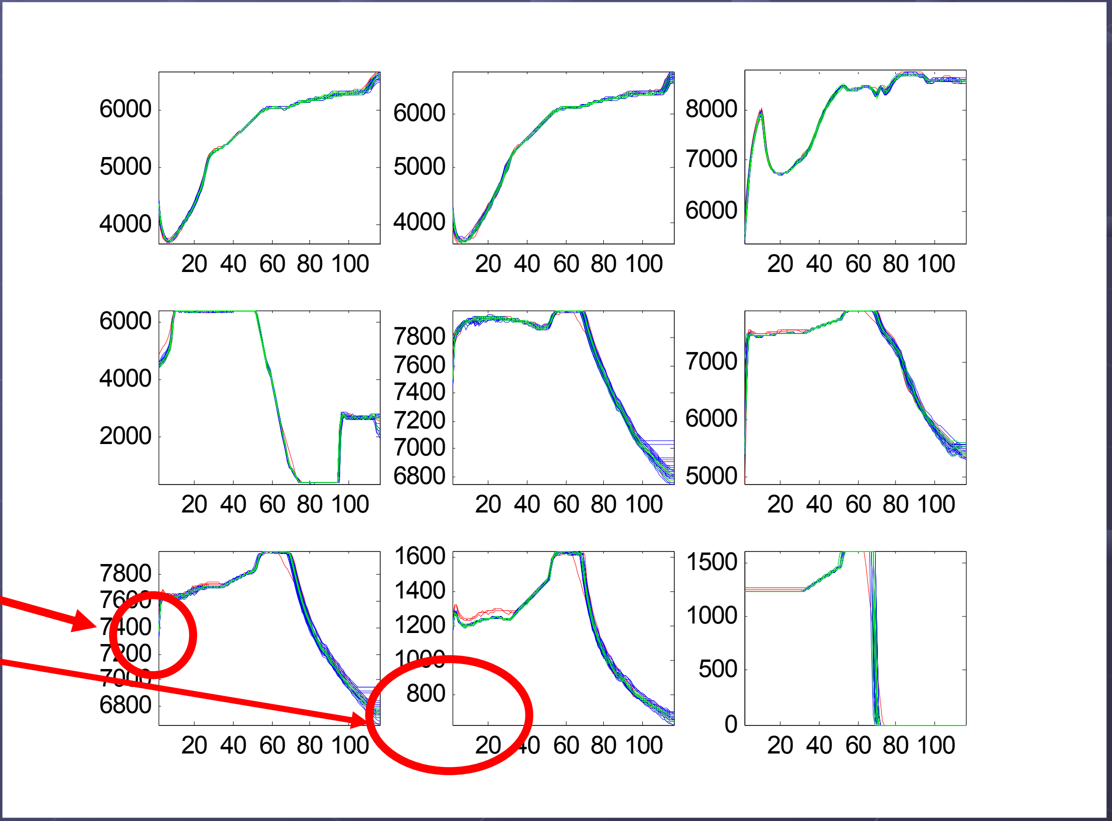
PCA-based On-line Monitoring of Batch Processes

Outline

1. **PCA-based On-line Monitoring of Batch Processes**
2. Materials and Methods
3. Results and Discussion
4. Conclusions

- Determine on-line if the product of a batch is produced under NOC.

Detect, diagnose and understand



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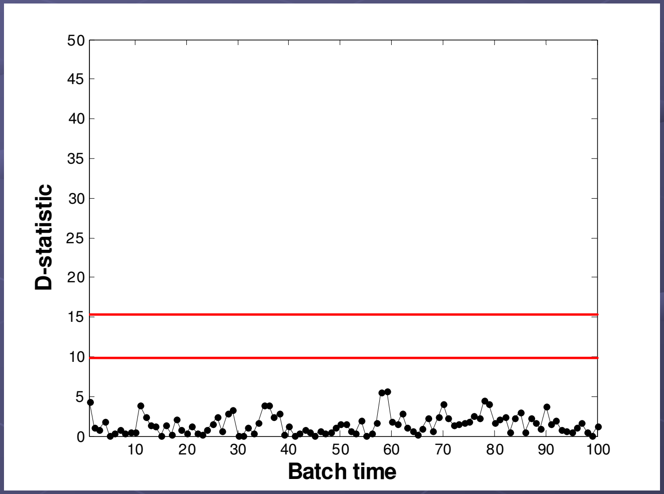
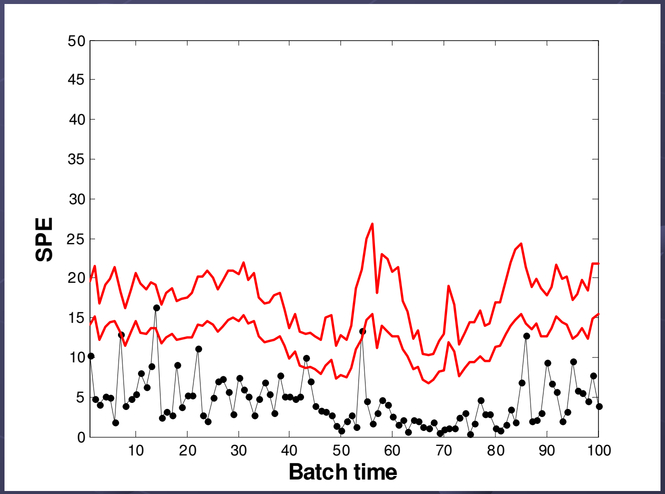
- Monitoring Charts: D-statistic and SPE

Batch under **NOC**





- Saccharomyces cerevisiae cultivation

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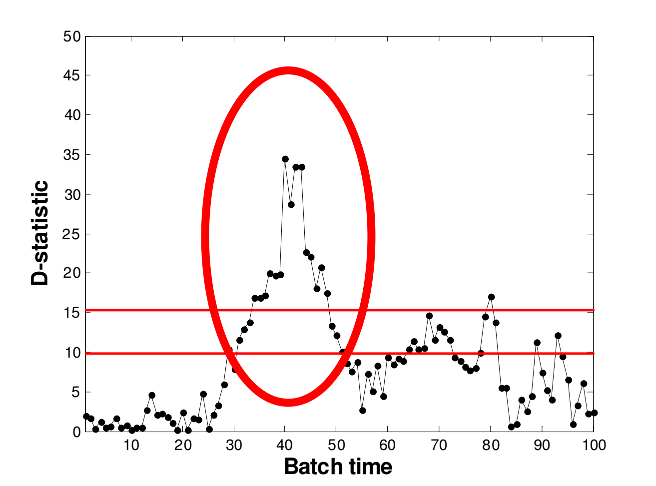
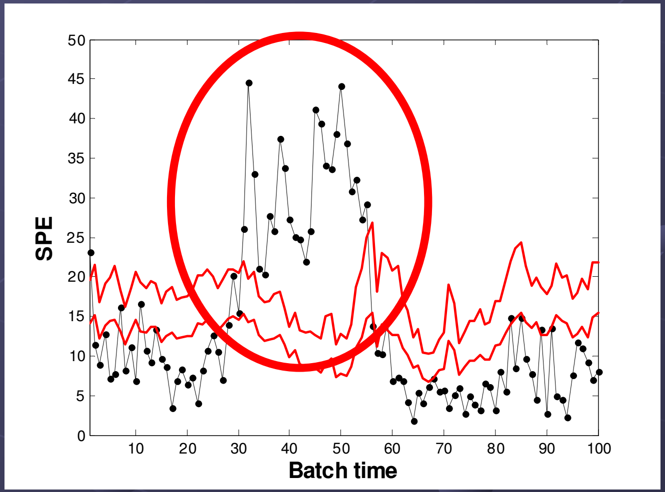
Abnormal Batch





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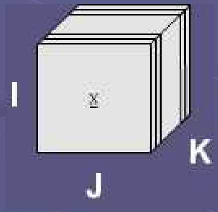
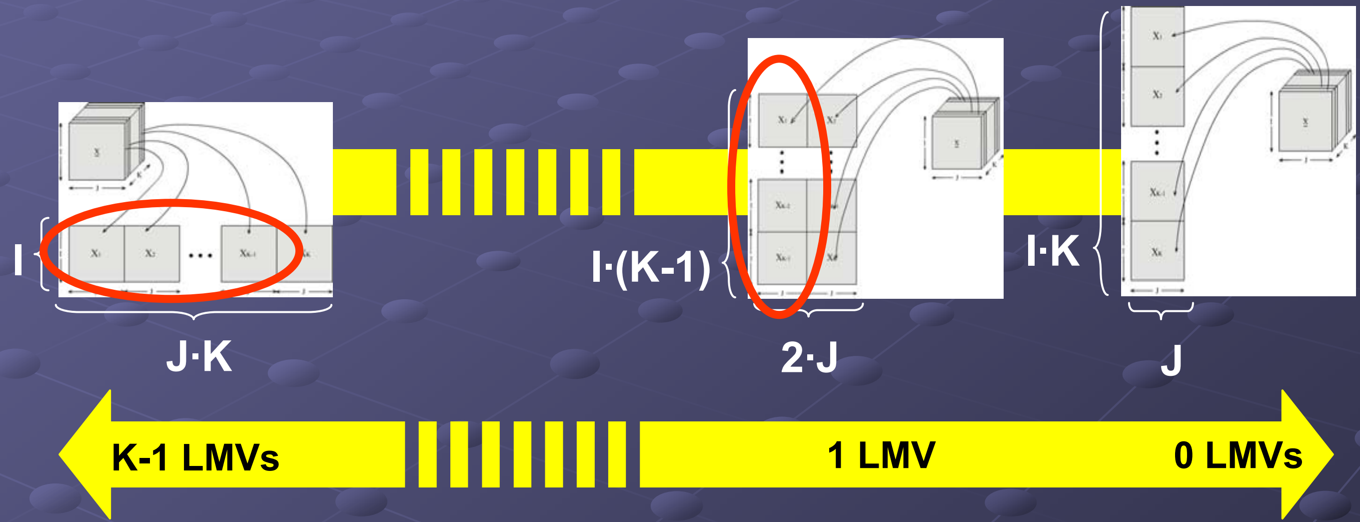


I batches
J variables
K sampling times

- Convert into two-way data ➔ Unfolding



+ LMVs	- LMVs
- Parsimonious	+ Parsimonious
+ Dynamics captured	- Dynamics captured
- Constrained Dynamics	+ Constrained Dynamics
+ Auto-corr Stats.	– Auto-corr. Stats.

J. Camacho, J. Picó and A. Ferrer. *Bilinear modelling of batch processes. Part I: Theoretical discussion*, Journal of Chemometrics, 2008, 22(5): 299-308.

Materials and Methods

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- Identify the dynamics of the process is important for prediction purposes
- **Is the monitoring performance improved by using the true dynamic structure of the process in the PCA model???**
- "Toy" process (simulink-matlab):
  - Simplified process where we know the dynamics a priori.
  - A PCA model containing the true dynamics of the process can be compared to predefined approaches (BW, VW, …)
  - Different types of faults can be induced without side-effect factors.

J. Camacho, J. Picó and A. Ferrer. *Bilinear modelling of batch processes. Part II: Comparison of PLS softsensors*, Journal of Chemometrics, 2008, In PRESS.

Materials and Methods

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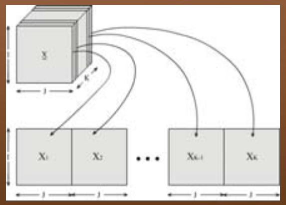
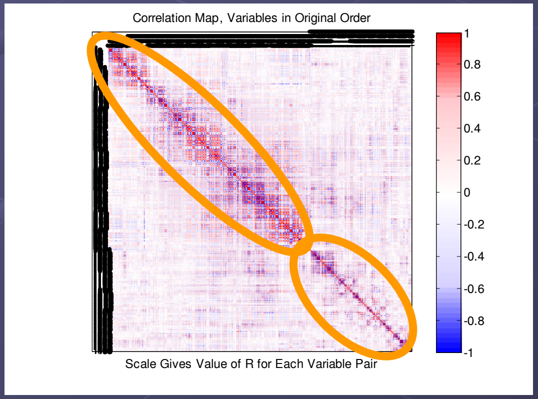
- "Toy" process (simulink-matlab):
  - Two processes with different dynamics.

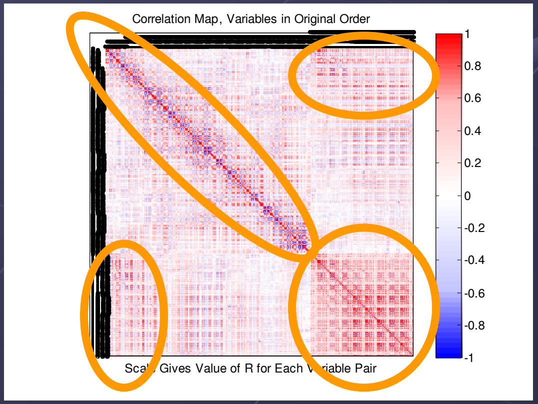


$M = (1/I) \cdot X^T \cdot X =$

X autoscaled



Process 1: 2 phases, short-term dynamics



Process 2: 2 phases, long-term dynamics

Materials and Methods

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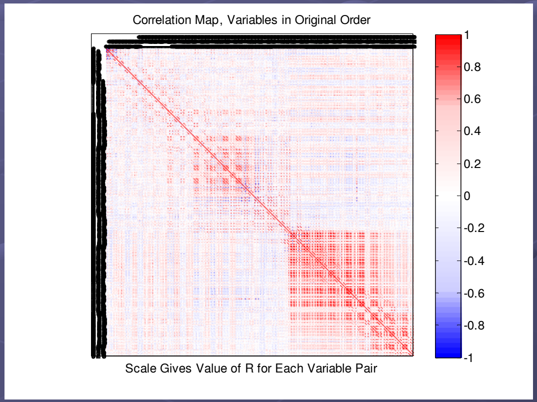
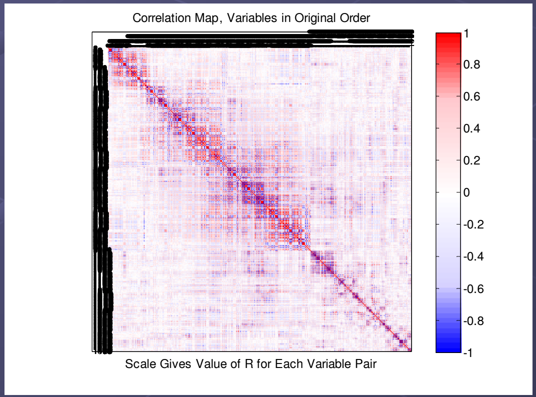


Real data from nylon 6'6 polymerization



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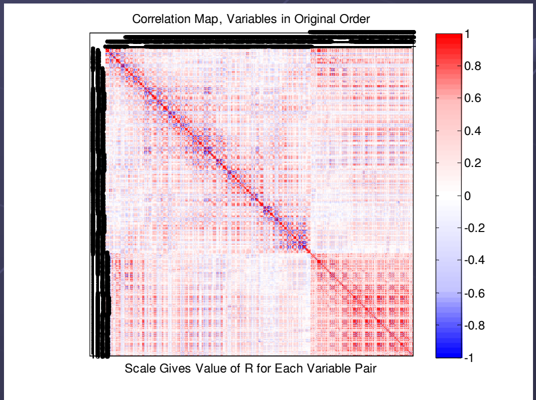


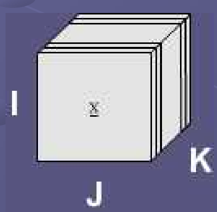
Process 2: 2 phases, long-term dynamics

Materials and Methods

- "Toy" process (simulink-matlab).
  - Two processes with different dynamics
- Generate a number of data-sets:
  - Calibration batches (30).
  - Test NOC batches (15).
  - Abnormal batches (40).
  - The same experiment is repeated 5 times per process.

Materials and Methods

Outline



I batches
J variables
K sampling times

- "Toy" process (simulink-matlab).
  - Two processes with different dynamics.
- Generate a number of data-sets.
- Comparison of different modelling structures.
  - **BW-PMP:** BW and Projection to Model Plane.
  - **BW-CV:** BW and current values.
  - **BW-ZV:** BW and zero values.
  - **VW:** VW after trajectory centering (TC).
  - **Local:** Local modelling.
  - **BD1:** BD (1LMV) after TC.
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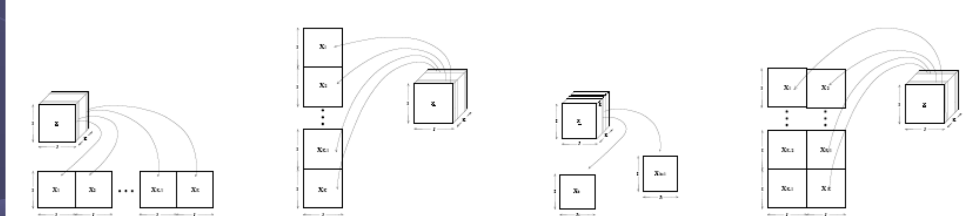

(a) Batch-wise (b) Variable-wise (c) Local (d) Batch Dynamic

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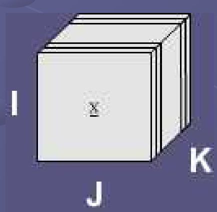

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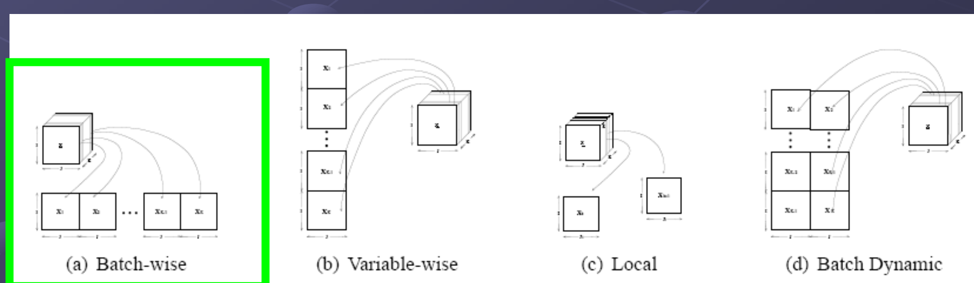

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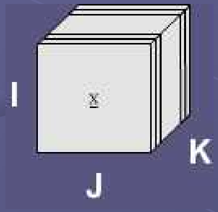

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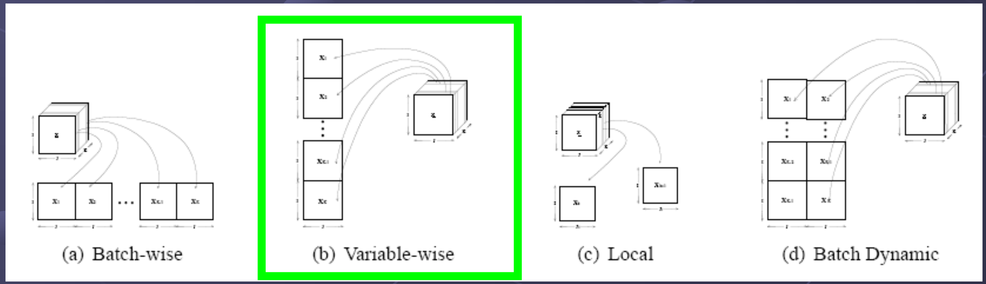

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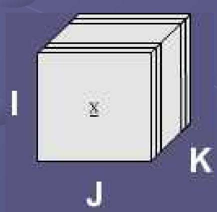

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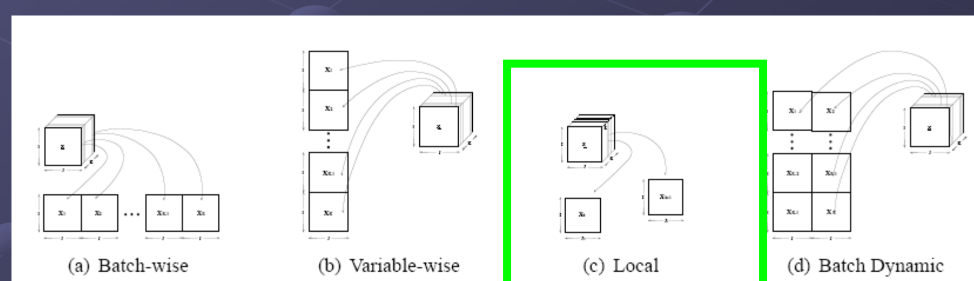

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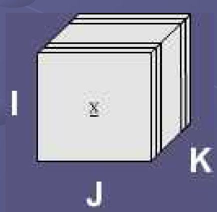

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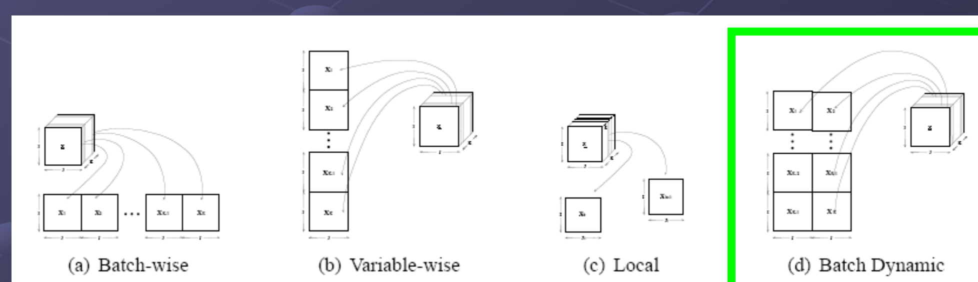

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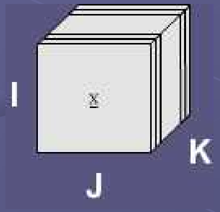

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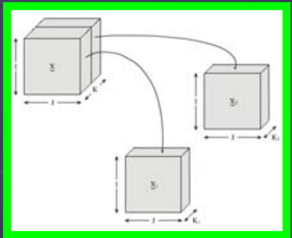

Materials and Methods

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- "Toy" process (simulink-matlab):
  - Two processes with different dynamics.
- Generate a number of data-sets.
- Comparison of different modelling structures.
- Indices used:
  - **Type I (TI) Risk** ➔ % NOC batches detected as abnormal
  - **Type II (TII) Risk** ➔ % abnormal batches detected as NOC
  - **Overall Type I (OTI) Risk** ➔ % faults in a NOC batch
  - **Overall Type II (OTII) Risk** ➔ % non-faults in an abn. interval
  - **Overall Type I f (OTI^f) Risk** ➔ % faults in a NOC interval after an abn interval.

$$OTI = 100 \cdot \frac{nf}{I_{NOC} \cdot K} \%$$

$$OTII = 100 \cdot \frac{nnf}{I_{ab} \cdot l} \%$$

Results and Discussion

Outline

TI = % NOC batches detected as abnormal

OTI = % faults in a NOC batch

OTI^f = % faults in a NOC batch after an abnormality

- **Process 1: 2 phases, short-term dynamics**

Model	Structure	TI		Test-NOC OTI$_D$	Test-NOC OTI$_{SPE}$	Test-Ab$_{a+}$ & Test-Ab$_{b+}$ OTI^f_D	Test-Ab$_{a+}$ & Test-Ab$_{b+}$ OTI$^f_{SPE}$
BW-PMP	BW	0%	(0/75)	0.08%	1.08%	40.9%	15.6%
BW-CV	BW	0%	(0/75)	0.47%	1.10%	41.1%	14.4%
BW-ZV	BW	0%	(0/75)	0.08%	0.86%	40.9%	13.4%
VW	VW	0%	(0/75)	0.87%	0.96%	1.2%	1.7%
Local	Local	0%	(0/75)	0.74%	1.08%	0.8%	3.2%
BD1	BD1	0%	(0/75)	0.64%	0.93%	4.1%	3.8%
VW-2ph	[VW, VW]	0%	(0/75)	0.60%	0.44%	0.9%	0.5%
BD1-2ph	[BD1, BD1]	0%	(0/75)	0.56%	1.06%	5.9%	7.0%
BD-2ph	[BD1, BD3]	0%	(0/75)	0.70%	1.07%	10.8%	11.5%

- **Process 2: 2 phases, long-term dynamics**

Model	Structure	TI		Test-NOC OTI$_D$	Test-NOC OTI$_{SPE}$	Test-Ab$_{a+}$ & Test-Ab$_{b+}$ OTI^f_D	Test-Ab$_{a+}$ & Test-Ab$_{b+}$ OTI$^f_{SPE}$
BW-PMP	BW	4%	(3/75)	1.87%	1.70%	63.7%	67.4%
BW-CV	BW	4%	(3/75)	0.61%	1.80%	52.3%	58.4%
BW-ZV	BW	4%	(3/75)	1.87%	1.56%	63.7%	50.2%
VW	VW	0%	(0/75)	1.10%	0.99%	1.0%	1.8%
Local	Local	2.7%	(2/75)	1.24%	3.20%	0.5%	3.0%
BD1	BD1	0%	(0/75)	1.19%	0.66%	3.7%	4.3%
VW-2ph	[VW, VW]	0%	(0/75)	1.09%	0.68%	0.5%	1.5%
BD1-2ph	[BD1, BD1]	0%	(0/75)	0.94%	1.28%	5.7%	7.9%
BD-2ph	[BD1, BW]	1.3%	(1/75)	1.04%	1.10%	100.0%	92.0%

J. Camacho and J. Picó. *Online Monitoring of Batch Processes using Multi-Phase Principal Component Analysis*, Journal of Process Control, 10(16):1021-1035 (2006).

Results and Discussion

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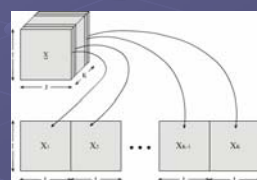
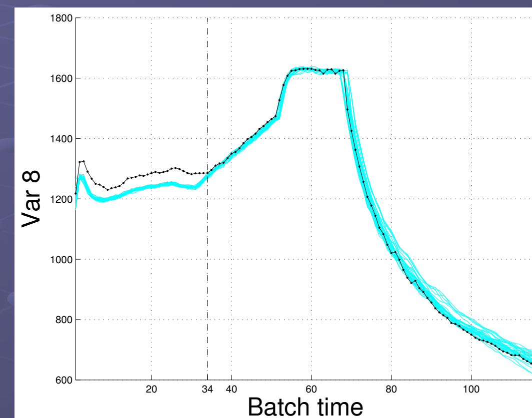
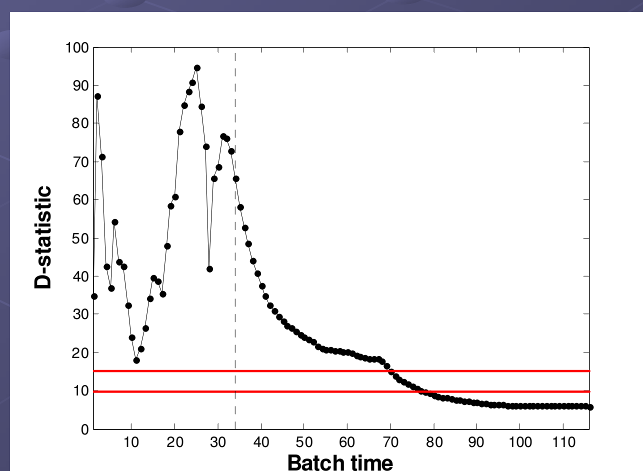
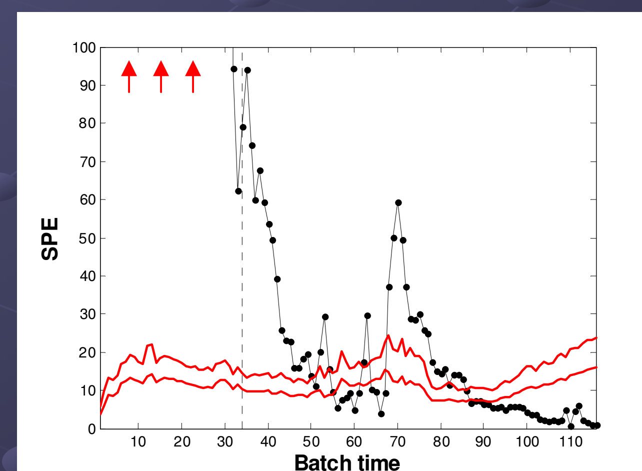
- Nylon 6'6 Polymerization









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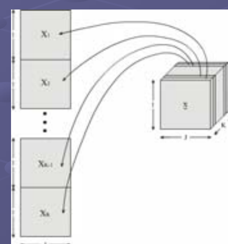

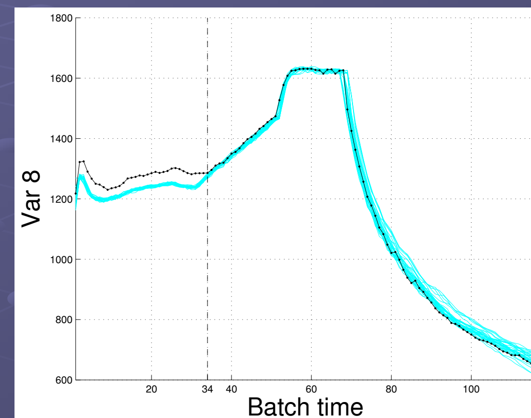

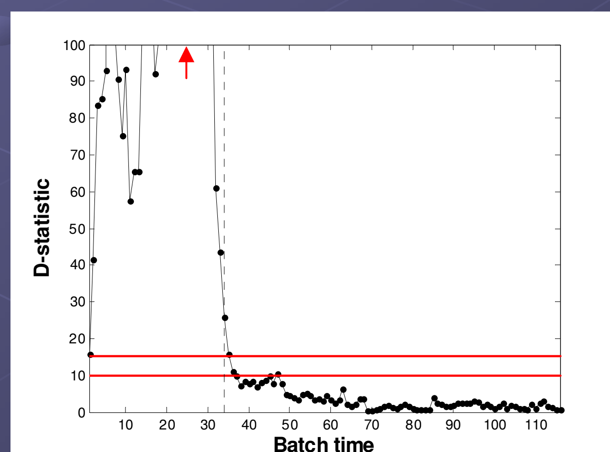

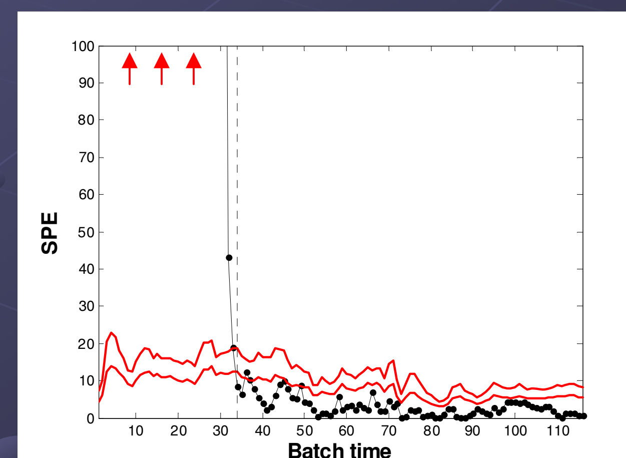

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☺ Best approach (ANOVA + LSD p-value=0.05)

$Test\text{-}Ab_a$ = High meas. noise

$Test\text{-}Ab_c$ = Ph.1 takes longer

$Test\text{-}Ab_f$ = Breakage of the inst. relat. Proc. Var.

- **Process 1: 2 phases, short-term dynamics**

Model	Test-Ab TII	$Test\text{-}Ab_a$ OTII	$Test\text{-}Ab_b$ OTII	$Test\text{-}Ab_c$ OTII	$Test\text{-}Ab_d$ OTII	$Test\text{-}Ab_e$ OTII	$Test\text{-}Ab_f$ OTII
BW-PMP	21.5% (43/200)	12%	19%	78%	6% ☺	100%	76%
BW-CV	22.0% (44/200)	13%	19%	76%	16%	100%	76%
BW-ZV	21.5% (43/200)	13%	19%	78%	5% ☺	100%	78%
VW	18.5% (37/200)	10%	17%	63%	41%	100%	49%
Local	15.0% (30/200)	6%	18%	42%	46%	100%	17%
BD1	9.5% (19/200)	9%	12%	56%	41%	82%	50%
VW-2ph	12.5% (25/200)	0% ☺	17%	7% ☺	50%	100%	3% ☺
BD1-2ph	1.5% (3/200)	5%	5% ☺	29%	49%	48% ☺	12%
BD-2ph	3.0% (6/200)	7%	5% ☺	39%	48%	54%	18%

- **Process 2: 2 phases, long-term dynamics**

Model	Test-Ab TII	$Test\text{-}Ab_a$ OTII	$Test\text{-}Ab_b$ OTII	$Test\text{-}Ab_c$ OTII	$Test\text{-}Ab_d$ OTII	$Test\text{-}Ab_e$ OTII	$Test\text{-}Ab_f$ OTII
BW-PMP	24.0% (48/200)	29%	33%	89%	9% ☺	100%	61%
BW-CV	23.5% (47/200)	23%	33%	88%	17%	100%	59%
BW-ZV	24.5% (49/200)	27%	33%	90%	8% ☺	100%	63%
VW	19.5% (39/200)	12%	32%	71%	42%	100%	40%
Local	17.5% (35/200)	4%	25%	57%	39%	100%	32%
BD1	17.0% (34/200)	12%	25%	88%	37%	94%	49%
VW-2ph	13.5% (27/200)	0% ☺	26%	6% ☺	46%	100%	4% ☺
BD1-2ph	1.0% (2/200)	5%	9% ☺	29%	46%	44% ☺	9%
BD-2ph	6.0% (12/200)	15%	20%	78%	34%	69%	25%

Results and Discussion

Outline

1. PCA-based On-line Monitoring of Batch Processes
2. Materials and Methods
3. **Results and Discussion**
4. Conclusions

☺ **Best approach (ANOVA + LSD p-value=0.05)**

Test-Ab$_b$ = High values but no correlation breakage

Test-Ab$_e$ = Dynamics change

- **Process 1: 2 phases, short-term dynamics**

Model	Test-Ab TII	Test-Ab$_a$ OTII	Test-Ab$_b$ OTII	Test-Ab$_c$ OTII	Test-Ab$_d$ OTII	Test-Ab$_e$ OTII	Test-Ab$_f$ OTII
BW-PMP	21.5% (43/200)	12%	19%	78%	6% ☺	100%	76%
BW-CV	22.0% (44/200)	13%	19%	76%	16%	100%	76%
BW-ZV	21.5% (43/200)	13%	19%	78%	5% ☺	100%	78%
VW	18.5% (37/200)	10%	17%	63%	41%	100%	49%
Local	15.0% (30/200)	6%	18%	42%	46%	100%	17%
BD1	9.5% (19/200)	9%	12%	56%	41%	82%	50%
VW-2ph	12.5% (25/200)	0% ☺	17%	7% ☺	50%	100%	3% ☺
BD1-2ph	1.5% (3/200)	5%	5% ☺	29%	49%	48% ☺	12%
BD-2ph	3.0% (6/200)	7%	5% ☺	39%	48%	54%	18%

- **Process 2: 2 phases, long-term dynamics**

Model	Test-Ab TII	Test-Ab$_a$ OTII	Test-Ab$_b$ OTII	Test-Ab$_c$ OTII	Test-Ab$_d$ OTII	Test-Ab$_e$ OTII	Test-Ab$_f$ OTII
BW-PMP	24.0% (48/200)	29%	33%	89%	9% ☺	100%	61%
BW-CV	23.5% (47/200)	23%	33%	88%	17%	100%	59%
BW-ZV	24.5% (49/200)	27%	33%	90%	8% ☺	100%	63%
VW	19.5% (39/200)	12%	32%	71%	42%	100%	40%
Local	17.5% (35/200)	4%	25%	57%	39%	100%	32%
BD1	17.0% (34/200)	12%	25%	88%	37%	94%	49%
VW-2ph	13.5% (27/200)	0% ☺	26%	6% ☺	46%	100%	4% ☺
BD1-2ph	1.0% (2/200)	5%	9% ☺	29%	46%	44% ☺	9%
BD-2ph	6.0% (12/200)	15%	20%	78%	34%	69%	25%

Results and Discussion

Outline

1. PCA-based On-line Monitoring of Batch Processes
2. Materials and Methods
3. **Results and Discussion**
4. Conclusions

☺ **Best approach (ANOVA + LSD p-value=0.05)**

Test-Ab_d = Change in initial conditions

- **Process 1: 2 phases, short-term dynamics**

Model	Test-Ab TII	Test-Ab_a OTII	Test-Ab_b OTII	Test-Ab_c OTII	Test-Ab_d OTII	Test-Ab_e OTII	Test-Ab_f OTII
BW-PMP	21.5% (43/200)	12%	19%	78%	6% ☺	100%	76%
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- **Process 2: 2 phases, long-term dynamics**

Model	Test-Ab TII	Test-Ab_a OTII	Test-Ab_b OTII	Test-Ab_c OTII	Test-Ab_d OTII	Test-Ab_e OTII	Test-Ab_f OTII
BW-PMP	24.0% (48/200)	29%	33%	89%	9% ☺	100%	61%
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Conclusions

Outline

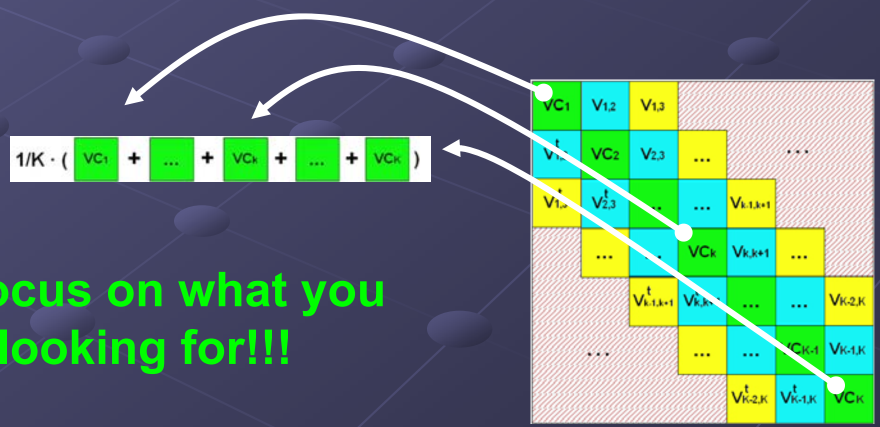
- **The best monitoring approach depends of the type of fault.** To detect:
  - **Breakage of the inst. corr. structure: Multi-Phase VW**
  - **Dynamic chage: Multi-Phase BD1**
  - **Overall change: BW**

Variable-wise

$$\#Par. = \frac{(J+1)J}{2}$$

Batch-wise

$$\#Par. = \frac{(JK+1)JK}{2}$$



Try to focus on what you are looking for!!!

J. Camacho, J. Picó and A. Ferrer. *Multi-Phase Analysis Framework for Handling Batch Process Data*, Journal of Chemometrics, 2008, available on-line, DOI: 10.1002/cem.1151

Conclusions

Outline

- **The best monitoring approach depends of the type of fault.** To detect:
  - **Breakage of the inst. corr. structure: Multi-Phase VW**
  - **Dynamic chage: Multi-Phase BD1**
  - **Overall change: BW**
- One note: **This results are for PCA monitoring, not for PLS !!!!**

  ★ **For prediction with PLS: Identify the order of dynamics.**

★ J. Camacho, J. Picó and A. Ferrer. *Bilinear modelling of batch processes. Part II: Comparison of PLS softsensors*, Journal of Chemometrics, 2008, In PRESS.

Conclusions

Outline

- **The best monitoring approach depends of the type of fault.** To detect:
  - **Breakage of the inst. corr. structure: Multi-Phase VW**
  - **Dynamic chage: Multi-Phase BD1**
  - **Overall change: BW**
- One note: **This results are for PCA monitoring, not for PLS !!!!**
- For those approaches that subtract the average trajectory:
  - **The unfolding (#LMVs) depends on the types of fault we want to detect.**
  - **The number of sub-models depends on #LMVs and the data of the process:**
    - The changes in the correlation structure may be identified from the data of the process (MP Framework)

J. Camacho, J. Picó and A. Ferrer. *Multi-Phase Analysis Framework for Handling Batch Process Data*, Journal of Chemometrics, 2008, In PRESS, DOI: 10.1002/cem.1151

On-line monitoring of batch processes: Does the modelling structure matter?

Monitoring Systems Design

Outline

1. **Monitoring Systems Design**
2. Toy Process

- Two steps:
  - Modelling step:
    - Align the data
    - Preprocess
    - Convert the three-way data into two-way
    - PCA Modelling $X = T \cdot P^T + E$

  - Construct a pair of monitoring charts based on:
    - The D-statistic (from the scores ***T***)
    - The SPE (from the residuals ***E***)

Monitoring Systems Design

Outline

- Alignment or outliers: detection non-necessary for this example.
- Preprocessing:
  - Data is already centered.
  - Data is scaled to unit variance in each sampling time.
- Modelling:
  - Determine the number of PCs
- Desing the monitoring system:
  - Compute the control limits

LEAVE-ONE-BATCH-OUT CROSS-VALIDATION

Monitoring Systems Design

Outline

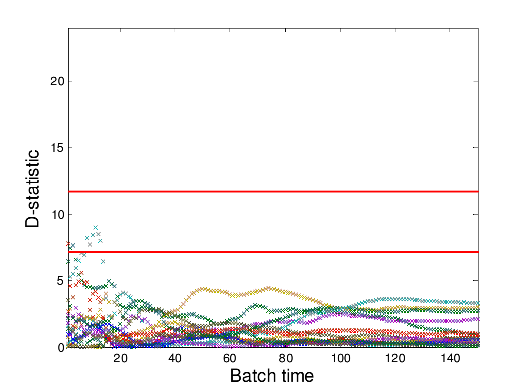
1. **Monitoring Systems Design**
2. Toy Process

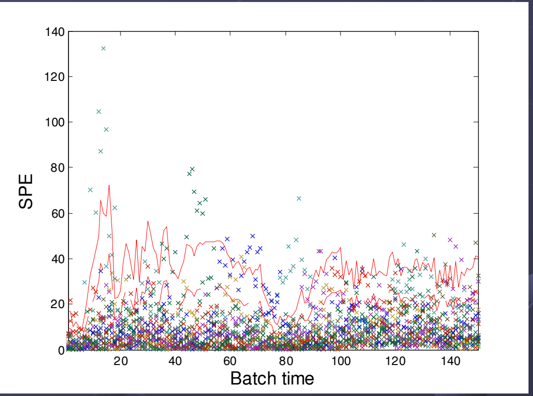
- Theoretical upper control limits:
  - α: imposed significant level (ISL).

$$UCL(D)_\alpha = \frac{A\cdot(I^2-1)}{I\cdot(I-A)}F_{(A,(I-A)),\alpha}$$

$$UCL(Q)_\alpha = \theta_1 \cdot \left[\frac{z_\alpha\sqrt{2\theta_2 h_0^2}}{\theta_1} + 1 + \frac{\theta_2 h_0 (h_0-1)}{\theta_1^2}\right]^{\frac{1}{h_0}}$$

  - OTI risk leave-one-batch-out CV: OTI-CV





★ The OTI-CV for α = 1% depends very much on the structure of the model (unfoldings, phases, etc.)

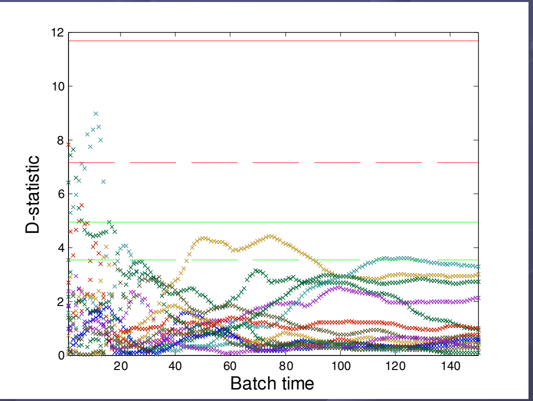
★ J. Camacho and J. Picó. *Online Monitoring of Batch Processes using Multi-Phase Principal Component Analysis*, Journal of Process Control, 10(16):1021-1035 (2006).

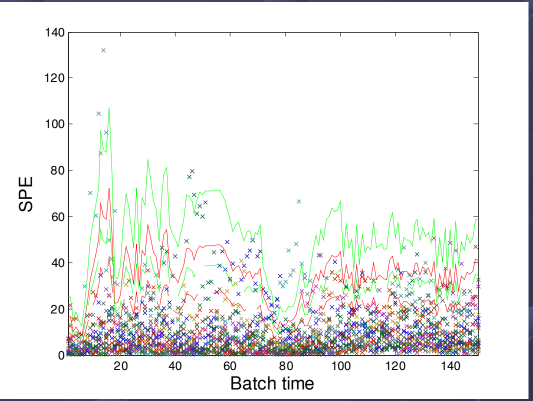
Monitoring Systems Design

Outline

1. **Monitoring Systems Design**
2. Toy Process

- Approaches: e.g. 99% confidence level.
  - Traditional: α = 1%
  - Proposed: set α so that OTI-CV = 1%
- Toy process:





Monitoring Systems Design

Outline

- Approaches: e.g. 99% confidence level.
  - Traditional: α = 1%
  - Proposed: set α so that OTI-CV = 1%

- Toy process: OTI (Test NOC set)

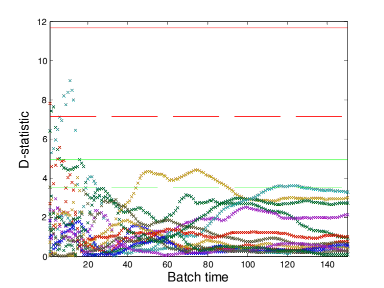
	Traditional		Proposed	
Model	OTI_D	OTI_{SPE}	OTI_D	OTI_{SPE}
NMG-PMP	0.00	1.70	0.08	1.08
NMG-CV	0.23	1.67	0.47	1.10
NMG-ZV	0.00	1.48	0.08	0.86
VW	0.86	1.23	0.87	0.96
Local	0.60	0.82	0.74	1.08
BD1	0.72	1.04	0.64	0.93
VW-2ph	0.46	0.51	0.60	0.44
BD1-2ph	0.52	0.42	0.56	1.06
BD-2ph	0.61	0.36	0.70	1.07

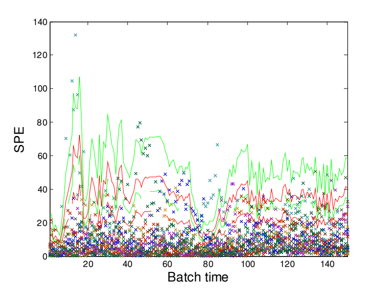
J. Camacho, J. Picó and A. Ferrer. *Multi-Phase Analysis Framework for Handling Batch Process Data*, Journal of Chemometrics, Early view (2008).

Monitoring Systems Design

Outline

1. **Monitoring Systems Design**
2. Toy Process





- Approaches: e.g. 99% confidence level.
  - Traditional: α = 1%
  - Proposed: set α so that OTI-CV = 1%
- Toy process: Number of PCs
  - α in BW-PMP: 1 PC

	α_D (OTICV=1%)	α_Q (OTICV=1%)	α_D (OTICV=5%)	α_Q (OTICV=5%)
1 PC	1.6	0.7	4.9	3.1
2 PCs	3.3	0.5	9.3	2.4
3 PCs	4.9	0.2	15.2	1.6
4 PCs	5.3	0.2	13.5	1.3

J. Camacho, J. Picó and A. Ferrer. *Multi-Phase Analysis Framework for Handling Batch Process Data*, Journal of Chemometrics, Early view (2008).

Toy Process

Outline

1. Monitoring Systems Design
2. **Toy Process**

- "Toy" process (simulink-matlab):

Error coherent with PCA sub-space

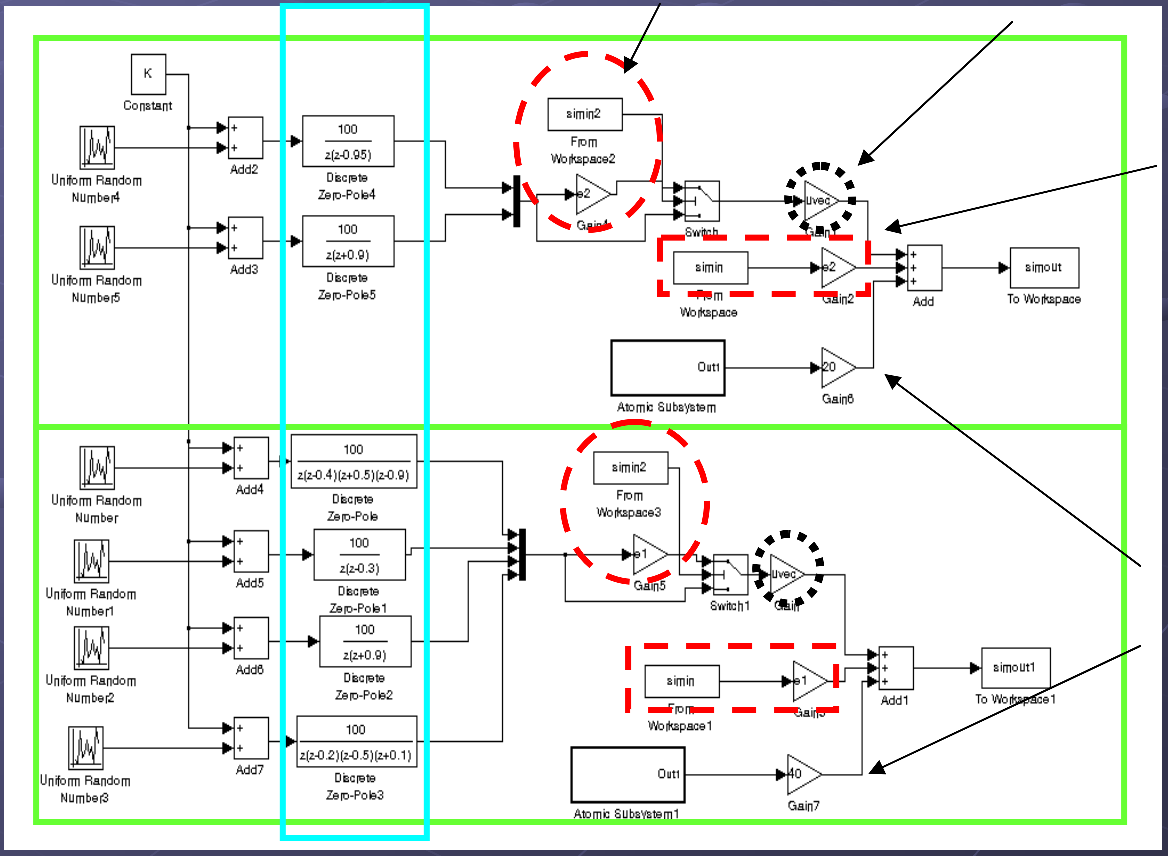
Conversion from LVs to OVS

Error not coherent with PCA sub-space

First phase (2 LVs, 1st OD)

Second phase (4 LVs, 3rd OD)

Measurement noise



Dynamics (ARs)

On-line monitoring of batch processes: Does the modelling structure matter?

CAC 2008

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