SCORES 4 CHEM
Knowledge Platform
www.scores4chem.be

The impact of process variability on Statistical Process Monitoring

Geert Gins, Jef Vanlaer, Jan Van Impe
KU Leuven Dept. of Chemical Engineering (BioTeC)

BIL 2014 — Workshop on Data-driven Modeling Methods and Applications
14–15 July 2014, Leuven, Belgium

ASSOCIATIE K.U.LEUVEN

essenscia

Overview

Statistical Process Monitoring

Process variability

Case study

- Study #1: Batch-end quality prediction
- Study #2: Fault detection

Conclusions

Overview

Statistical Process Monitoring

Process variability

Case study

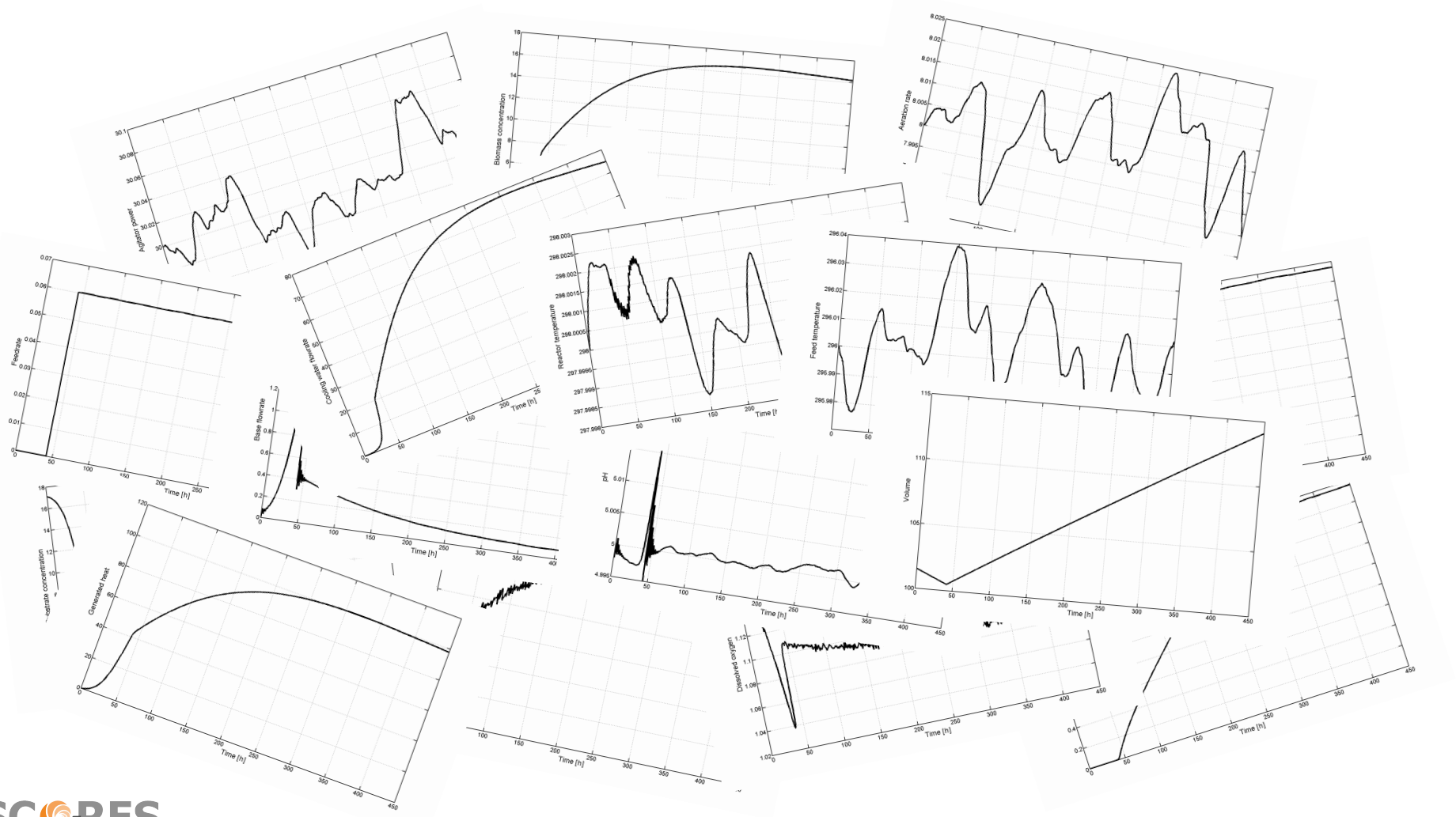
- Study #1: Batch-end quality prediction
- Study #2: Fault detection

Conclusions

Statistical Process Monitoring



Statistical Process Monitoring



Statistical Process Monitoring



Statistical Process Monitoring

Exploit available historical databases

- Quality prediction
- Fault detection
- Fault diagnosis

Development & benchmarking

- Known disturbances (amplitude, onset, …)
- Known quality parameters

⇒ Work with simulated processes

Overview

Statistical Process Monitoring

Process variability

Case study

- Study #1: Batch-end quality prediction
- Study #2: Fault detection

Conclusions

Process variability

Benchmark simulations

- Variability on initial conditions
- Non-perfect measurements & manipulated variables
- Constant model parameters

Reality

- Variability on initial conditions
- Non-perfect measurements & manipulated variables
- Stochastic, time-varying model parameters

Process variability

Benchmark simulations

Variability on initial conditions

Non-perfect measurements & manipulated variables

Constant model parameters

Reality

Variability on initial conditions

Non-perfect measurements & manipulated variables

Stochastic, time-varying model parameters

Process variability

Uncertainty about process

Negative influence on Statistical Process Monitoring

- Poorer prediction of quality parameters
- Slower detection of disturbances

⇒ Overestimate SPM performance

⇒ Should variability be included?

Overview

Statistical Process Monitoring

Process variability

Case study

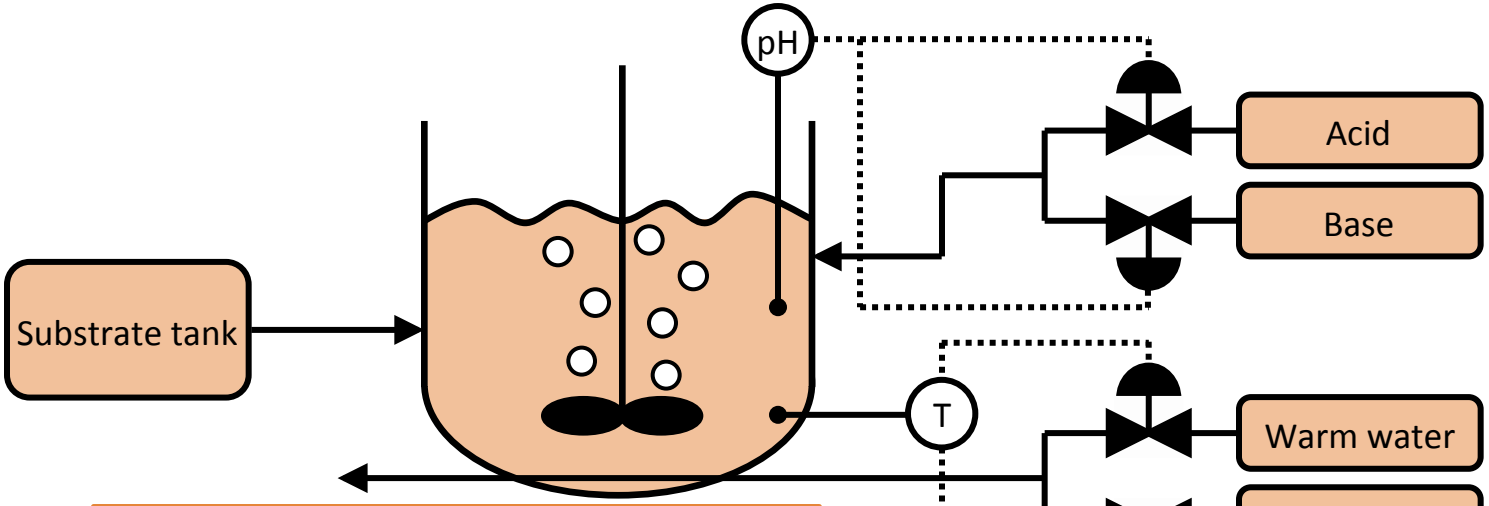
- Study #1: Batch-end quality prediction
- Study #2: Fault detection

Conclusions

Case study

PENSIM benchmark simulator

Industrial-scale penicillin production



$$\frac{dX}{dt} = \mu X + \frac{X}{V}\frac{dV}{dt}$$

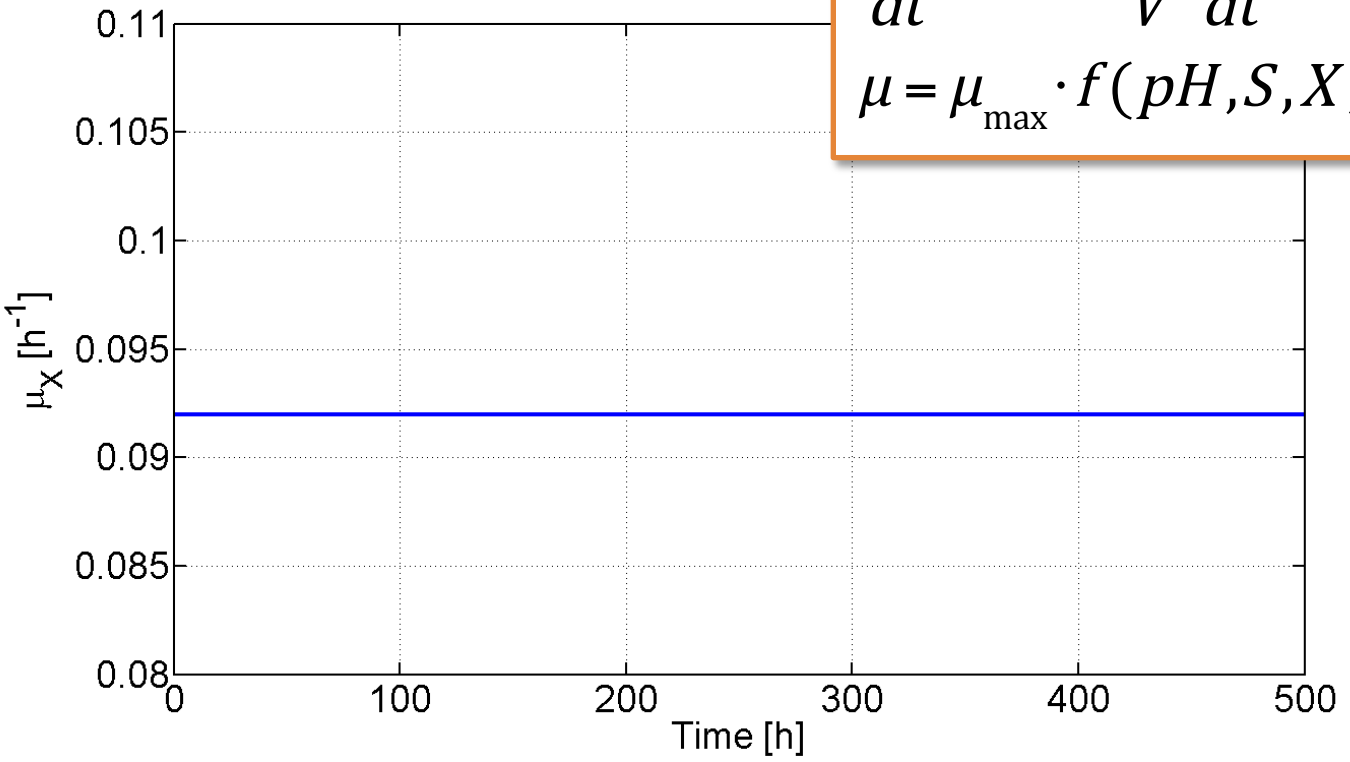
$$\mu = \mu_{\max} \cdot f(pH, S, X, DO, T)$$

Case study

Constant μ_{max}

$$\frac{dX}{dt} = \mu X + \frac{X}{V}\frac{dV}{dt}$$

$$\mu = \mu_{max} \cdot f(pH, S, X, DO, T)$$

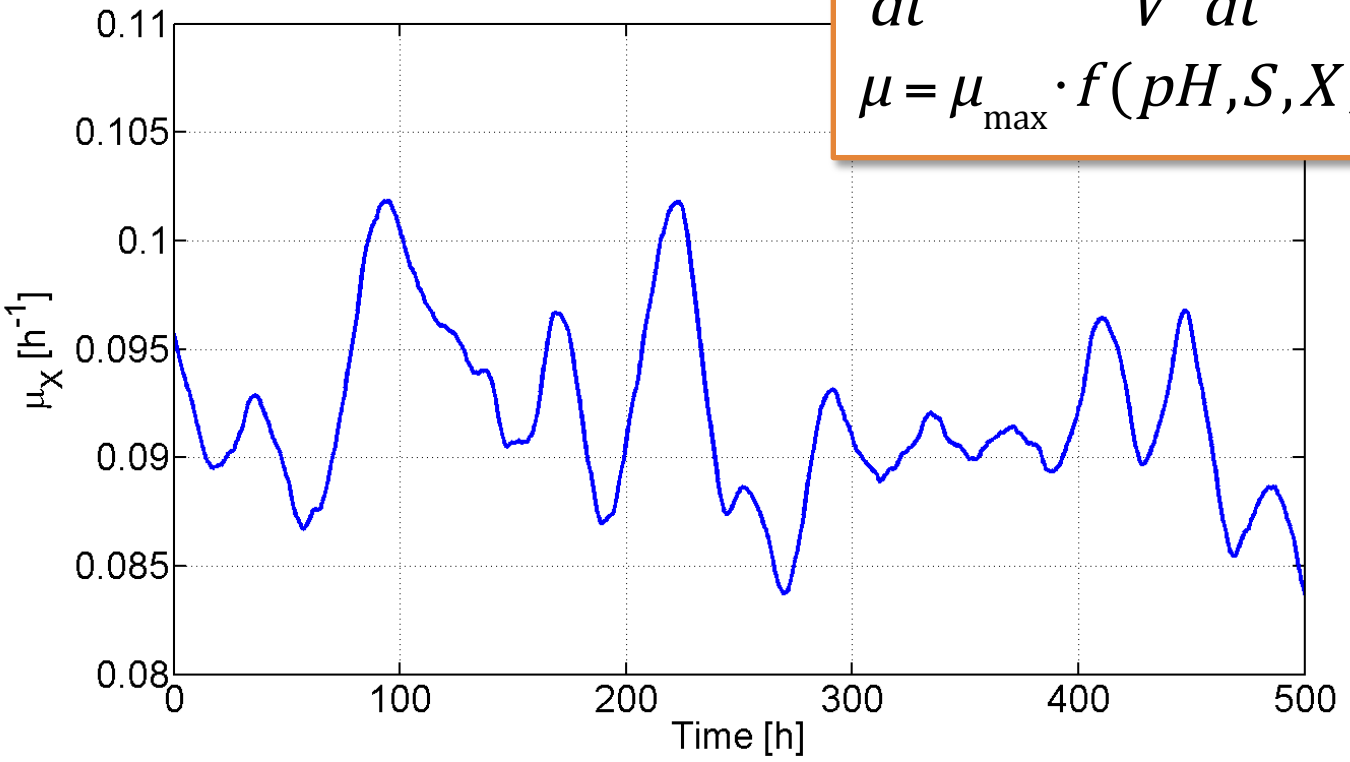


Case study

Time-varying μ_{max}

$$\frac{dX}{dt} = \mu X + \frac{X}{V}\frac{dV}{dt}$$

$$\mu = \mu_{max} \cdot f(pH, S, X, DO, T)$$



Overview

Statistical Process Monitoring

Process variability

Case study

- Study #1: Batch-end quality prediction
- Study #2: Fault detection

Conclusions

Batch-end quality prediction

Predict penicillin concentration at batch completion by exploiting online measurements

Partial Least Squares (PLS)

Capture underlying relationship between in- and outputs

Projection to low-dimensional space

$$\begin{cases} \mathbf{X} = \mathbf{T} \cdot \mathbf{P}^T + \mathbf{E}_X \\ \mathbf{Y} = \mathbf{T} \cdot \mathbf{Q}^T + \mathbf{E}_Y \end{cases}$$

Batch-end quality prediction

Investigate prediction accuracy for different levels of biological variability

Data set

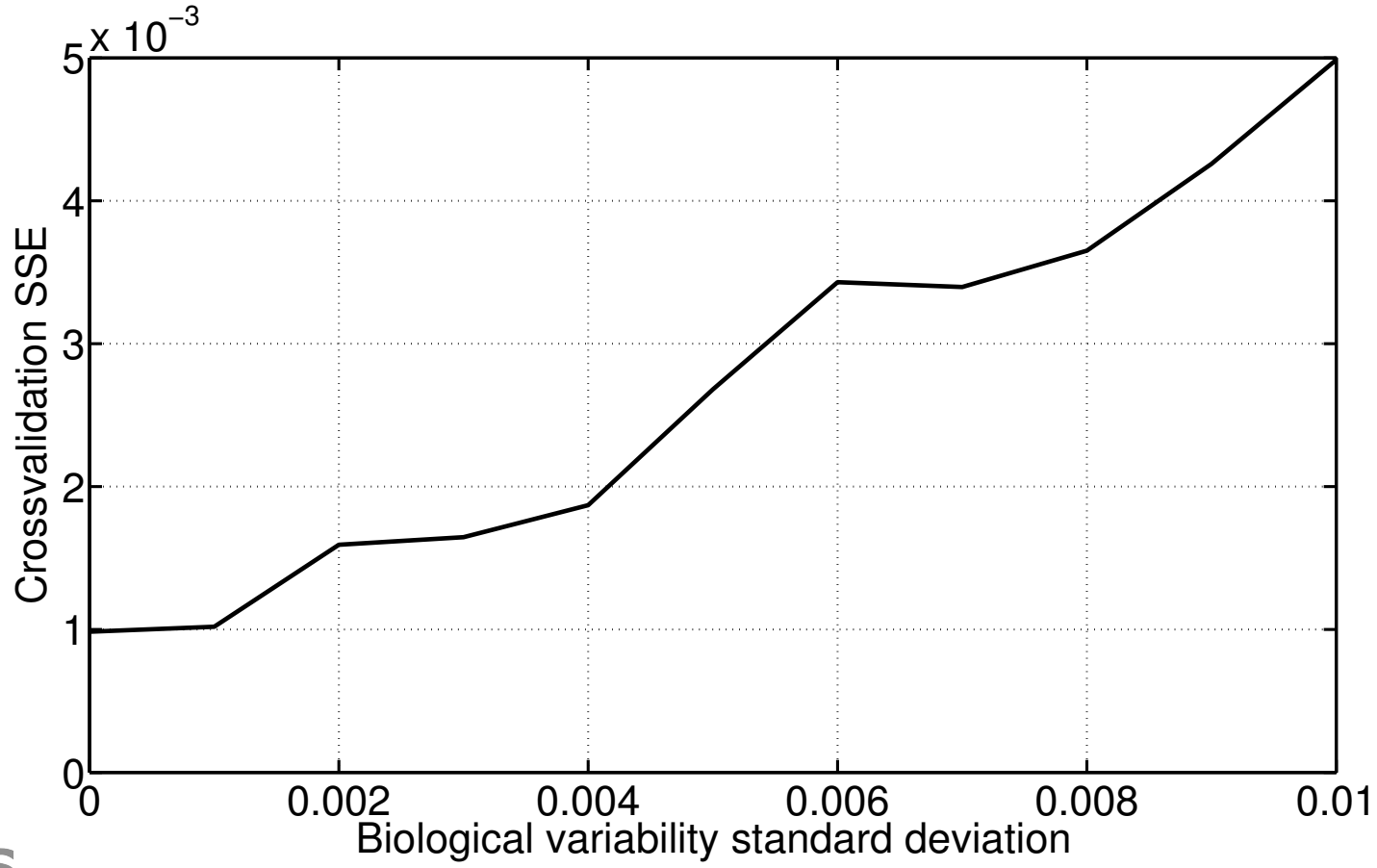
- 150 training batches with variability
- 50 validation with same variability

Performance

- Offline accuracy
- Online accuracy

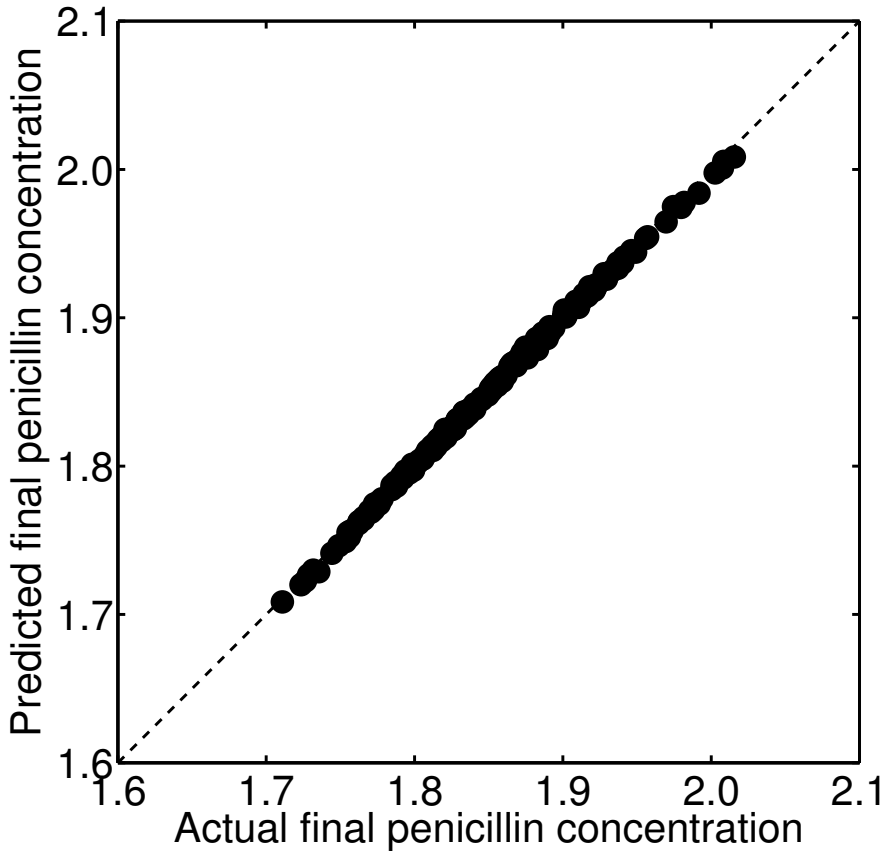
Batch-end quality prediction

Offline prediction



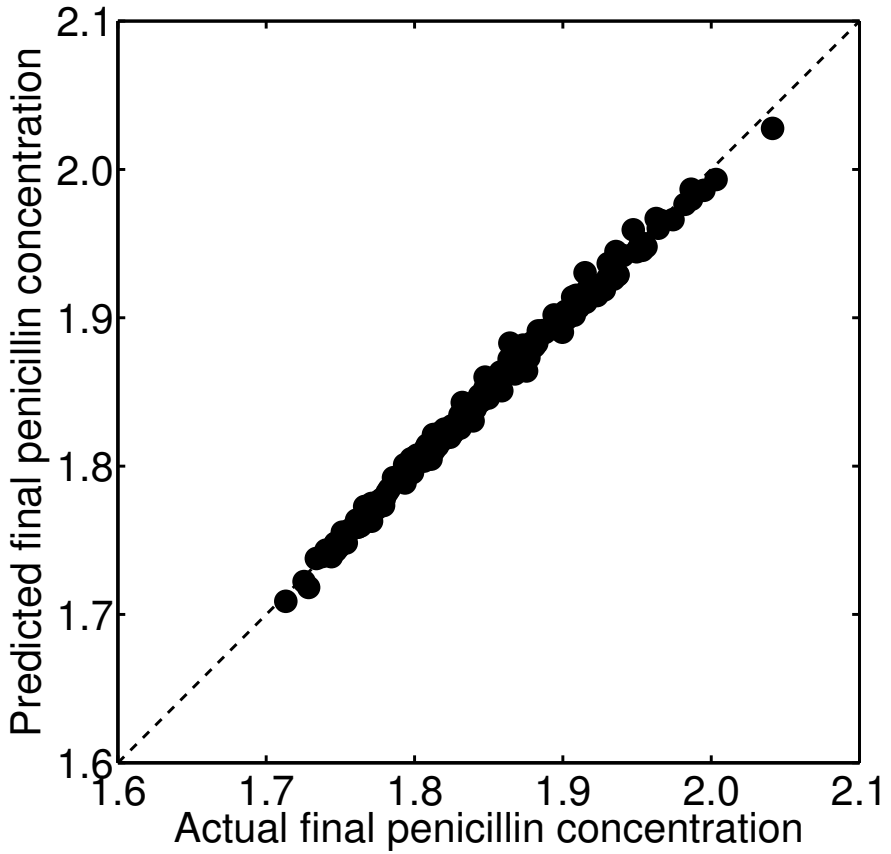
Batch-end quality prediction

Offline prediction: no biological variability



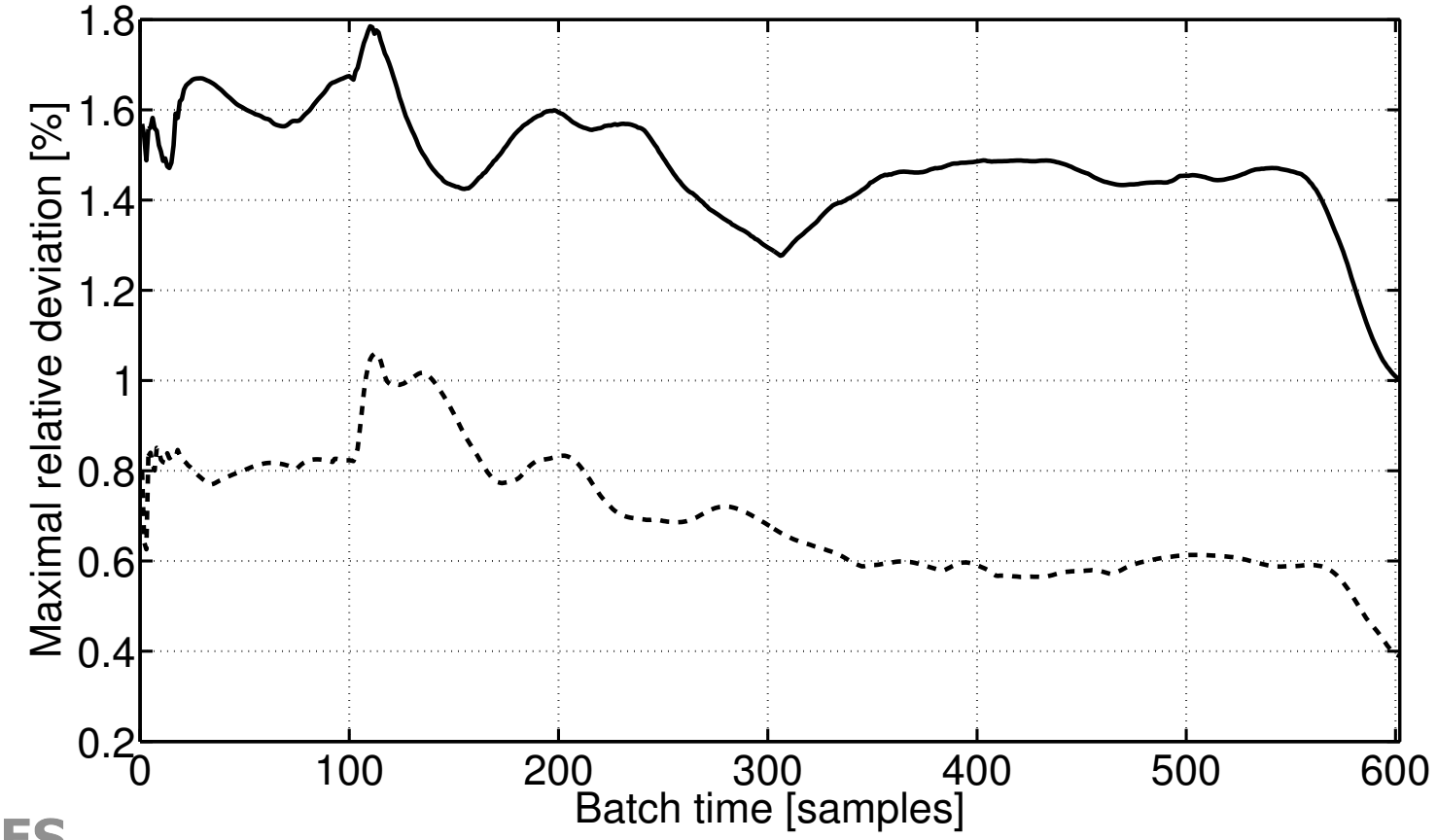
Batch-end quality prediction

Offline prediction: biological variability ($\sigma_{bv} = 0.01$)



Batch-end quality prediction

Online prediction



Conclusions

Do we overestimate the performance of SPM?

Should variability be included in benchmarks?

Batch-end quality prediction

Acceptable prediction accuracy

Slightly less accurate for increasing variability

$\Rightarrow$ *Negative influence of variability*

Fault detection

???

Overview

Statistical Process Monitoring

Process variability

Case study

- Study #1: Batch-end quality prediction
- Study #2: Fault detection

Conclusions

Fault detection

Detect deviations from normal behavior by exploiting online measurements

Principal Component Analysis (PCA)

Characterize normal operation

Projection to low-dimensional space

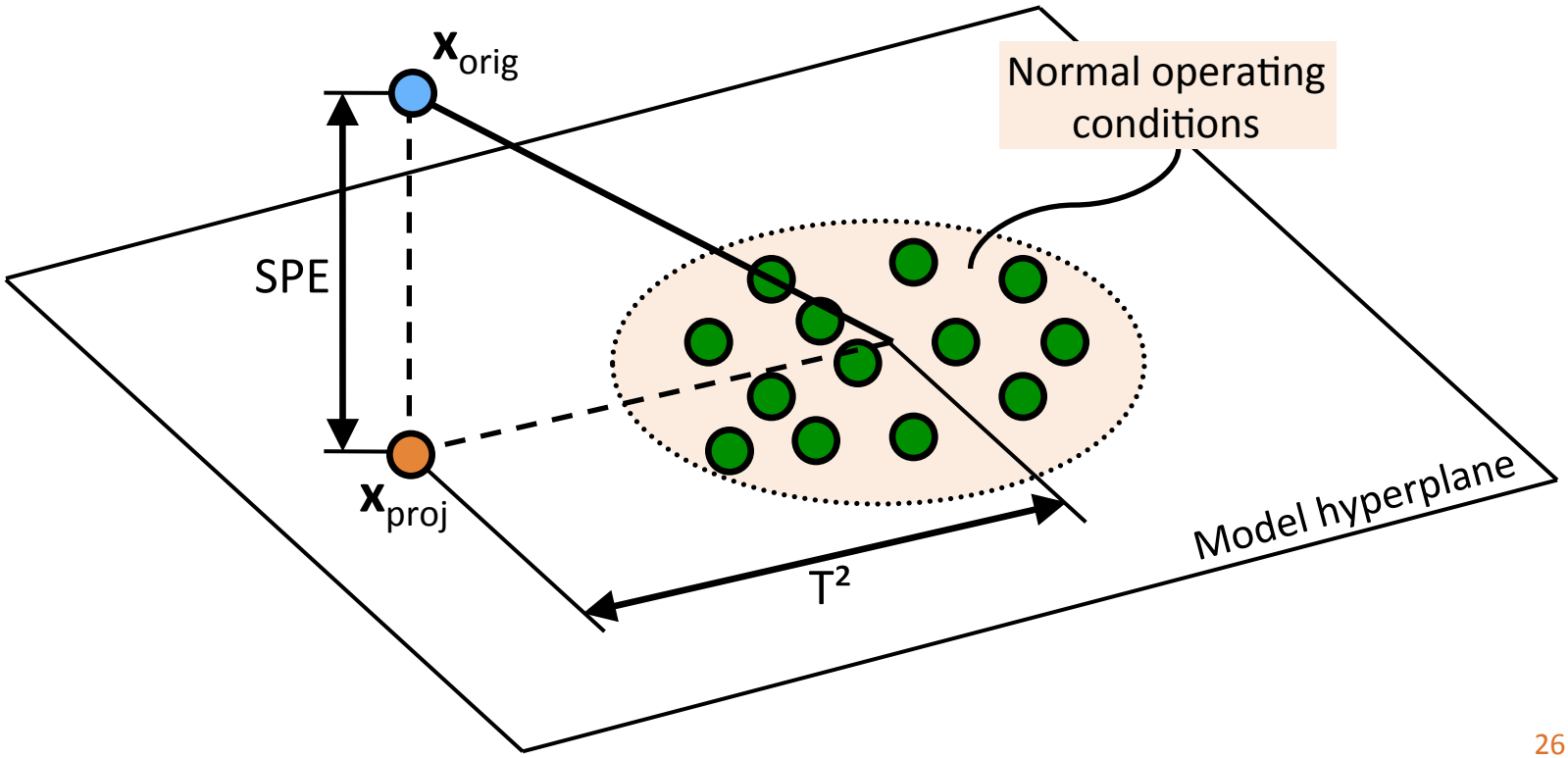
$$\mathbf{X} = \mathbf{T} \cdot \mathbf{P}^T + \mathbf{E}_X$$

Fault detection statistics

Detect deviations from normal operation

Fault detection

Detect deviations from normal behavior by exploiting online measurements



Fault detection

Investigate detection speed for different levels of biological variability

Data set

150 normal batches with variability

50 faulty batches with same variability

Performance

Detection speed

Fault detection

σ_{bv}	Detection [h]		p-value		
	μ	σ	p_0	$p_{0.001}$	$p_{0.005}$
Gradual feed rate decrease					
0	31.1	5.6	–	–	–
0.001	26.8	5.4	2.0×10^{-4}	–	–
0.005	25.3	3.8	3.8×10^{-8}	1.2×10^{-1}	–
0.01	23.2	5.7	3.6×10^{-10}	1.5×10^{-3}	2.9×10^{-2}
Gradual DO sensor failure					
0	21.4	0.8	–	–	–
0.001	19.9	1.1	3.1×10^{-12}	–	–
0.005	17.8	1.3	1.9×10^{-30}	3.6×10^{-14}	–
0.01	16.4	0.9	1.6×10^{-49}	5.2×10^{-32}	7.2×10^{-9}

Overview

Introduction

Process variability

Case study

- Study #1: Batch-end quality prediction
- Study #2: Fault detection

Conclusions

Conclusions

Do we overestimate the performance of SPM?

Should variability be included in benchmarks?

Batch-end quality prediction

Acceptable prediction accuracy

Slightly less accurate for increasing variability

⇒ *Negative influence of variability*

Fault detection

Faster detection for increasing variability

⇒ *Positive influence of variability*

Conclusions

Do we overestimate the performance of SPM?

Should variability be included in benchmarks?

⇒ Trade-off between different applications

Include variability in case studies …

… when comparing different techniques

… when assessing/estimating real-life performance

SCORES 4 CHEM
Knowledge Platform
www.scores4chem.be

The impact of process variability on Statistical Process Monitoring

Geert Gins, Jef Vanlaer, Jan Van Impe
KU Leuven Dept. of Chemical Engineering (BioTeC)

BIL 2014 — Workshop on Data-driven Modeling Methods and Applications
14–15 July 2014, Leuven, Belgium

ASSOCIATIE K.U.LEUVEN

essenscia