

UNIVERSITÀ  
DEGLI STUDI  
DI PADOVA

DEPARTMENT OF  
INDUSTRIAL ENGINEERING 

# Machine Learning Laboratory #3

Prof. Pierantonio Facco

CAPE-Lab, Computer-Aided Process Engineering Laboratory

Email: [pierantonio.facco@unipd.it](mailto:pierantonio.facco@unipd.it)

URL: <https://research.dii.unipd.it/capelab/>

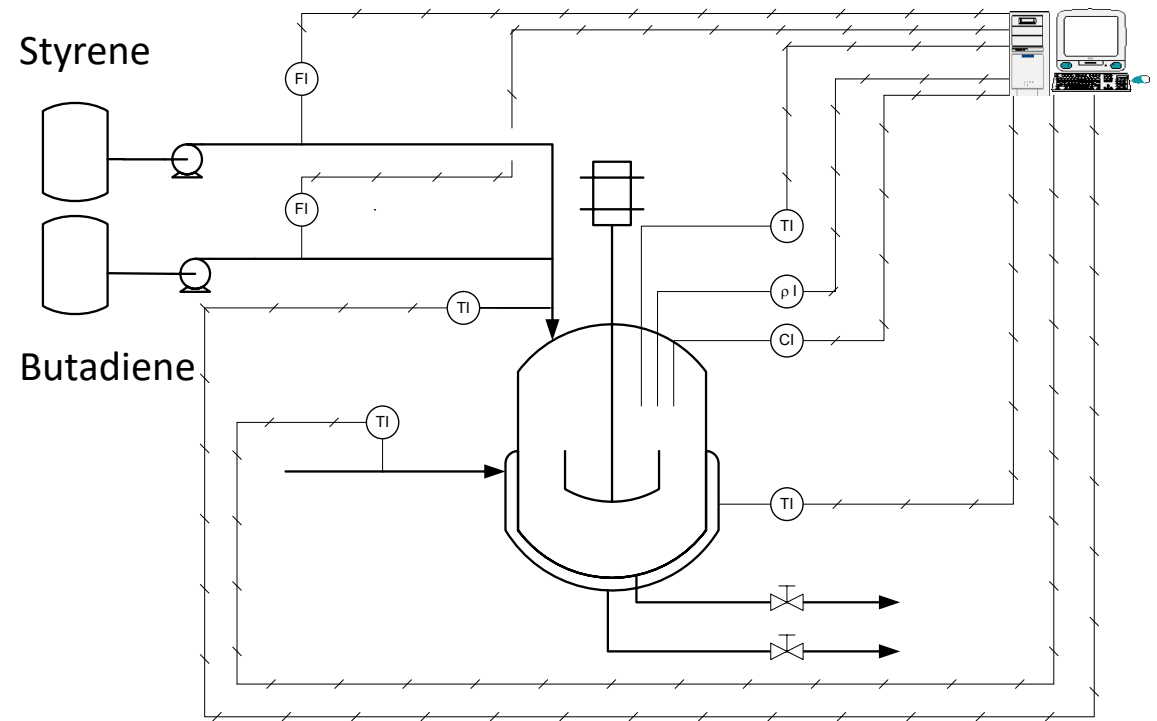
Example #3:

rubber process monitoring

# Process and objectives

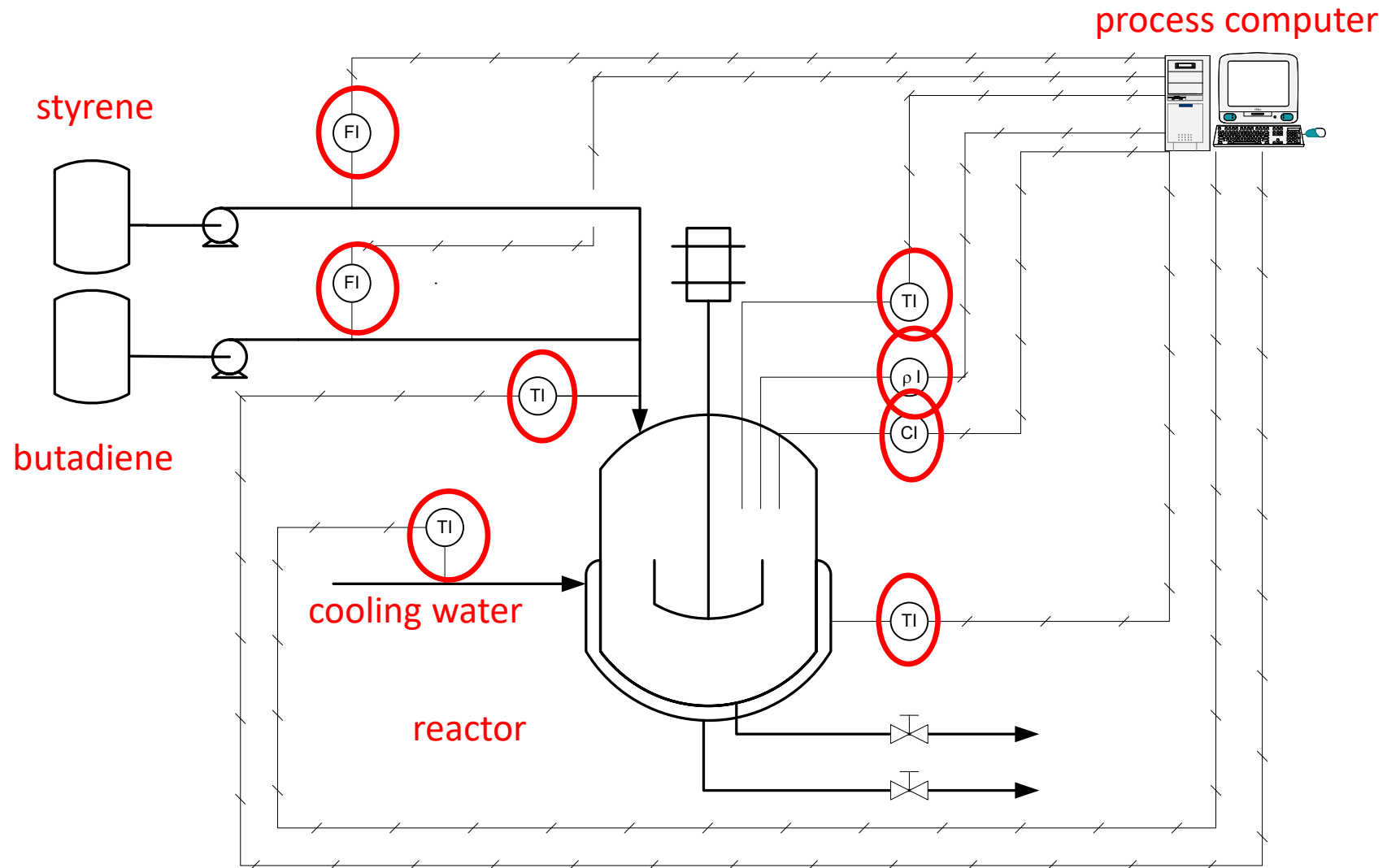
- Semi-batch process\*: styrene-butadiene polymerization for the production of rubber
- Objectives:
  - online monitoring
  - fault detection & diagnosis

	variable
1	styrene flowrate $F_{styr}$
2	butadiene flowrate $F_{buta}$
3	feed temperature $T_f$
4	reactor temperature $T_r$
5	coolant temperature $T_{cw}$
6	reactor jacket temperature $T_{rj}$
7	polymer density $R_o$
8	total conversion $c_{TOT}$
9	instant energy $E_r$



\* Nomikos, P., MacGregor, J.F., 1994. Monitoring batch processes using multiway principal component analysis. AIChE J. 40, 1361–1375

# P&ID



# Available data visualization

- Load: `styrenebutadienebatch.mat`

- find it in Moodle under: rubber production monitoring

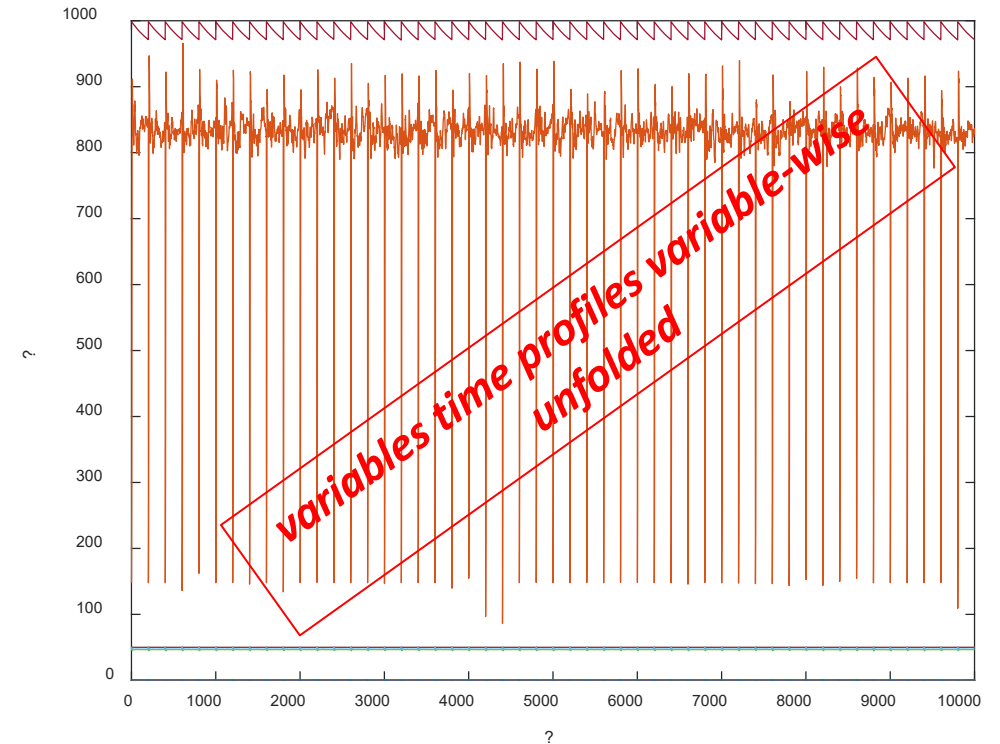
- Data:

- 50 standard batches
- 9 variables recorded in 200 time samples

- Data visualization:

```
plot(X); xlabel('?'); ylabel('?')
```

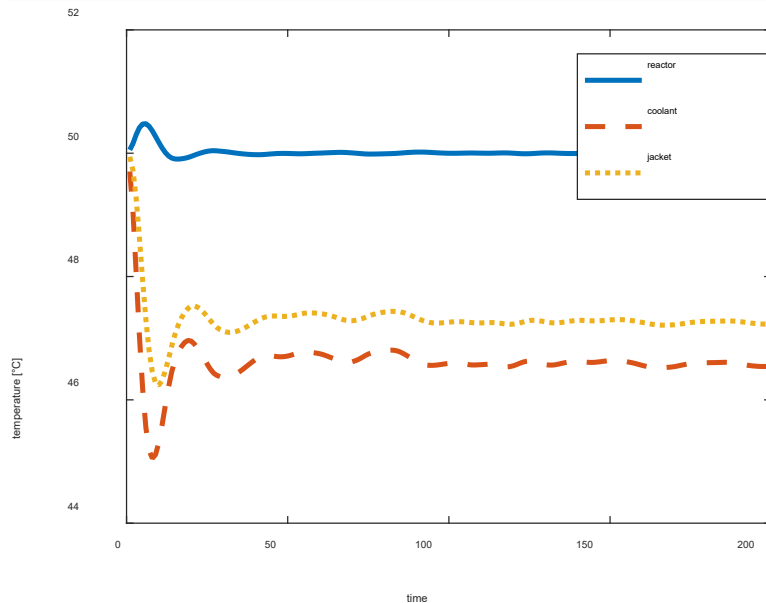
- what data structure?



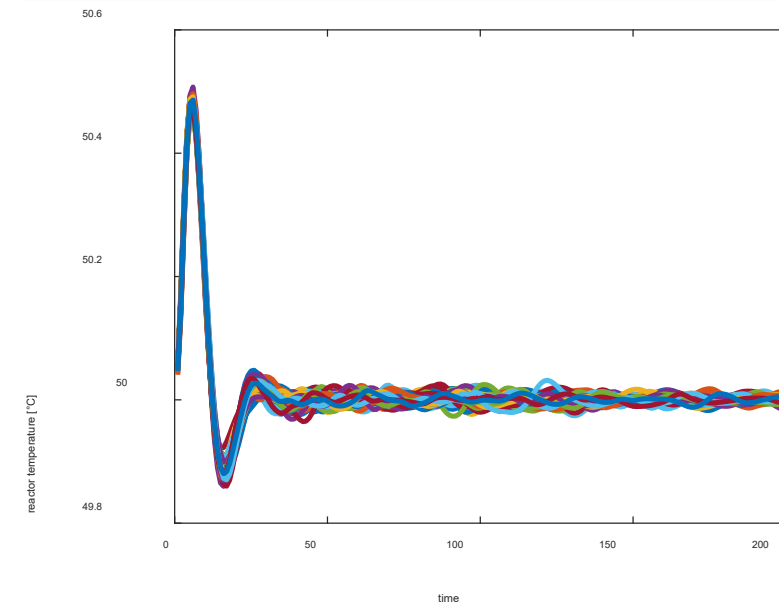
# Variables time profiles

- Variables time profiles do not show anomalies
  - high correlation is found
- All the batches seem to be standard

```
figure; plot(X(1:200,4:6));  
xlabel('time');  
ylabel('temperature [°C]');  
legend('reactor', 'coolant', 'jacket')
```

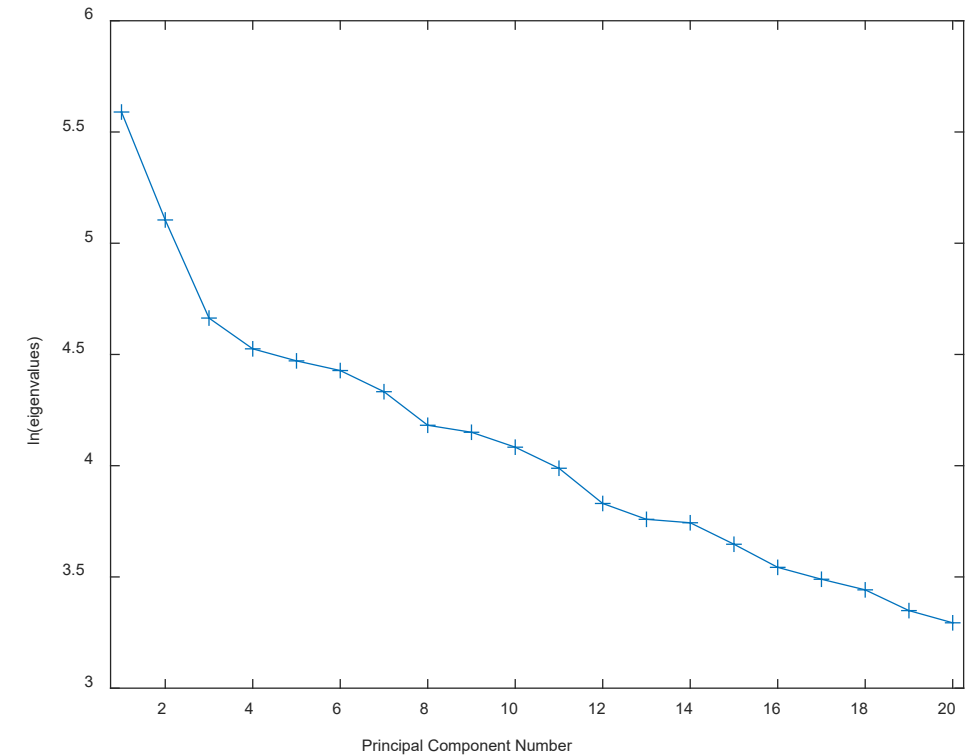


```
Tr(:, :)=X_3D(:, 4, :);  
figure; plot(Tr');  
xlabel('time');  
ylabel('reactor temperature [°C]');
```



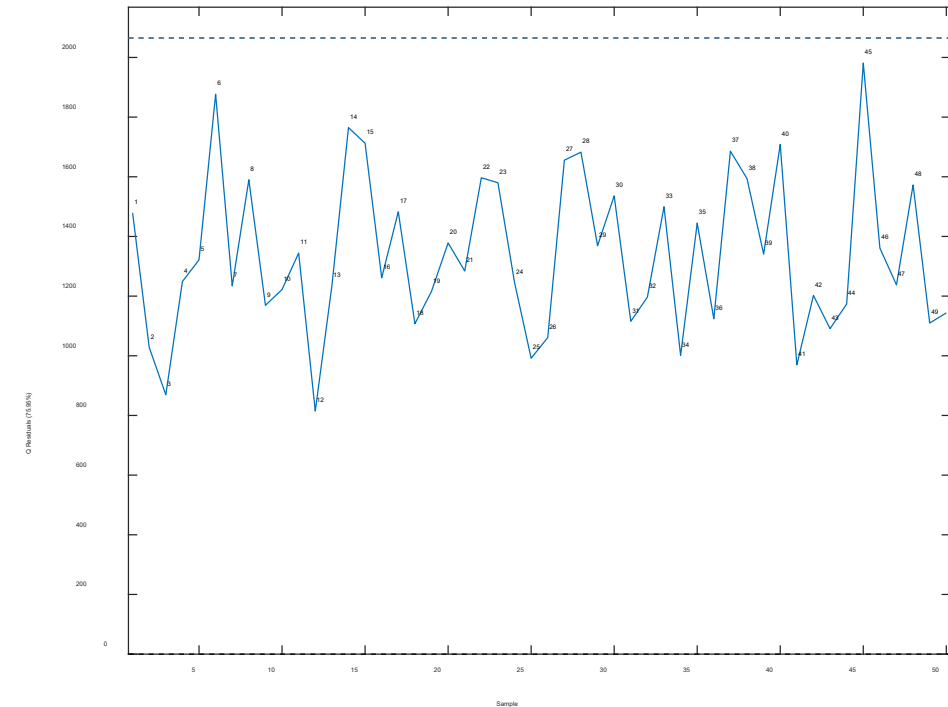
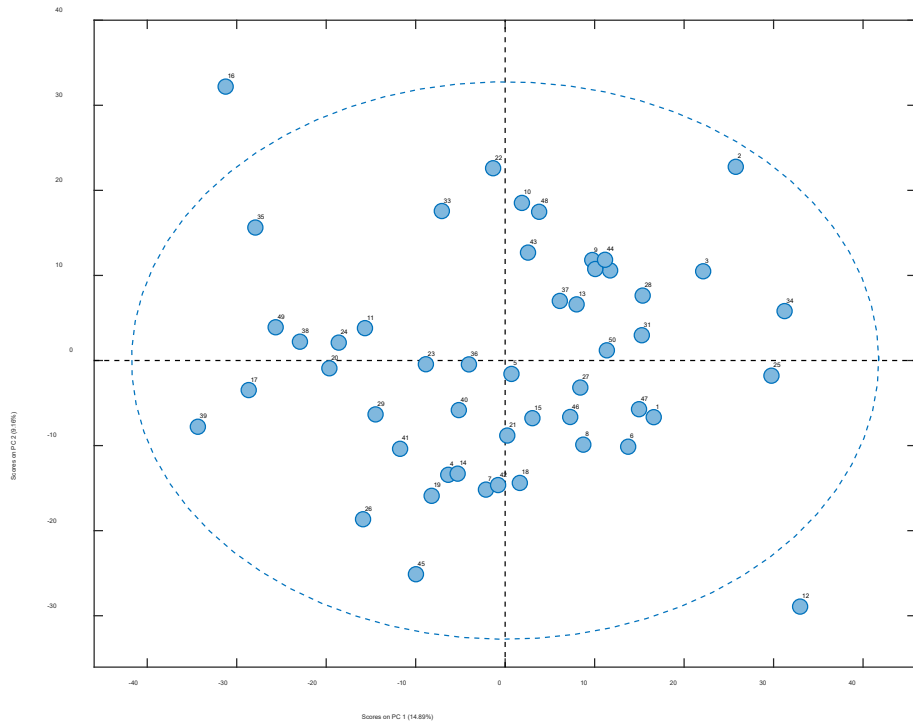
# PCA modelling

- **Batch-wise unfolding** considers process dynamics
  - consider commands: **unfoldm** and **unfoldmw**
- Build the PCA model on: **Xbwu**
- Pretreatment:
  - autoscaling: to survey the variables time profiles compared to the **average time profile and the respective variability**
- Number of selected PCs: 2-4



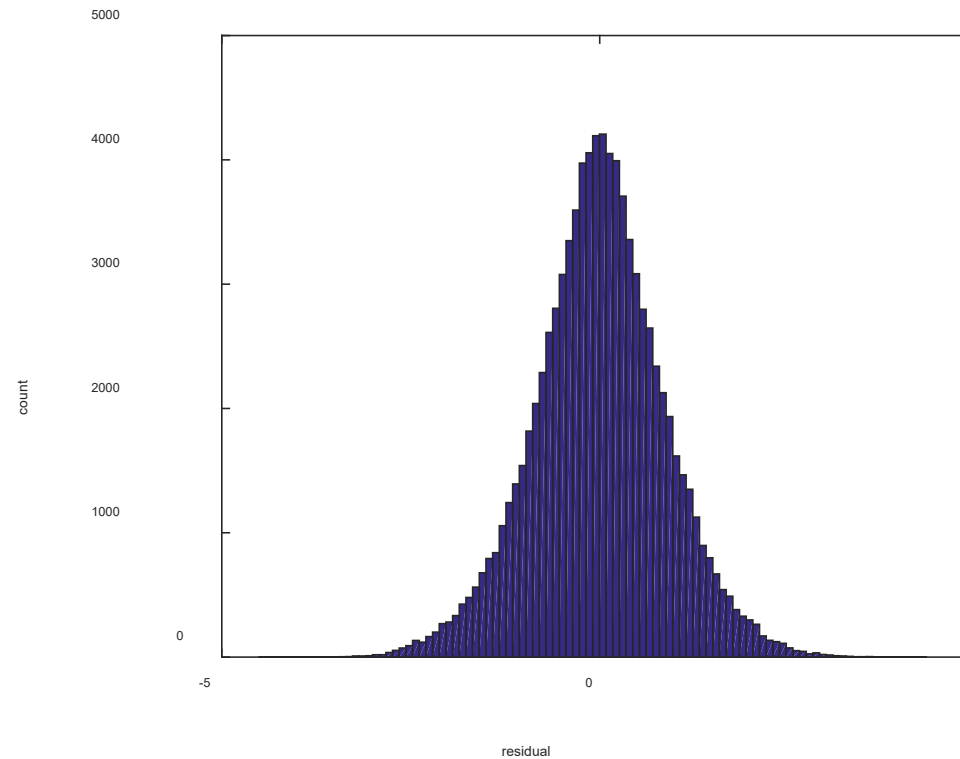
# Score plot and relation among batches

- The batches seems to be multi-normally distributed
- ~5% of the batches are out of the 95% confidence ellipse
- No anomalies are present in the Q residuals

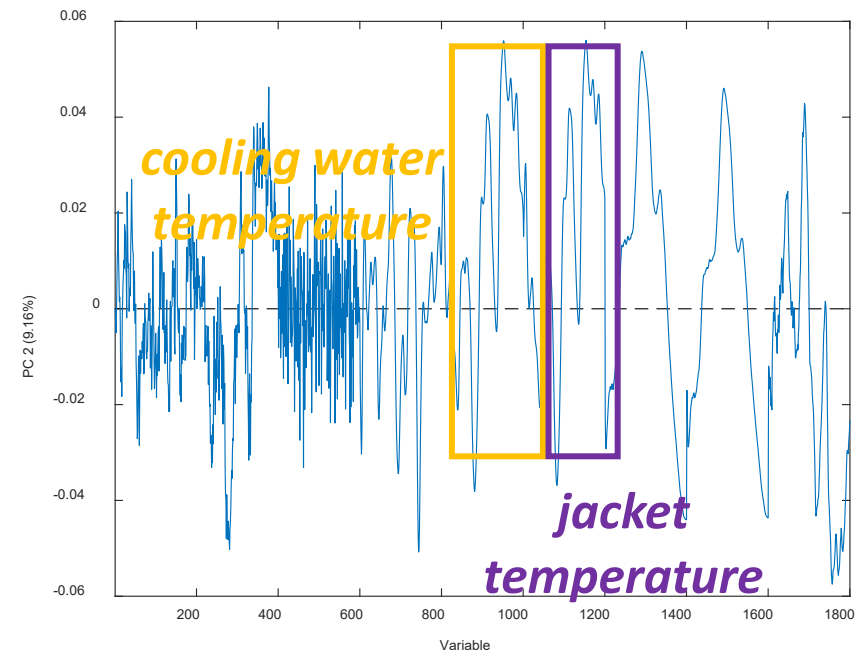
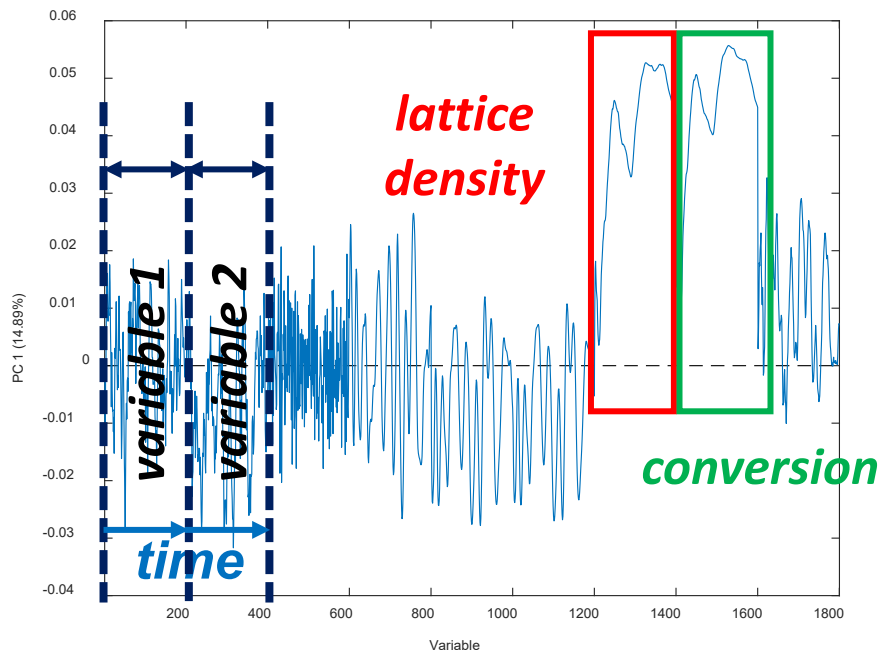


# Note that...

- The residuals are normally distributed and centered in zero
  - all the residuals are picked together here



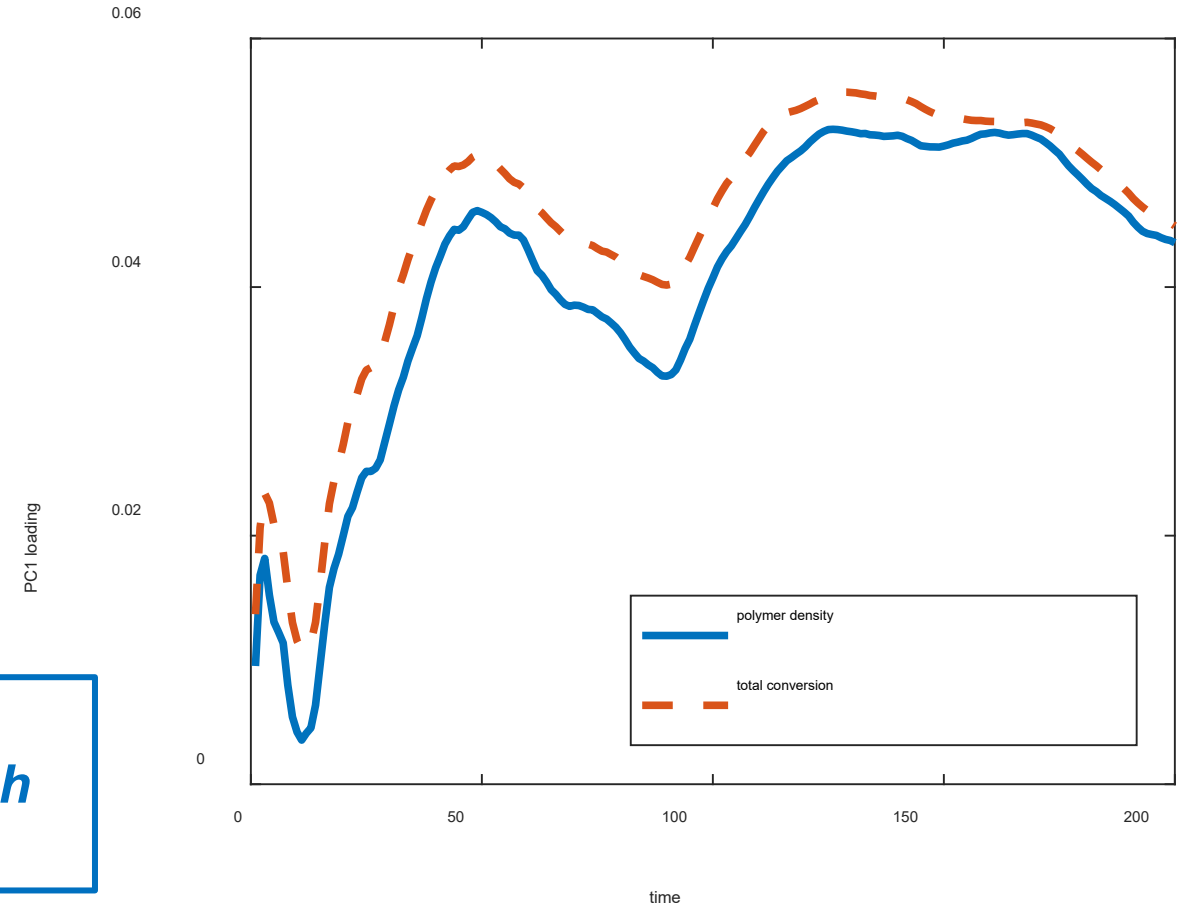
- The loading plot shows that:
  - variables correlation **in time**
  - **time trajectories** of the major sources of variability
    - lattice density and conversion (on PC1)
    - coolant and jacket temperatures (on PC2)



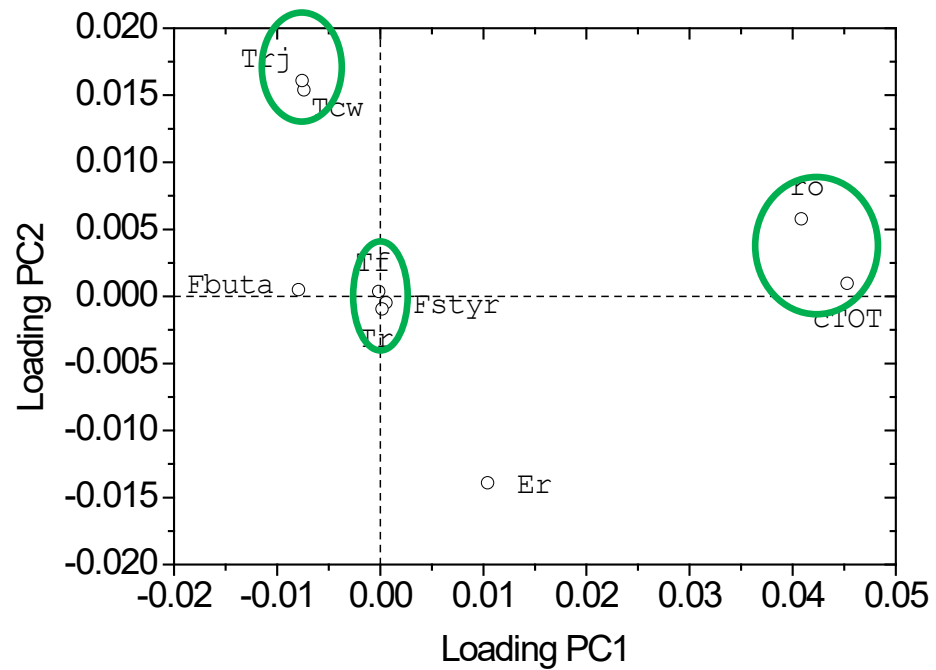
- The detail on the time profiles of the PC1 loadings of the most important variables:
  - polymer density
  - total conversion

***Increasing importance in time***

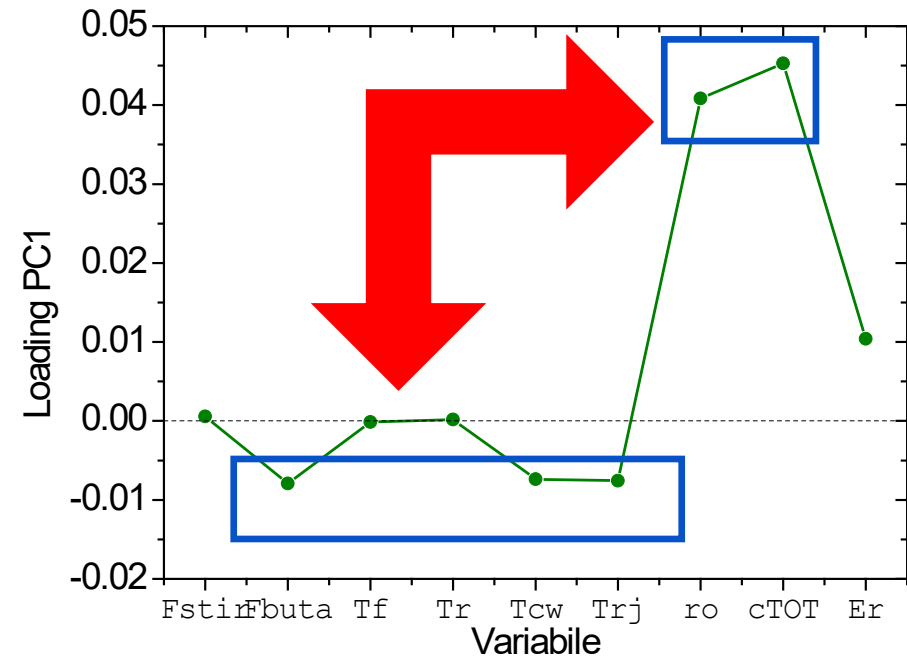
- ***not so important in the first part of the batch***
- ***important in the second half of the batch***



- **Cumulative loadings** show that:
  - the values are cumulated on the entire time trajectory
  - the same variability sources as in the previous slide



clusters

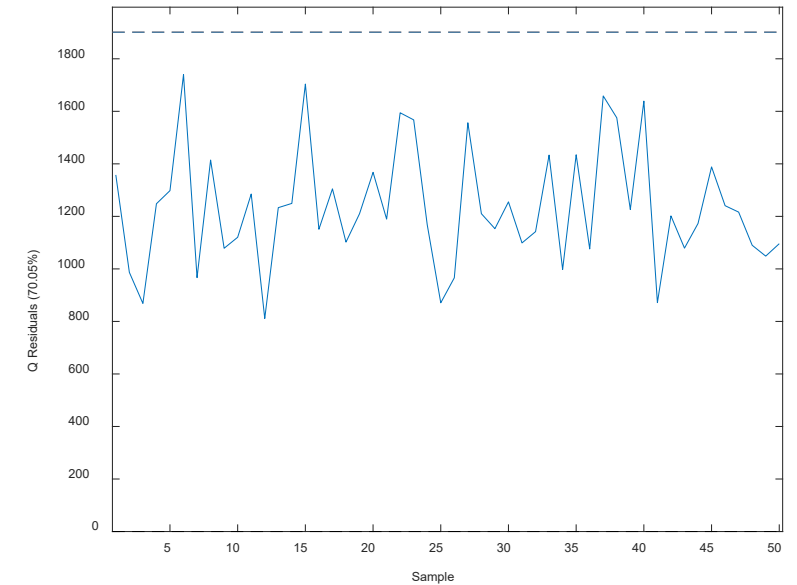
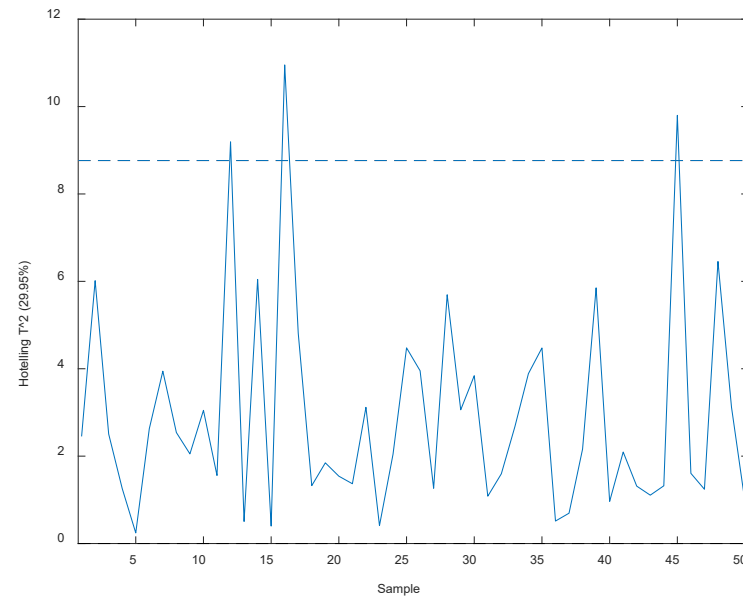
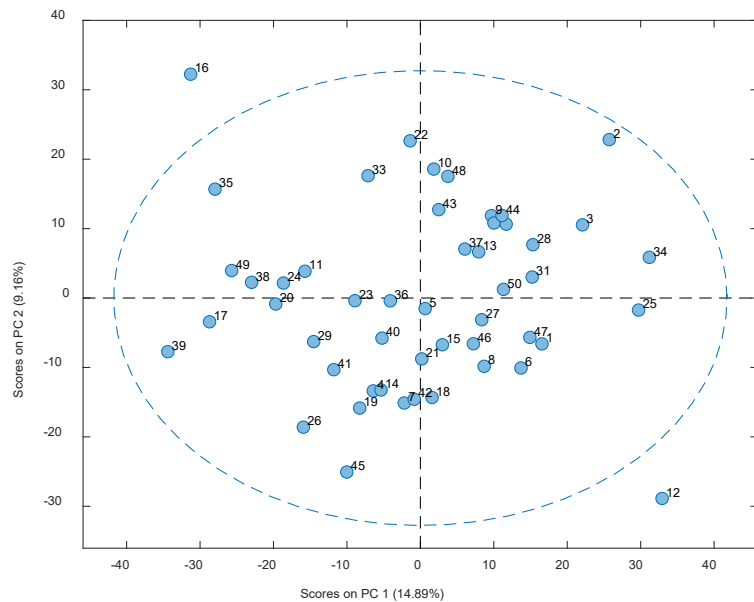


positive relations

anti-correlation

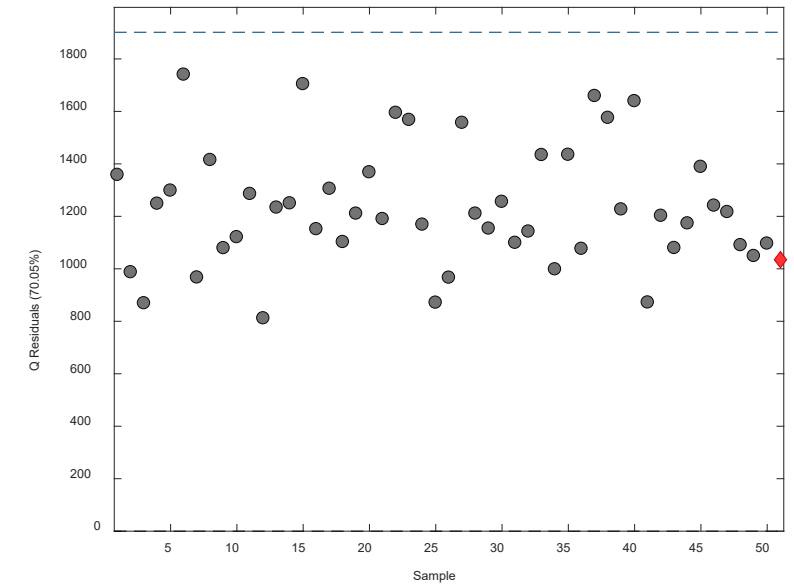
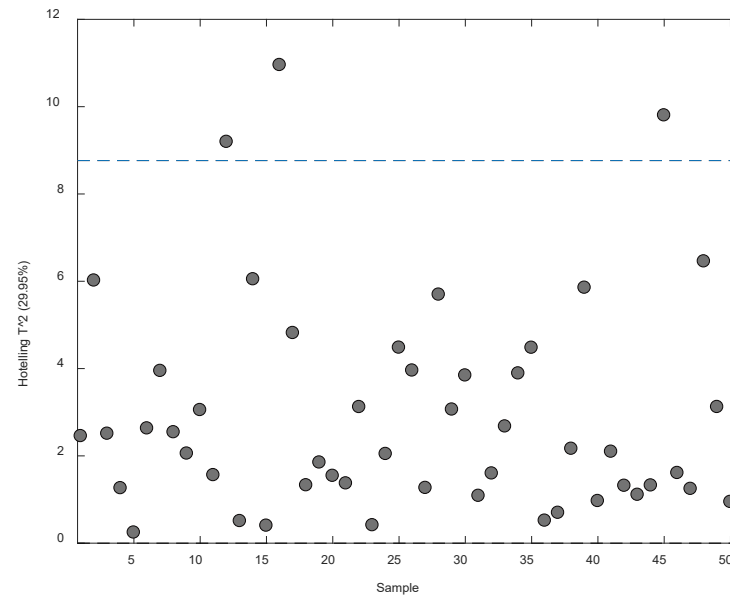
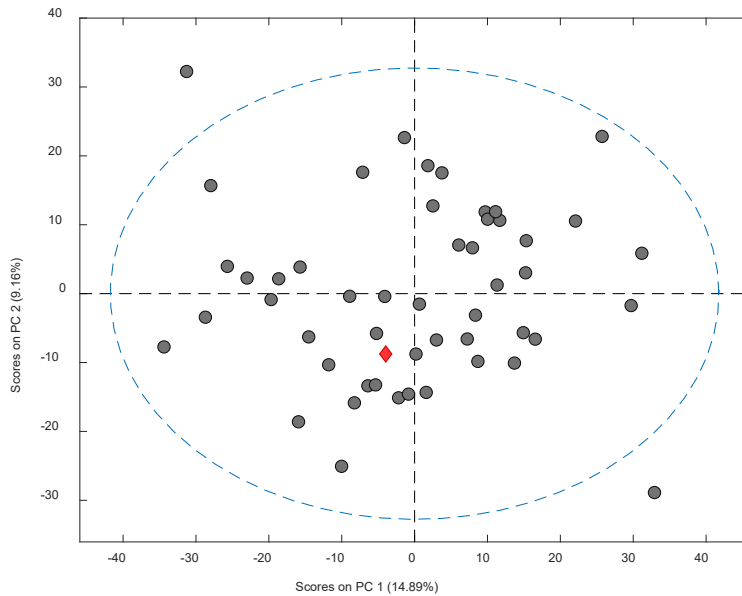
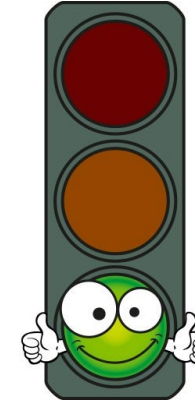
# Control charts

- $T^2$  and  $SPE$  control charts in a joint reading
  - complementary information



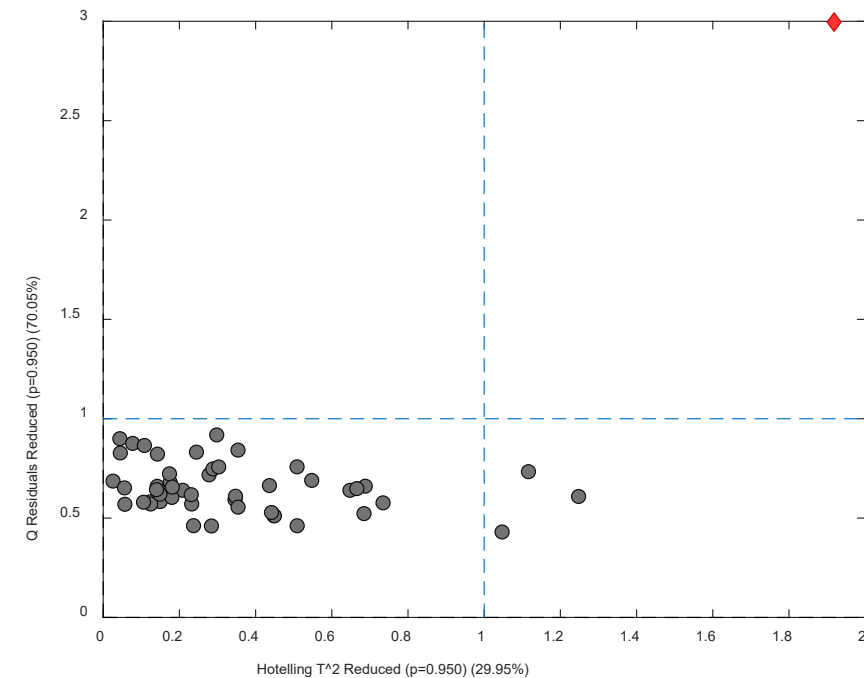
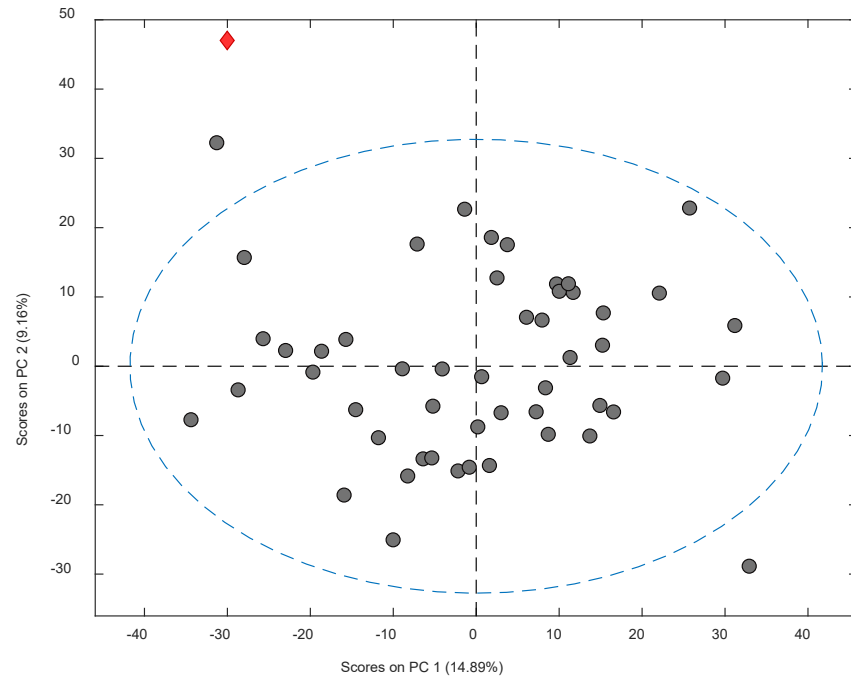
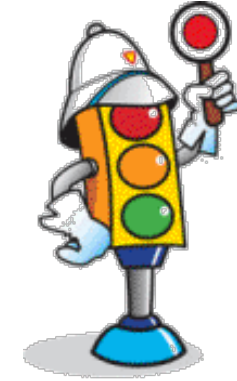
# «Post mortem» monitoring of batch 53

- Batch 53 is **normal**
  - project onto the model **x53\_bwu**

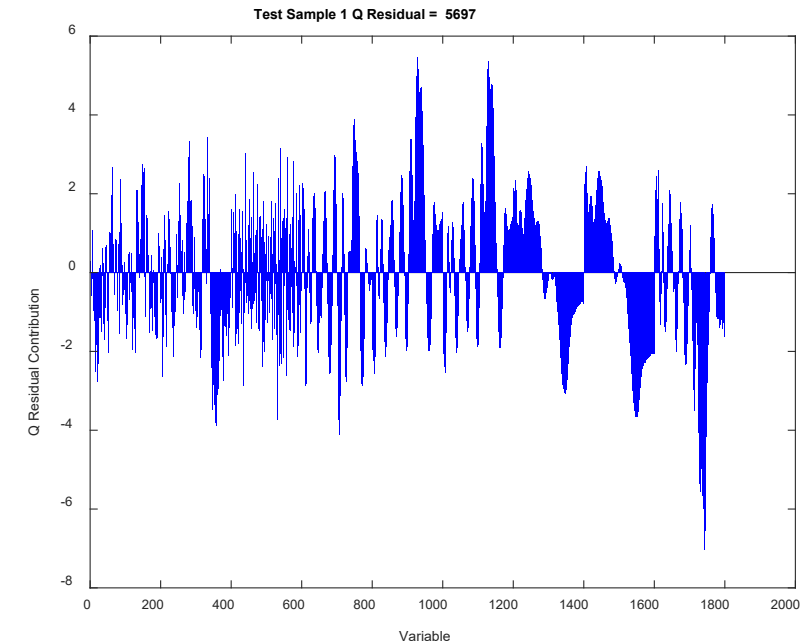
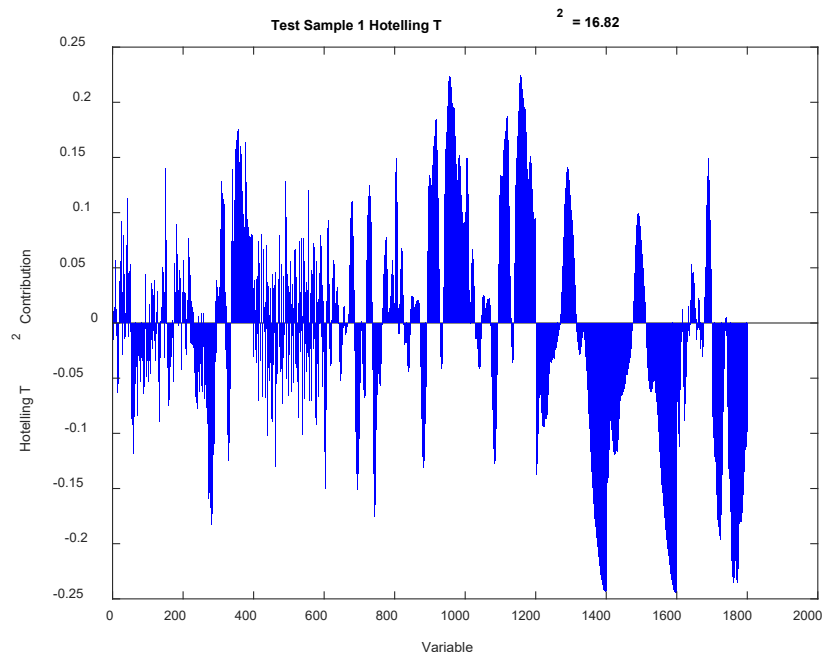


# «Post mortem» monitoring of batch 99

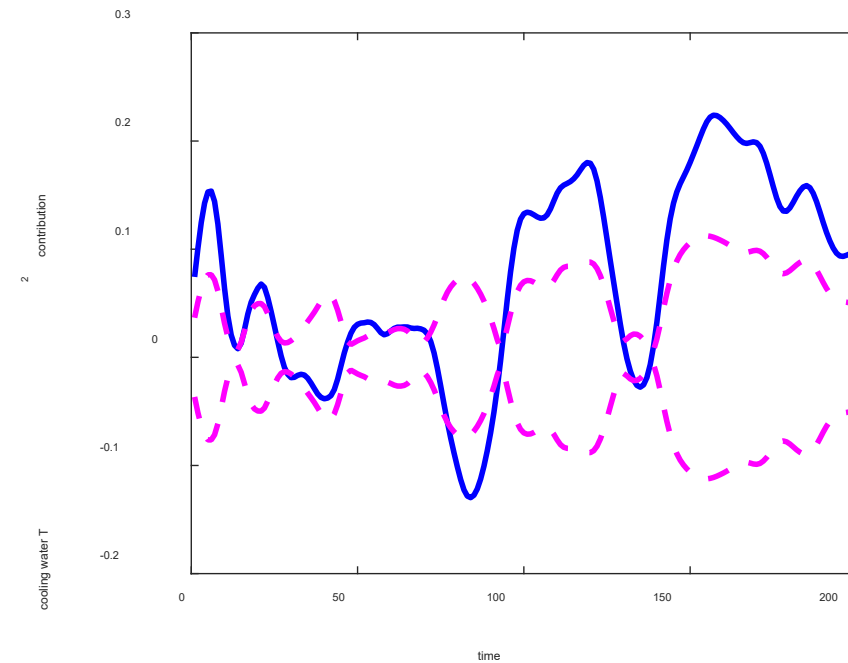
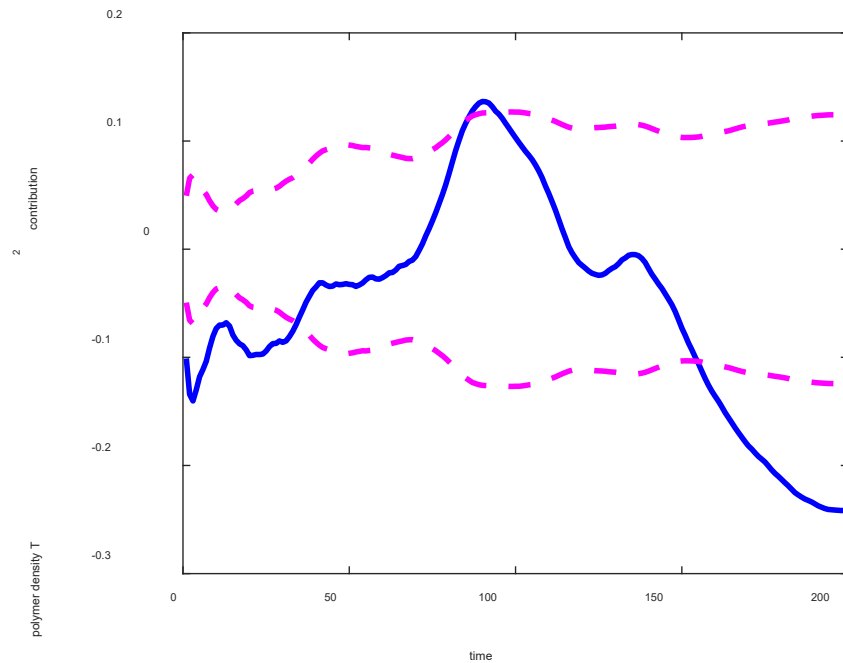
- Batch 99 is anomalous
  - project onto the model **x99\_bwu**
  - $T^2$  e SPE show a **malfunction**



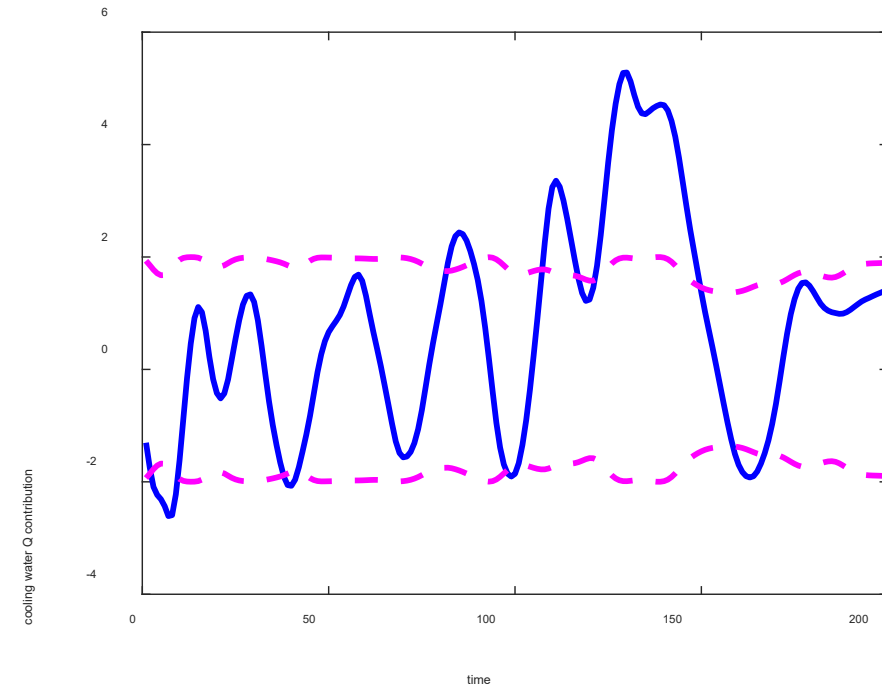
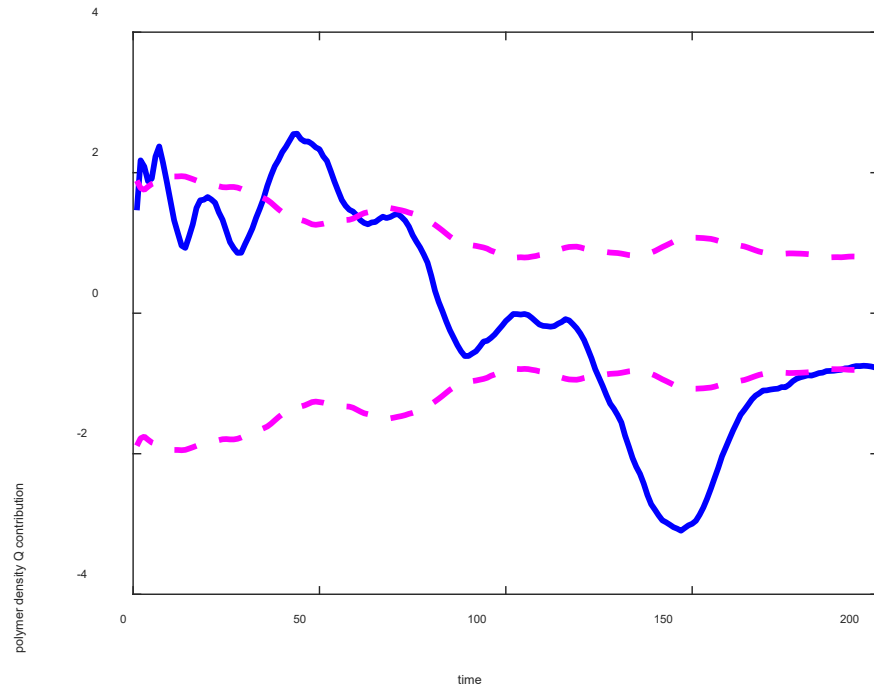
- Contribution plot
  - $T^2$  and Q contributions are examined
- The anomaly is correlated to:
  - low values of conversion and low polymer density
  - high temperature of the coolant in the jacket



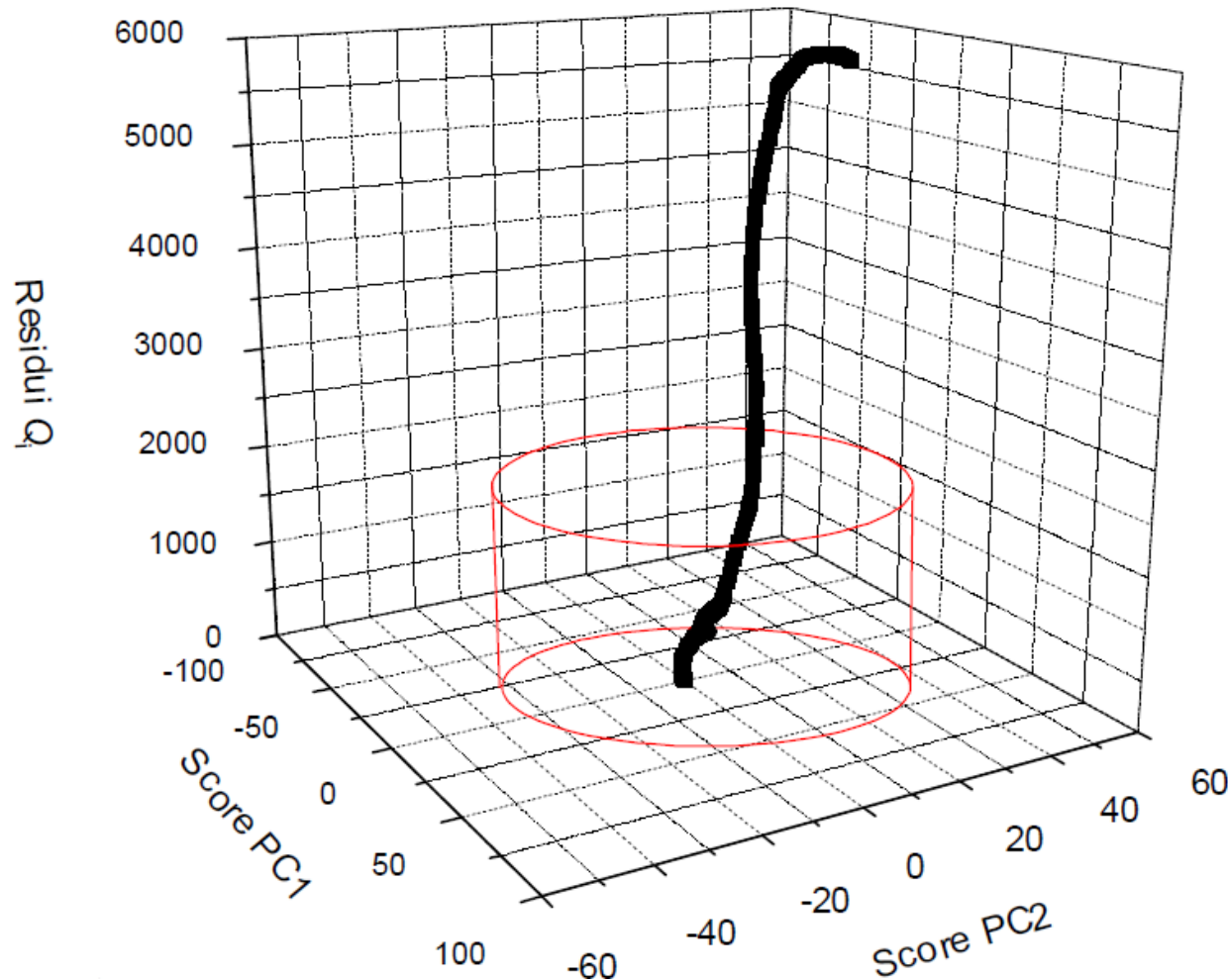
- The time profiles of the variables contribution plot are examined and show anomalies in the time profiles of several variables:
  - low values of conversion and low polymer density
  - high temperature of the coolant in the jacket



- Similar trends can be found also in the time profiles of the Q-residuals contributions



# Is it possible to anticipate fault detection?

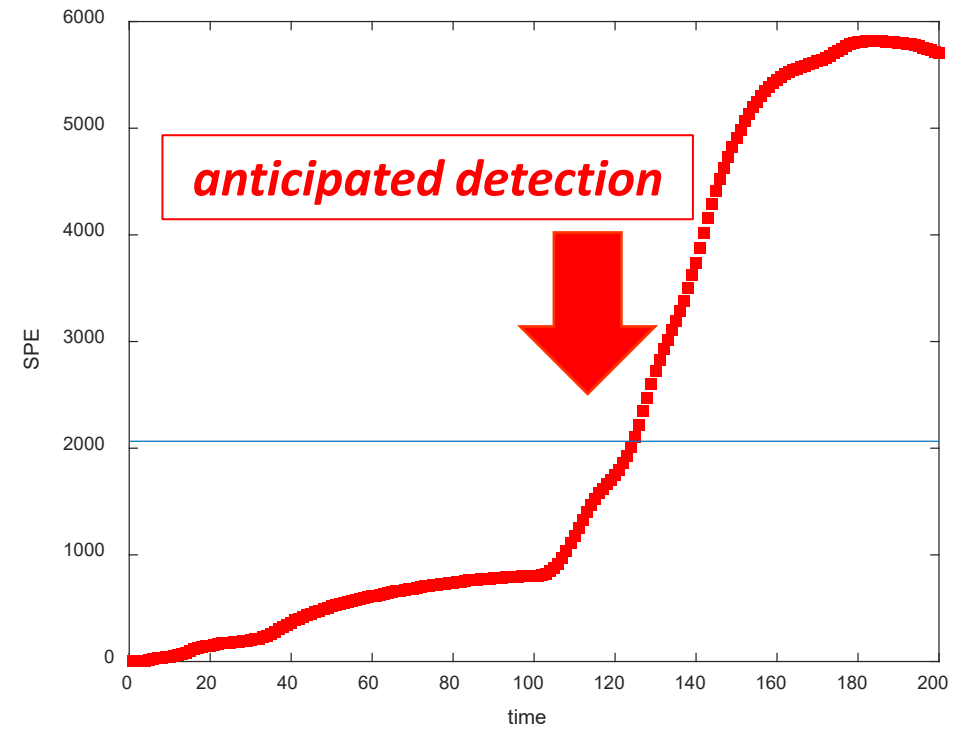
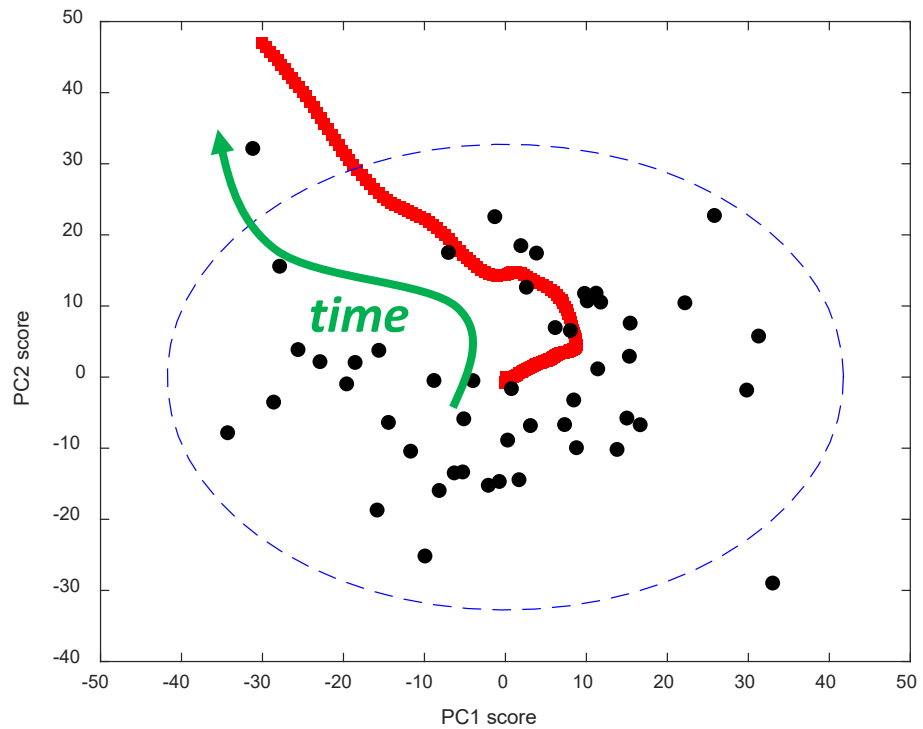


- The fault detection can be anticipated observing the **time trajectory of the model diagnostics during the batch within the control charts**
- Fixed confidence limits for the end of the batch
  - time dependent limits can be used, as well\*

\* Nomikos, P., MacGregor, J.F., 1994. Monitoring batch processes using multiway principal component analysis. AIChE J. 40, 1361–1375

# Online monitoring of batch 99

- **Anticipated detection** of the anomaly
  - possibility of making midcourse corrections
  - anticipated waste treatment and plant cleaning



# Take home message

- **Dynamic behavior of the processes can be accounted for in SPC**
  - *batch processes are monitored by means of **multy-way methodologies***
- Multivariate and multiway SPC can be utilized for:
  - batch-to-batch control («post mortem» monitoring)
  - **in real time for online monitoring** to judge the state of the system in all the time points
    - is the process in standard operating conditions?



```
close all
clear all
clc

% Dataset loading
% load styrenebutadienebatch_monitoring.mat

% Visual inspection
figure;plot(X(1:200,:), 'DisplayName', 'X(1:200,:)')
figure;plot(X(:,7))
figure;plot(X(:,8))
for v=1:9
    a(:,:)=X_3D(:,v,:);
    figure;
    plot(a');
    xlabel('time');ylabel(['variable ' num2str(v)]);
    box on
end
figure; plot(X(1:200,4:6));
```



% Unfolding

```
X_bwu=unfoldmw(X_3D,1);
```

```
X53bwu=[];
```

```
for n=1:200
```

```
    X53bwu=[X53bwu batch53(n,:)];
```

```
end
```

```
X99bwu=[];
```

```
for n=1:200
```

```
    X99bwu=[X99bwu batch99(n,:)];
```

```
end
```

```
X106bwu=[];
```

```
for n=1:200
```

```
    X106bwu=[X106bwu batch106(n,:)];
```

```
end
```



```
% PCA modelling
opca.display='off';
opca.plots='none';
opca.preprocessing='autoscale';
pcam=pca(X_bwu,2,opca);

T=pcam.loads{1,1};
P=pcam.loads{2,1};
Xhat=T*P';
E=auto(X_bwu)-Xhat;
histogram(E(:,3))
figure;normplot(E(:,3))
figure;hist(reshape(E,numel(E),1),40);

% Loadings time trajectories
for v=1:9
    figure;
    plot(P(v:9:end,1));
    xlabel('time');
    ylabel(['variable ' num2str(v) ' PC1 loading']);
    ylim([-0.08 0.08]);
end
```



```
%Cumulative loadings
for v=1:9
    b(v,1)=sum(P(v:9:end,1));
end
figure;bar(b);
xlabel('variable');
ylabel('PC1 cumulative loading');

% Validation batch projection
[s53,q53,T253]=pcapro(X53bwu,pcam,0);
tc=tconcalc(X_bwu,pcam);
qc=qconcalc(X_bwu,pcam);
tc99=tconcalc(X99bwu,pcam);
for v=1:9
    figure
    bar(tc99(:,v:9:end));
    hold on;
    plot(mean(tc(:,v:9:end))-1.96*std(tc(:,v:9:end)),'--m');
    plot(mean(tc(:,v:9:end))+1.96*std(tc(:,v:9:end)),'--m');
    box on;
    xlabel('time');
    ylabel(['variable ' num2str(v) ' - T^2 contribution']);
    hold off
end
```



**% Online monitoring**

```
for n=9:9:1800
    Xp=[X99bwu(1,1:n) mean(X_bwu(:,n+1:end))];
    [t(n,:),q(n,:),t2(n,:)]=pcapro(Xp,pcam,0);
end
T=pcam.loads{1,1};
```

**% Figure**

```
figure;scatter(t(9:9:1800,1),t(9:9:1800,2),'sr','filled');hold on;
scatter(T(:,1),T(:,2),'ok','filled');hold off;box on
xlabel('PC1 score');ylabel('PC2 score');ellps([0,0],[41.76 32.75],'--b');
SPElim=pcam.detail.reslim{1,1}(1,1);
figure;scatter(1:200,q(9:9:1800,1),'sr','filled');
line([0,200],[SPElim,SPElim]); box on
xlabel('time');ylabel('SPE');
```



... per sempre a fianco a me!

