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Machine Learning Laboratory #3

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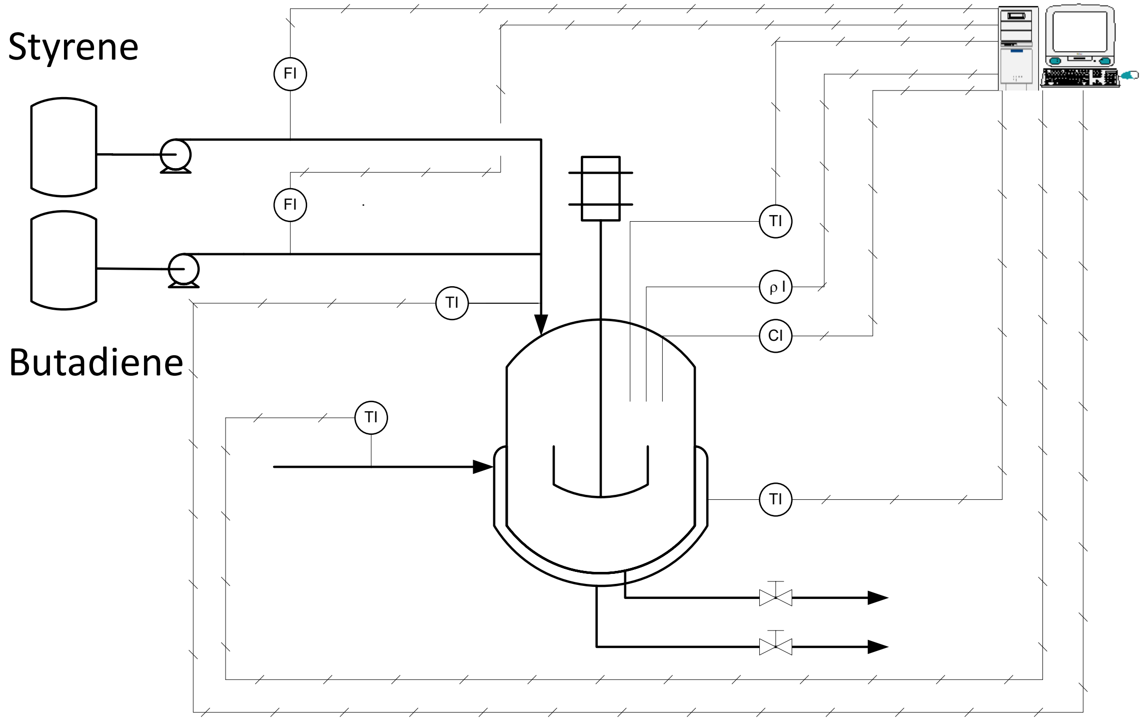
Example #3: rubber process monitoring

Process and objectives

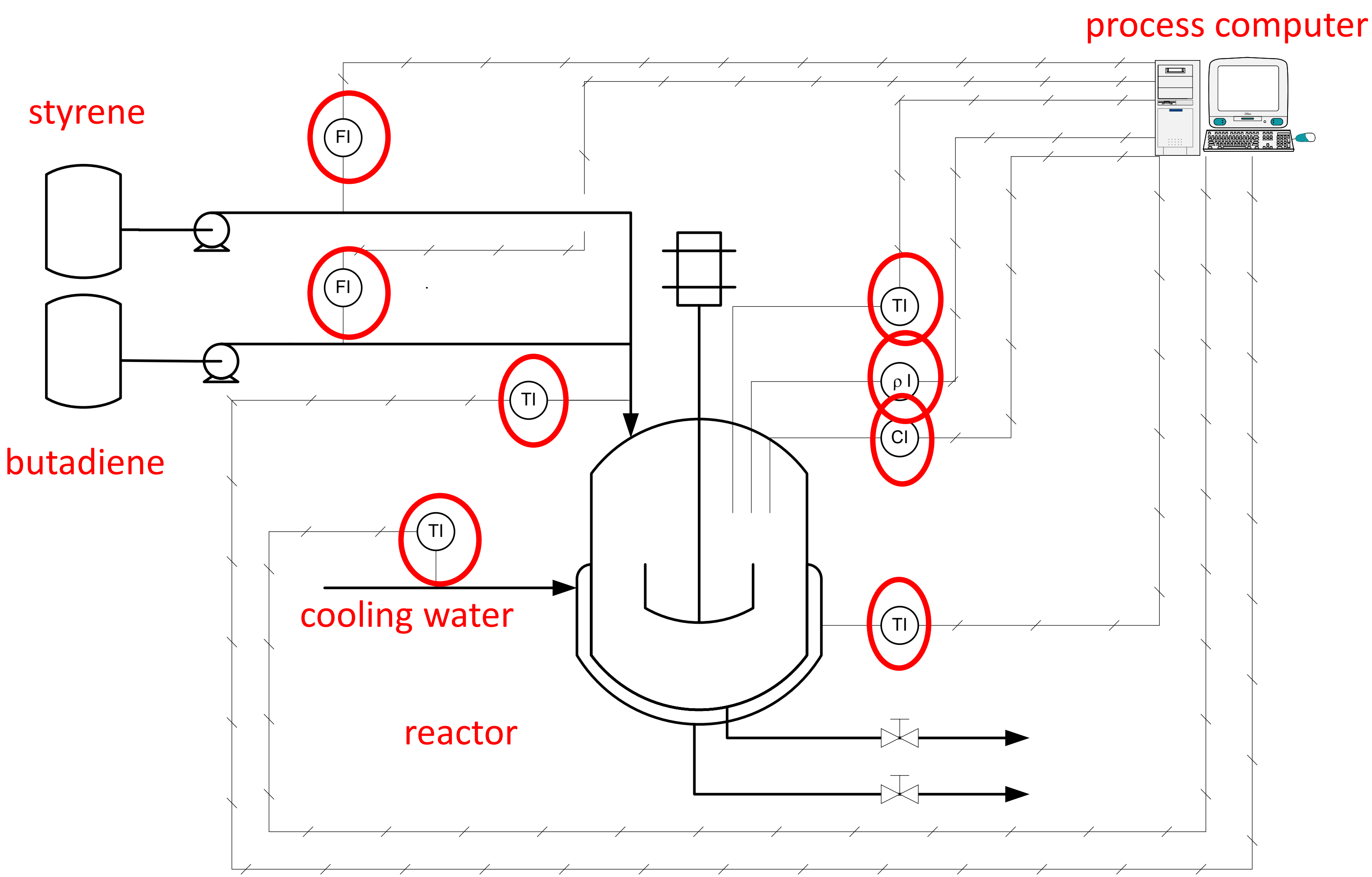
- Semi-batch process*: styrene-butadiene polymerization for the production of rubber
- Objectives:
  - **online monitoring**
  - **fault detection** & **diagnosis**

	variable
1	styrene flowrate Fstyr
2	butadiene flowrate Fbuta
3	feed temperature Tf
4	reactor temperature Tr
5	coolant temperature Tcw
6	reactor jacket temperature Trj
7	polymer density Ro
8	total conversion cTOT
9	instant energy Er



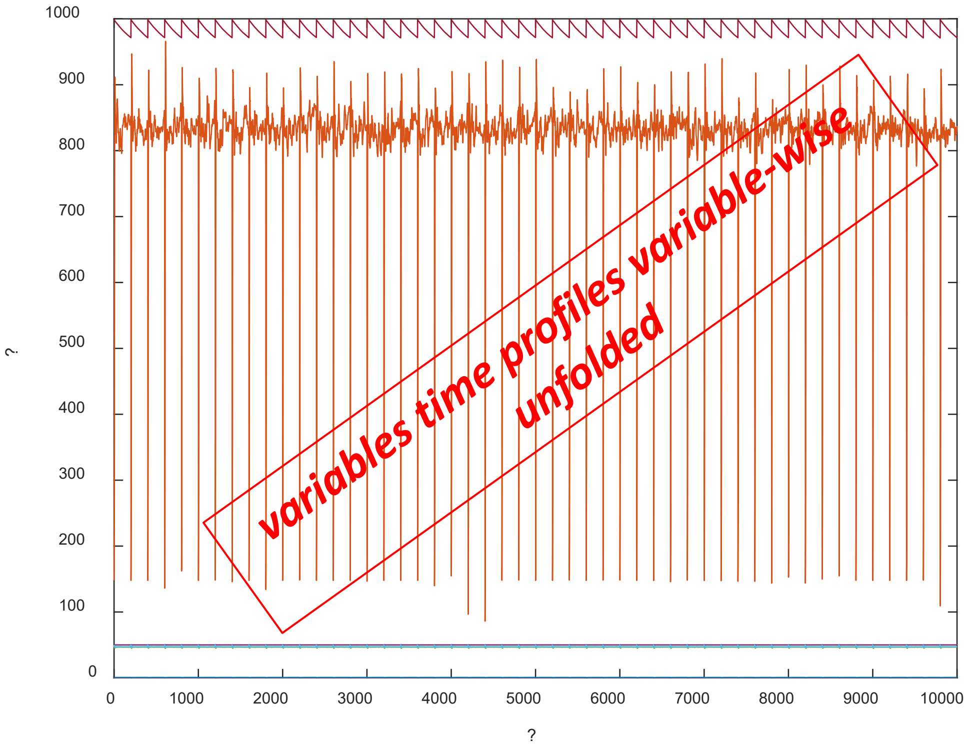
* Nomikos, P., MacGregor, J.F., 1994. Monitoring batch processes using multiway principal component analysis. AIChE J. 40, 1361–1375

P&ID


process computer
styrene
FI
FI
butadiene
TI
TI
cooling water
reactor
TI
ρ I
CI
TI

Available data visualization

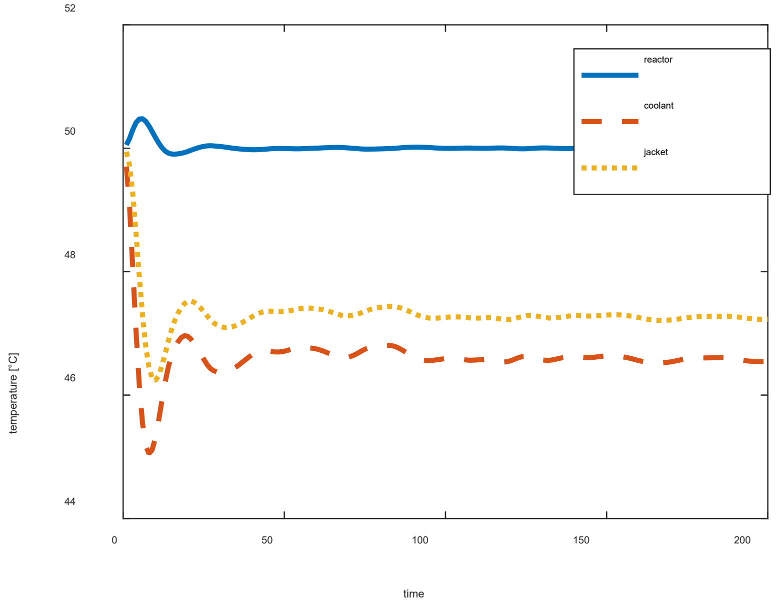
- Load: `styrenebutadienebatch.mat`
  - find it in Moodle under: rubber production monitoring
- Data:
  - 50 standard batches
  - 9 variables recorded in 200 time samples
- Data visualization: `plot(X);xlabel('?');ylabel('?')`
  - what data structure?



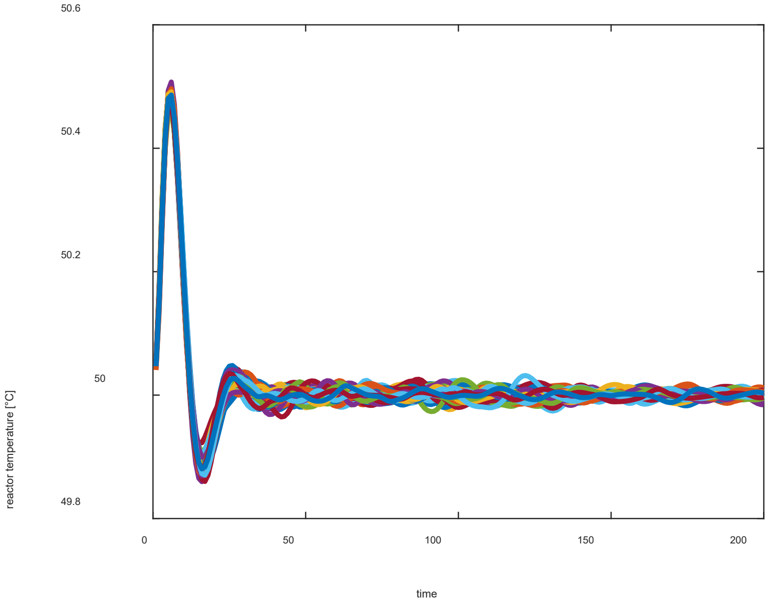
Variables time profiles

- 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')
```

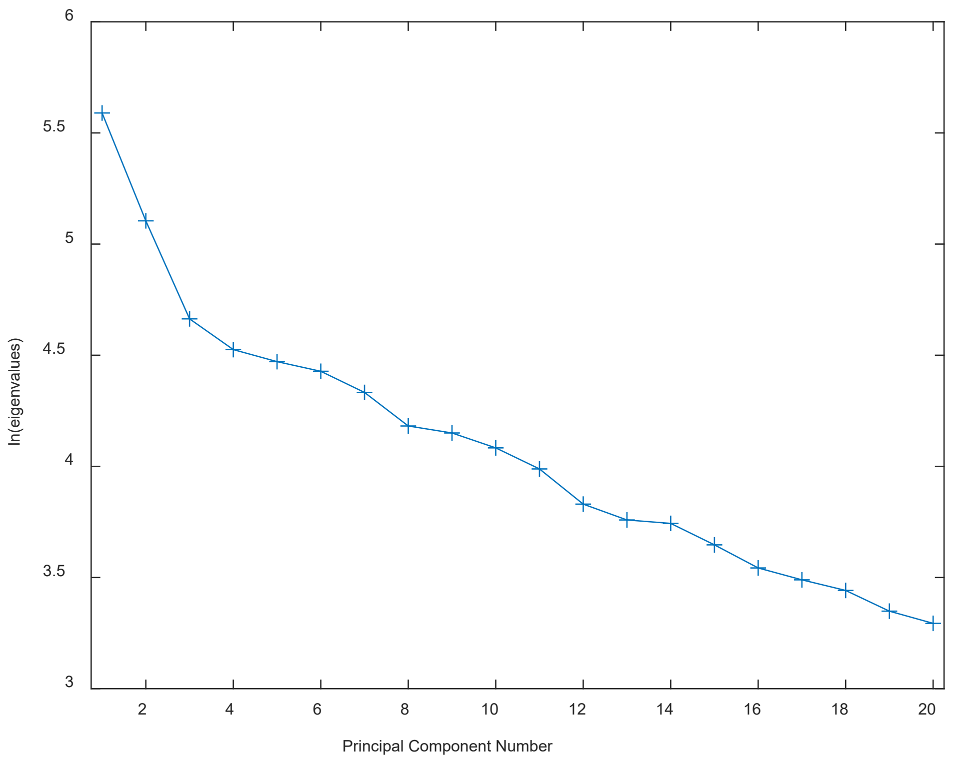



```
Tr(:,:)=X_3D(:,4,:);
figure; plot(Tr');
xlabel('time');
ylabel('reactor temperature [°C]');
```



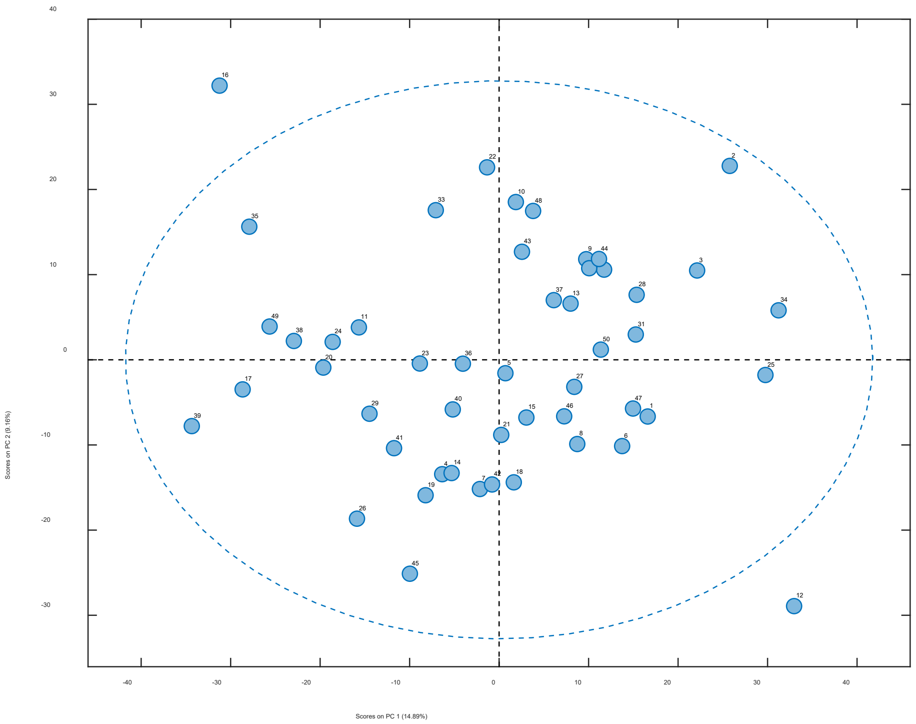
PCA modelling

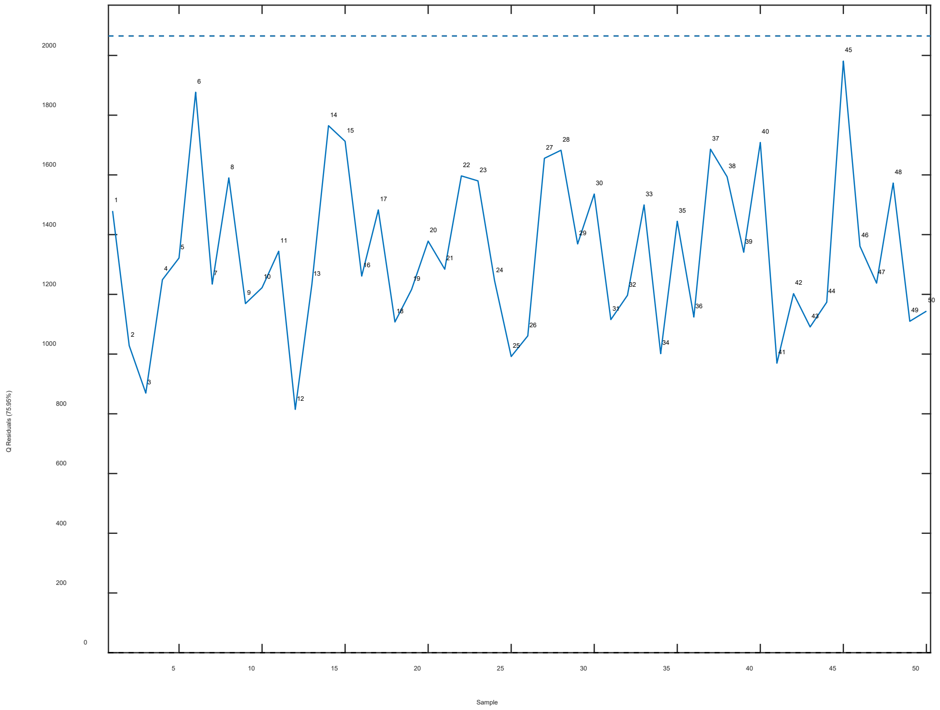
- **Batch-wise unfolding** considers process **dynamics**
  - consider commands: `unfoldm` and `unfoldmw`
- Build the PCA model on: `Xbwu`
- Pretreatment:
  - autoscaling: to survey the variables time profiles compared to the **average time profile and the respective variability**
- Number of selected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



Score plot and relation among batches

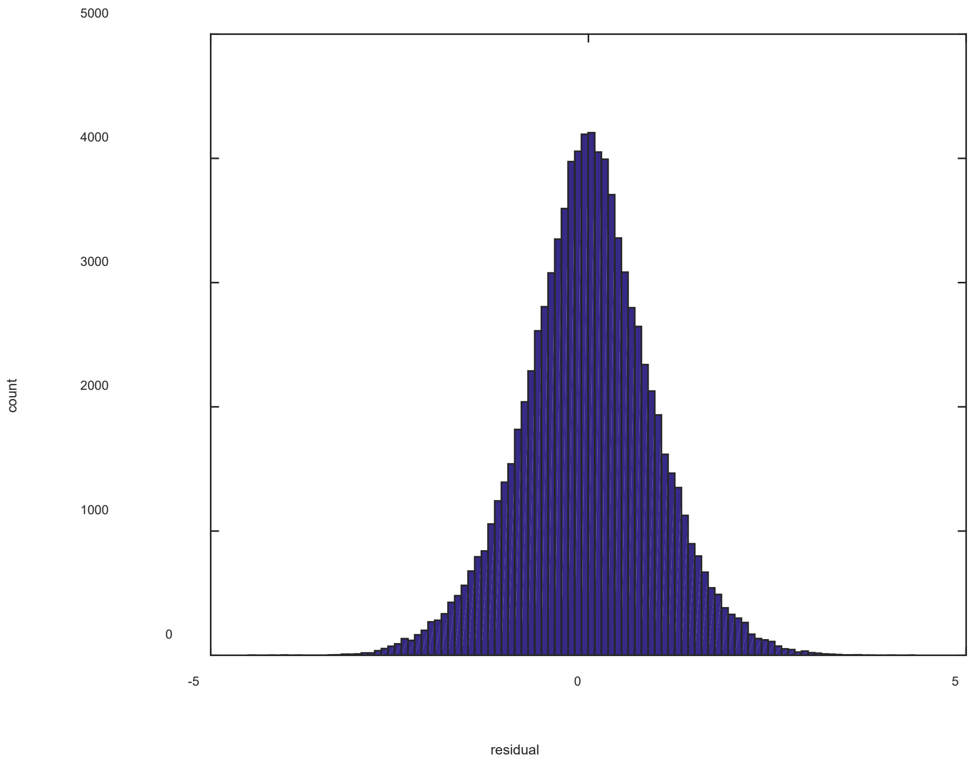
- The batches seems to be multi-normally distributed
- ~5% of the batches are out of the 95% confidence ellipse
- No anomalies are present in the Q residuals





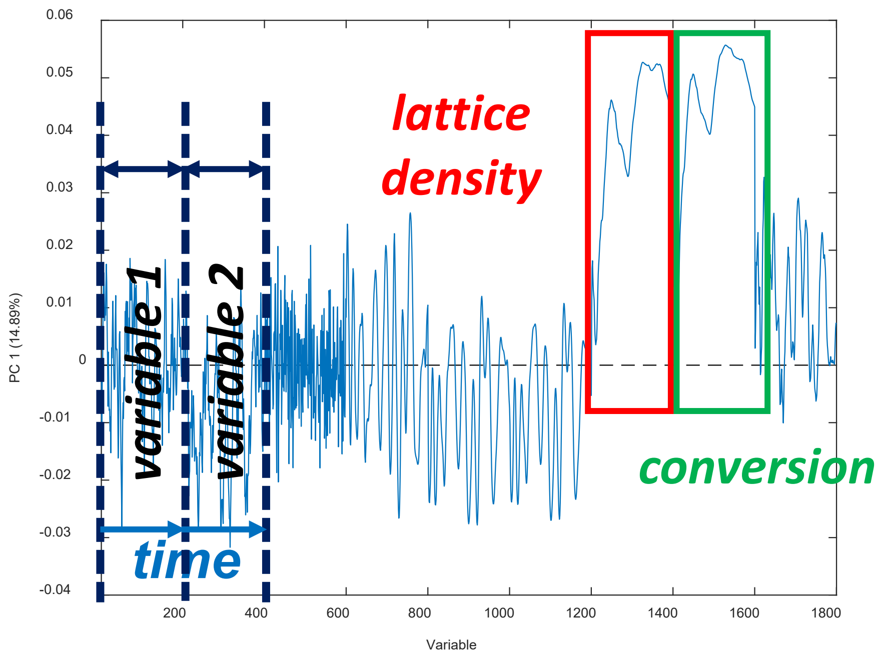
Note that…

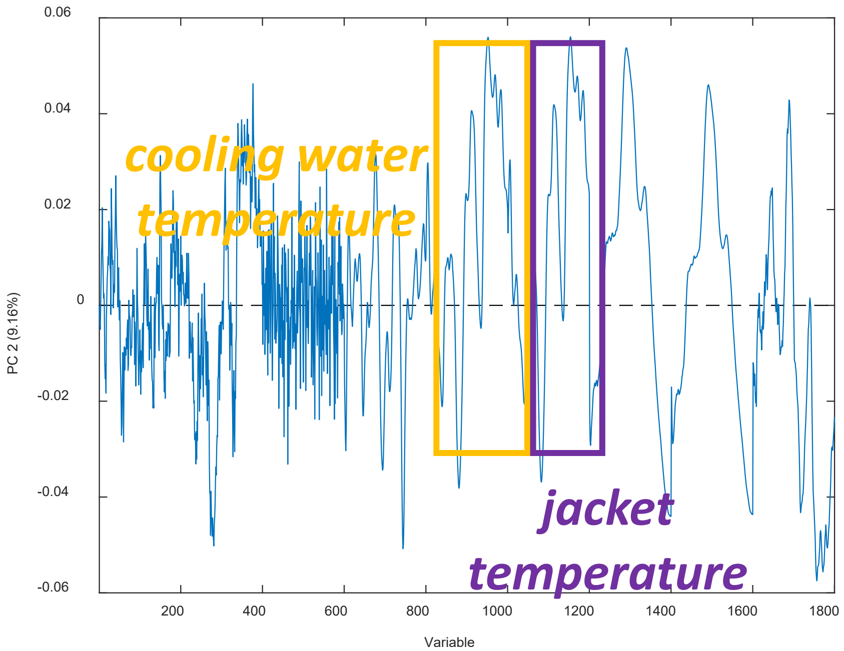
- The residuals are normally distributed and centered in zero
  - all the residuals are picked together here



Process understanding (1/3)

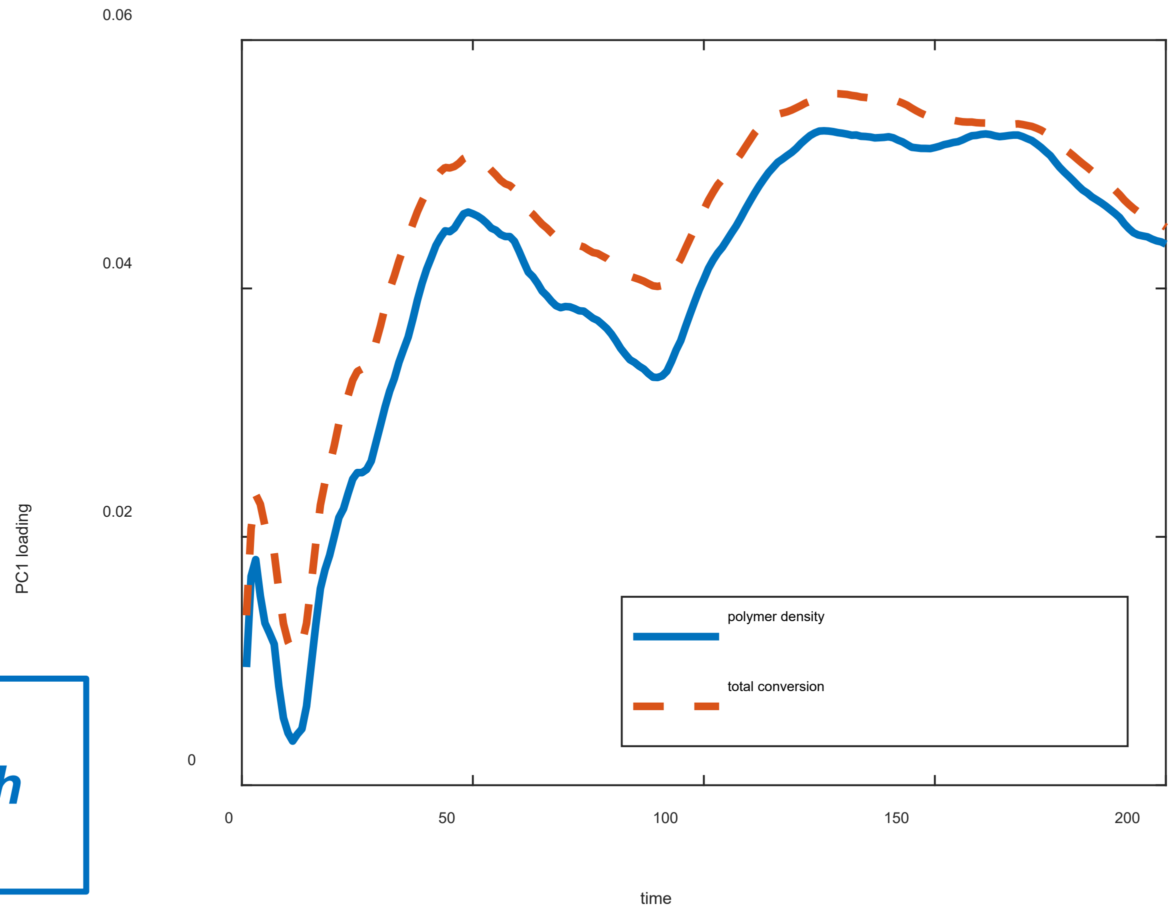
- The loading plot shows that:
  - variables correlation **in time**
  - **time trajectories** of the major sources of variability
    - lattice density and conversion (on PC1)
    - coolant and jacket temperatures (on PC2)





Process understanding (2/3)

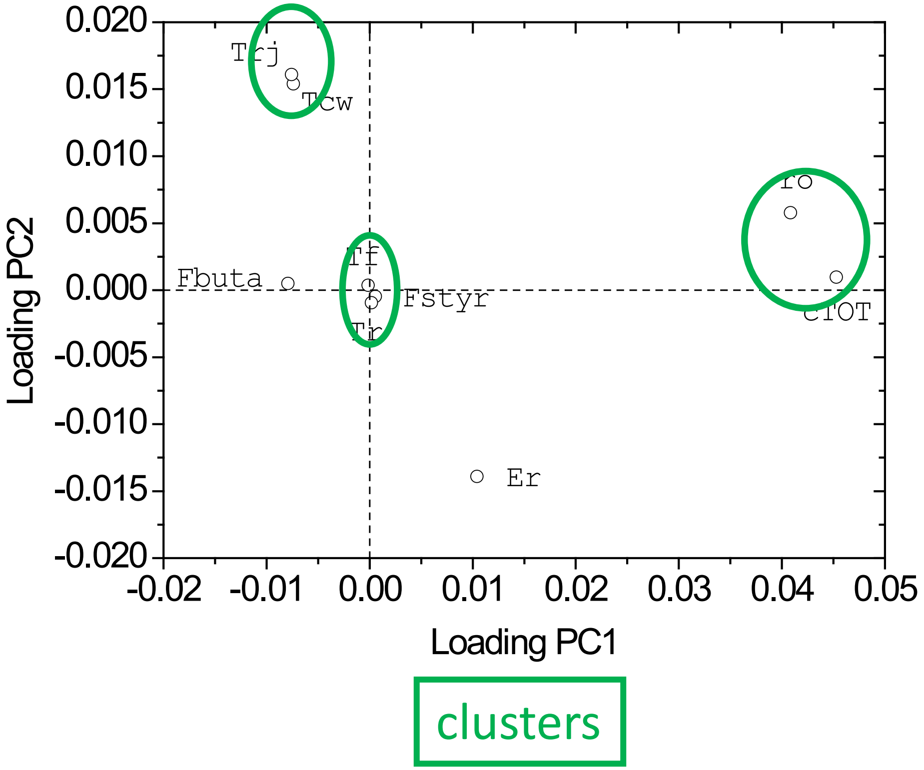
- The detail on the time profiles of the PC1 loadings of the most important variables:
  - polymer density
  - total conversion

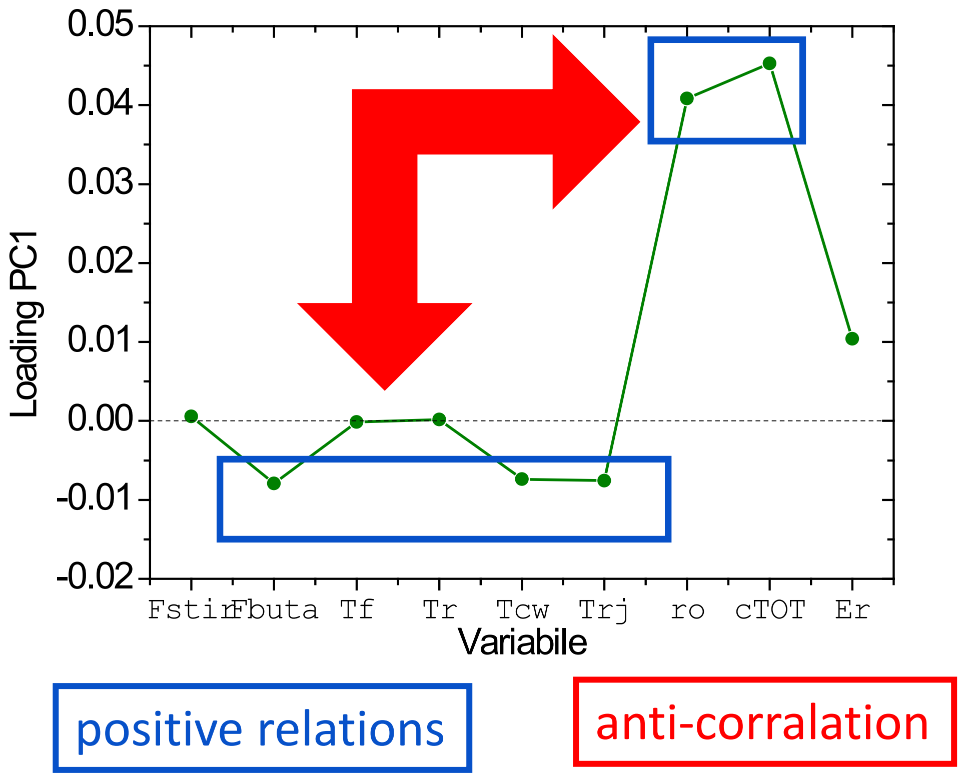


Increasing importance in time
- ***not so important in the first part of the batch***
- ***important in the second half of the batch***

Process understanding (3/3)

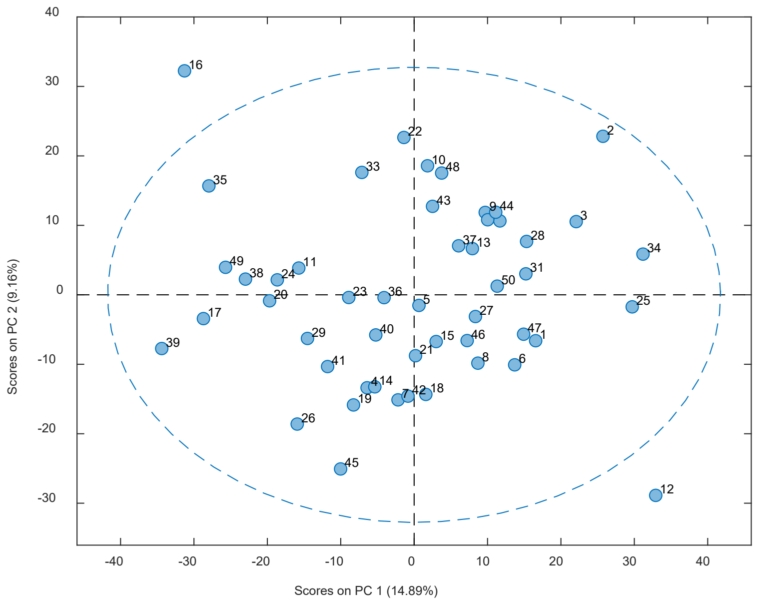
- **Cumulative loadings** show that:
  - the values are cumulated on the entire time trajectory
  - the same variability sources as in the previous slide

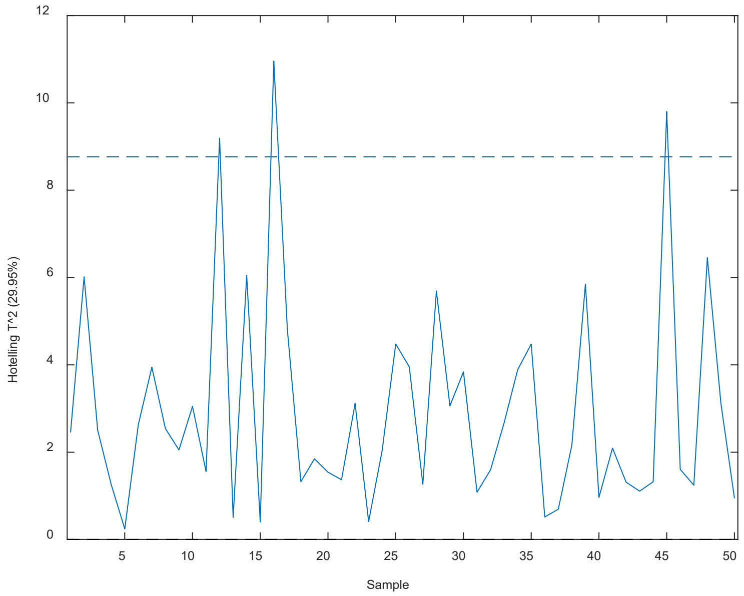


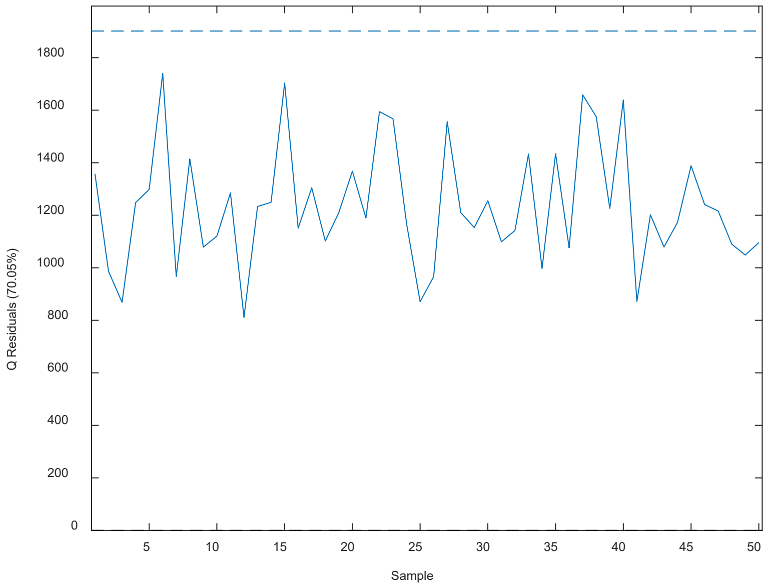


Control charts

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

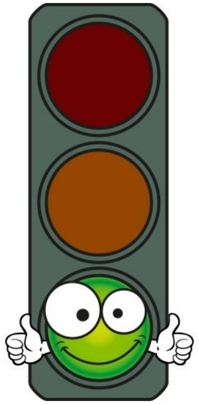


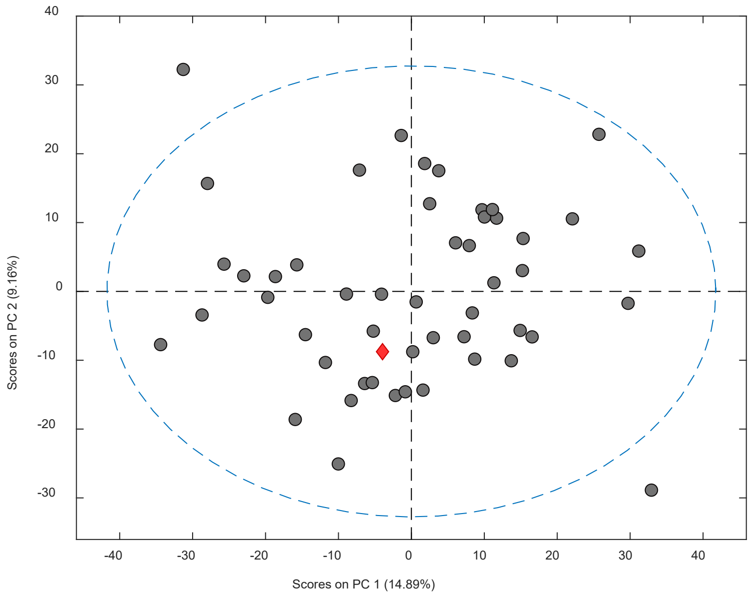


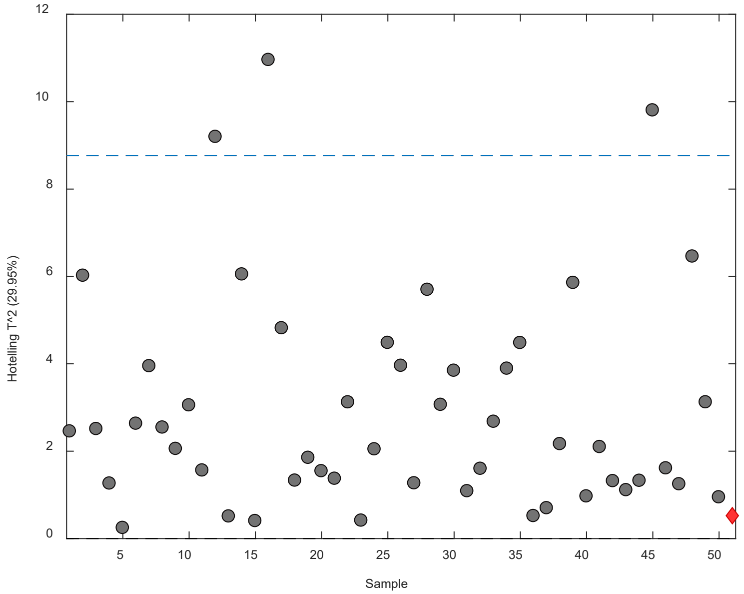


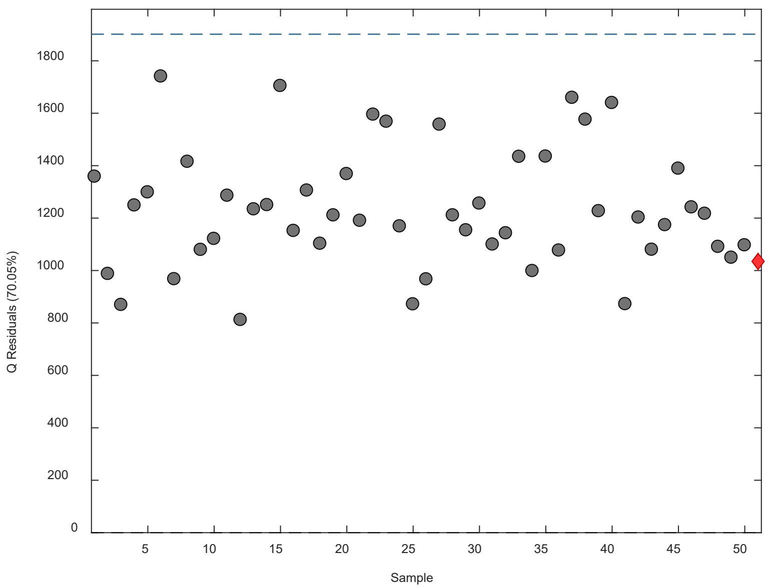
«Post mortem» monitoring of batch 53

- Batch 53 is **normal**
  - project onto the model `X53_bwu`



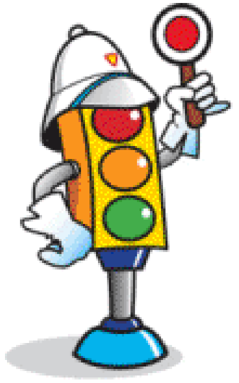


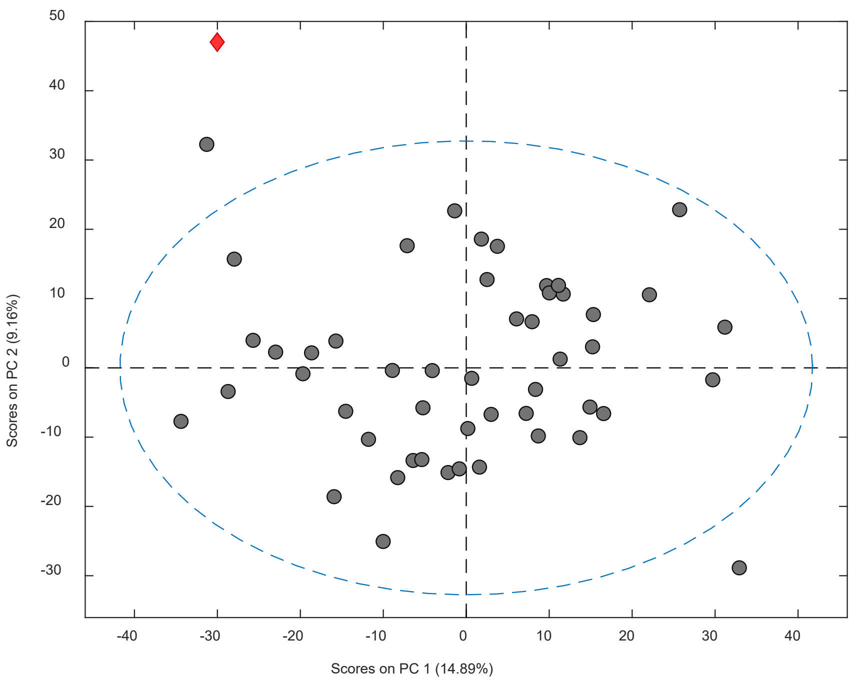


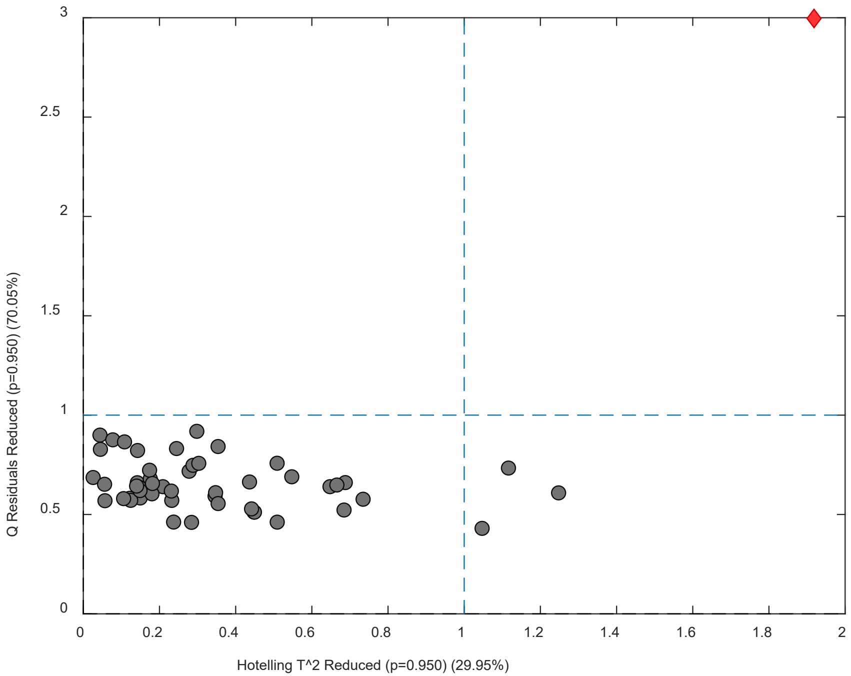


«Post mortem» monitoring of batch 99

- Batch 99 is anomalous
  - project onto the model **X99_bwu**
  - T^2 e SPE show a **malfunction**

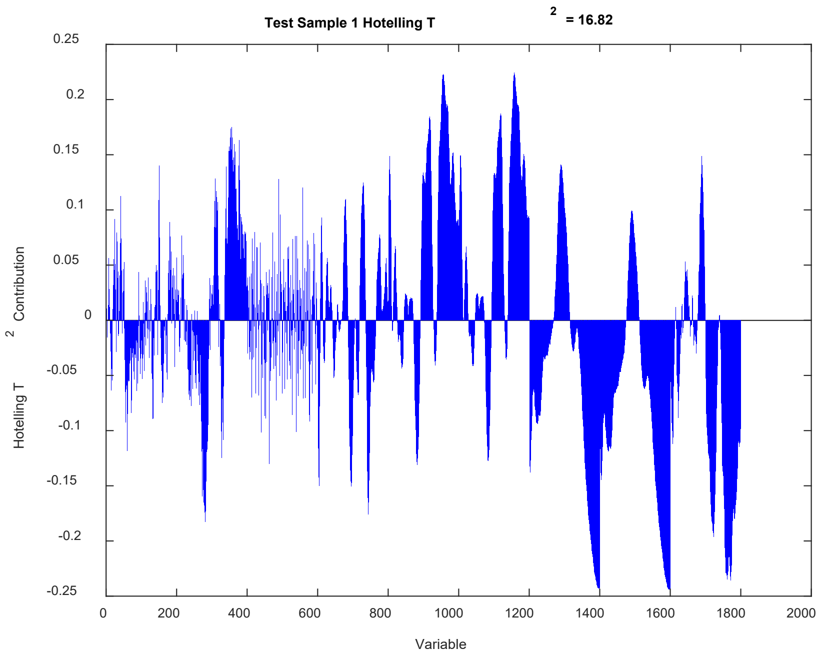


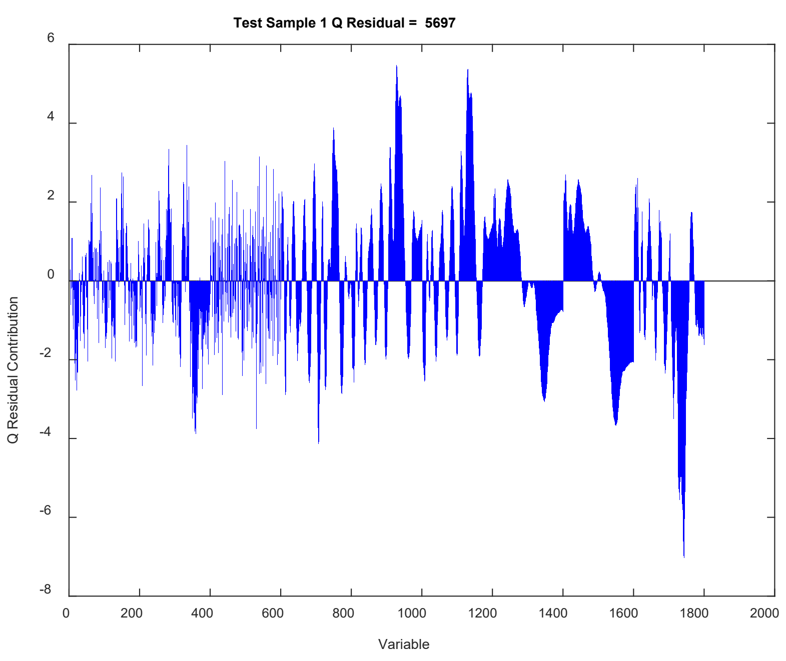




Diagnosis (1/3)

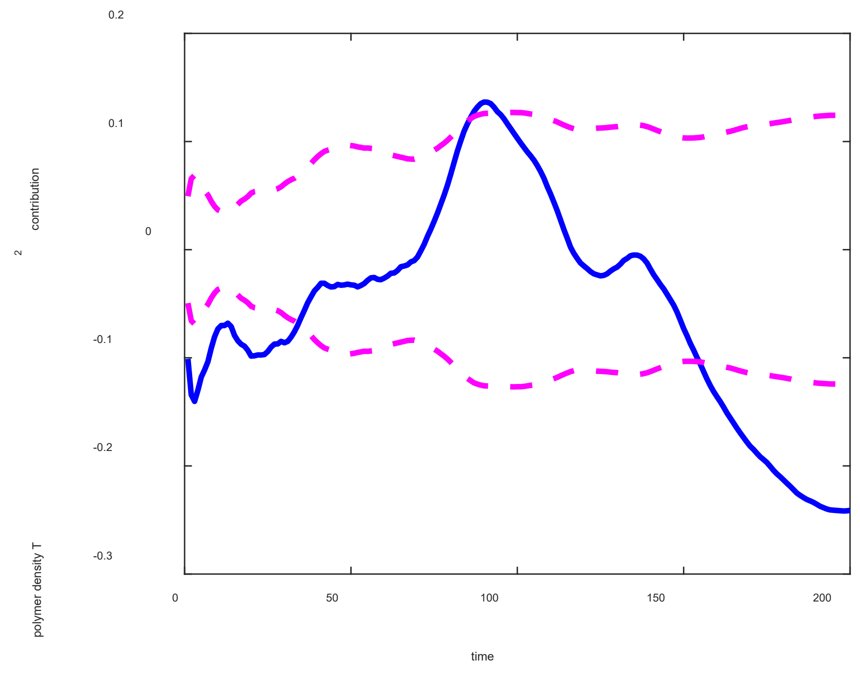
- Contribution plot
  - T^2 and Q contributions are examined
- The anomaly is correlated to:
  - low values of conversion and low polymer density
  - high temperature of the coolant in the jacket

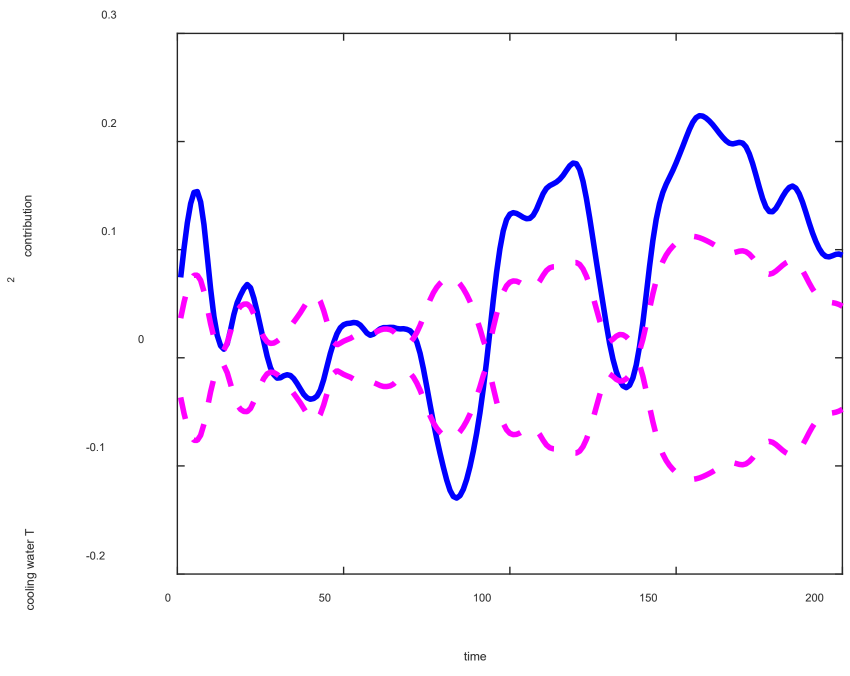




Diagnosis (2/3)

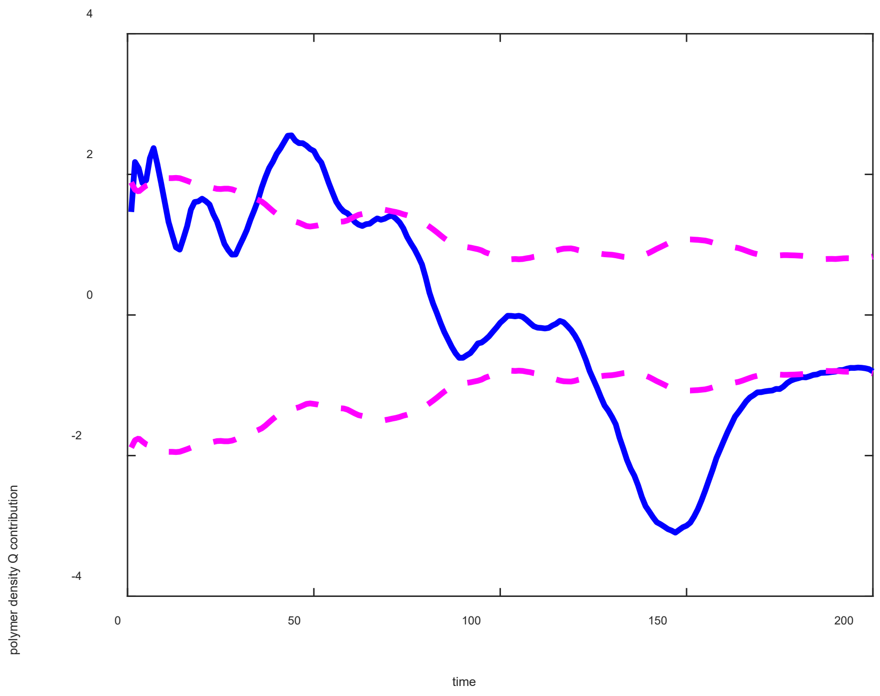
- The time profiles of the variables contribution plot are examined and show anomalies in the time profiles of several variables:
  - low values of conversion and low polymer density
  - high temperature of the coolant in the jacket

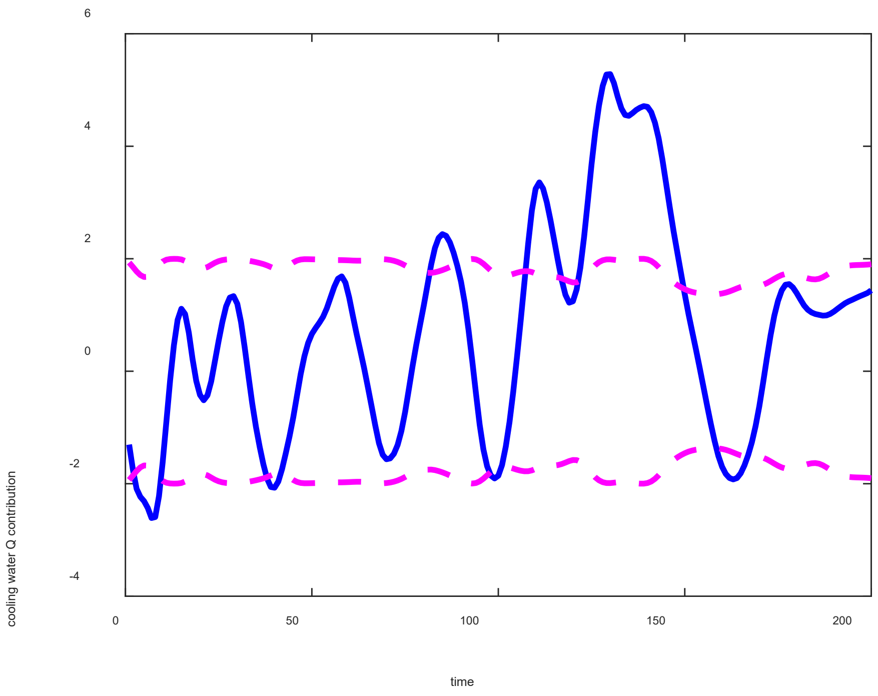




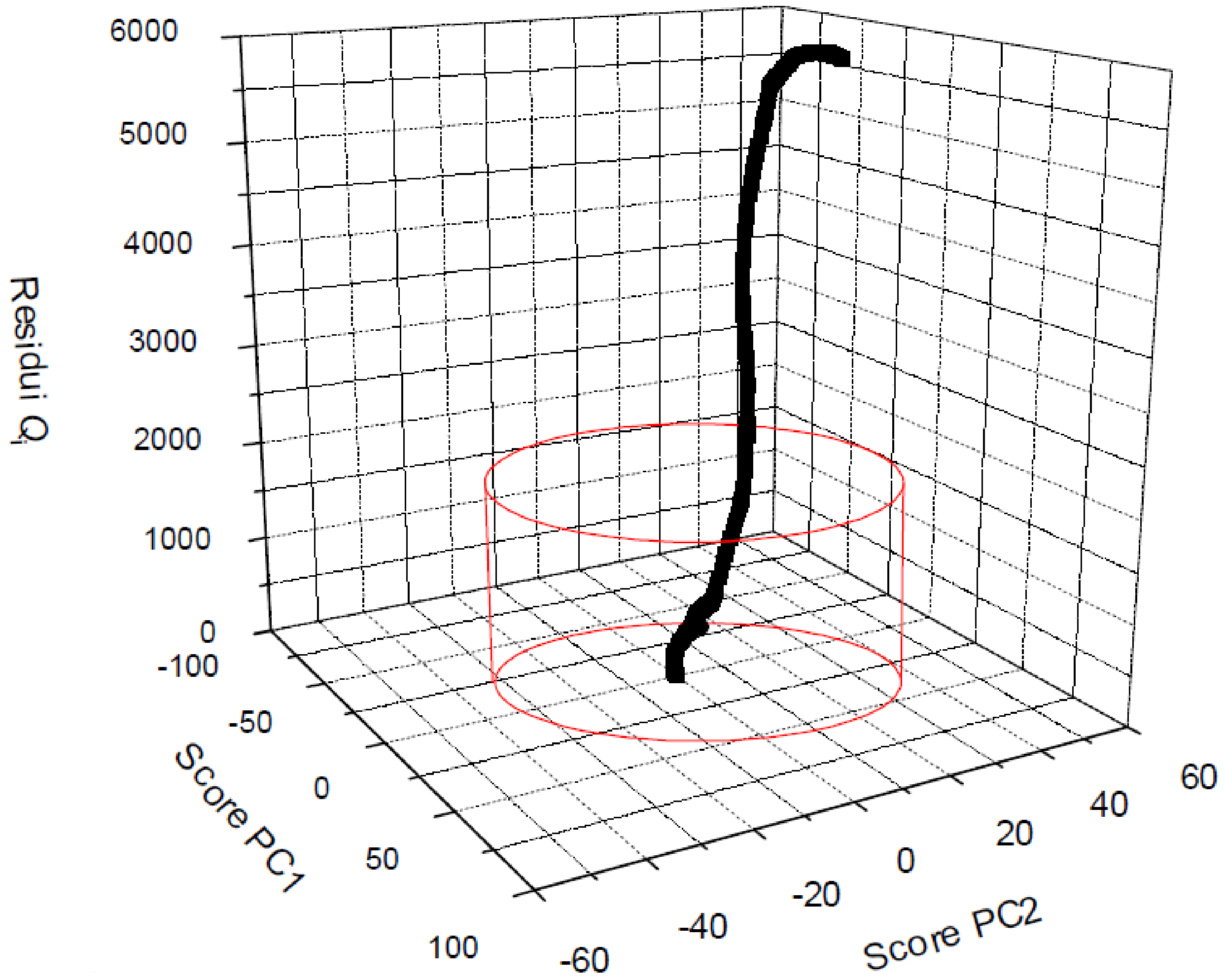
Diagnosis (3/3)

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





Is it possible to anticipate fault detection?

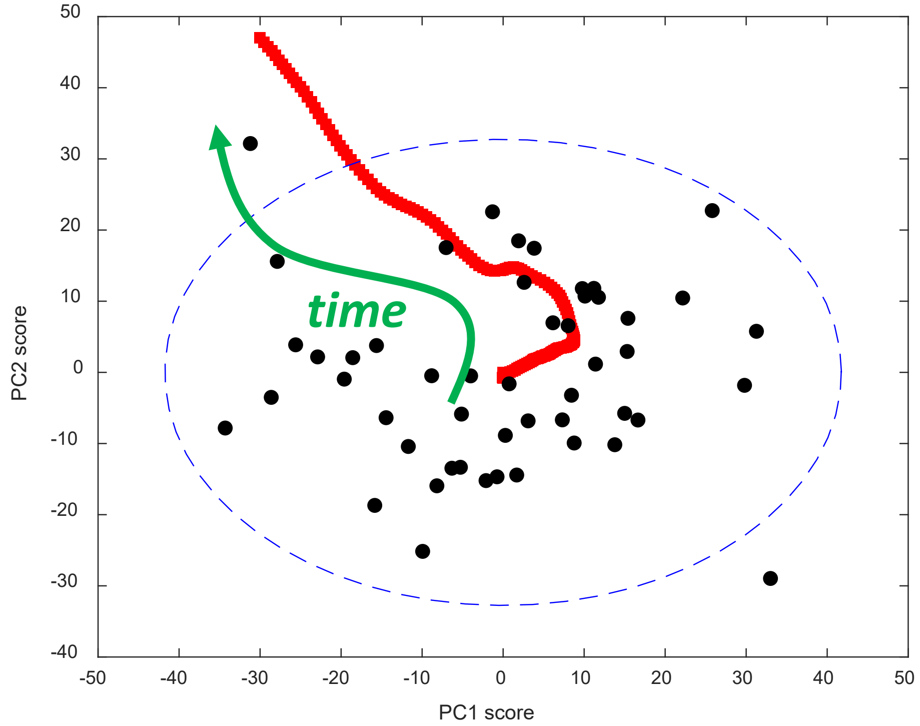


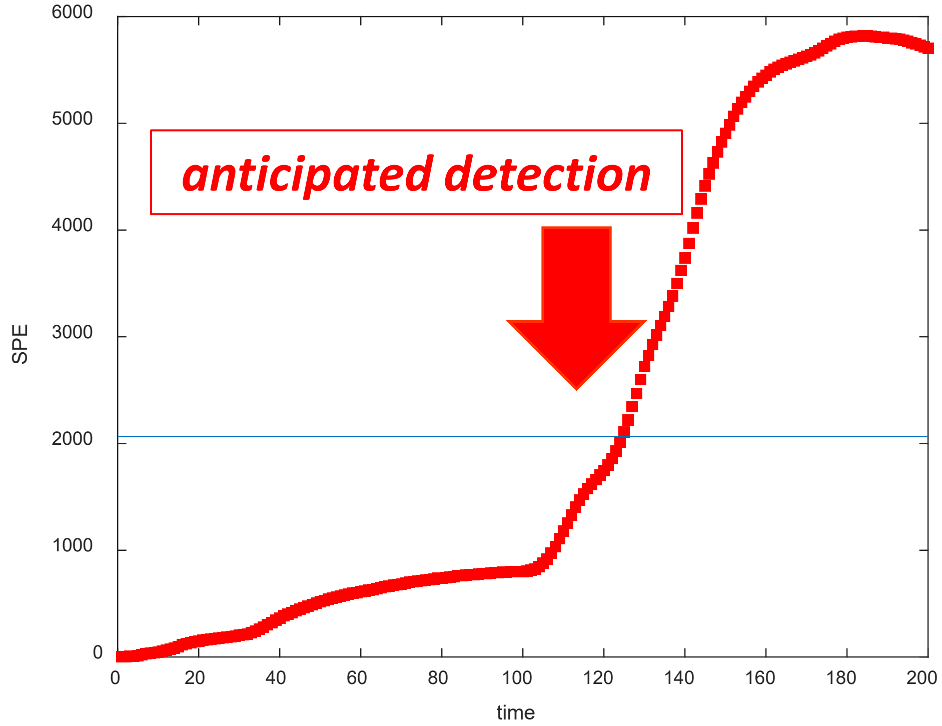
- The fault detection can be anticipated observing the **time trajectory of the model diagnostics during the batch within the control charts**
- Fixed confidence limits for the end of the batch
  - time dependent limits can be used, as well*

* 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?

Batch monitoring code (1/5)

```
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));
```

Batch monitoring code (2/5)

```
% 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
```

Batch monitoring code (3/5)

```
% 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
```

Batch monitoring code (4/5)

```
%Cumulatrive 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
```

Batch monitoring code (5/5)

```
% 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!