Large-Scale Process Monitoring using JMP®

Process Monitoring and Diagnosis by Multivariate Statistical Process Control (MSPC)

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Process Data Analysis - Purposes

- Monitoring the state of the process
  - Early detection
  - Diagnosis and adjustment

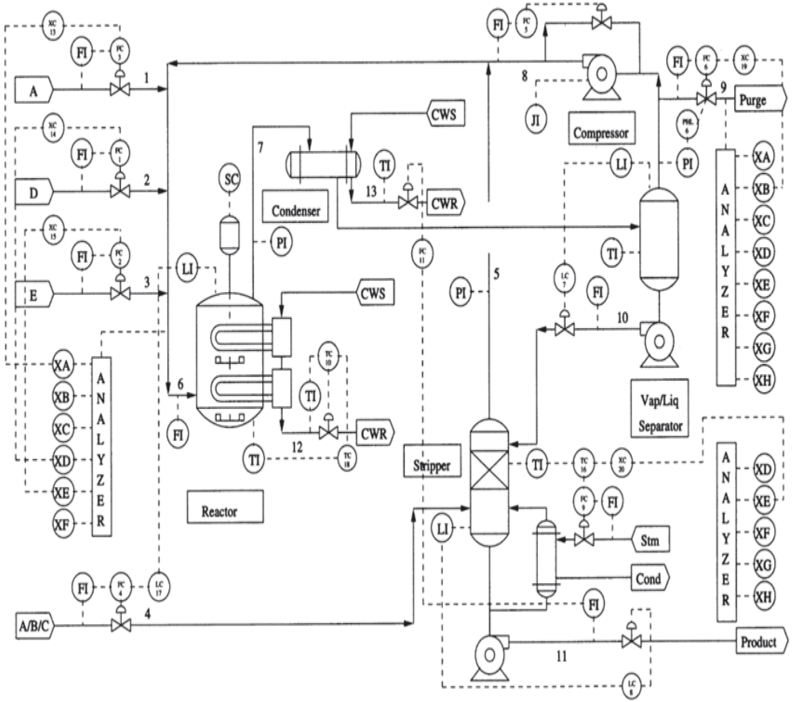
- Understanding the relationship between
  - Input variables, X (process data) and output data, Y (product quality, cost, amount, …)

- Optimization
  - Use process models to improve process

Challenge

- A few decades ago
  - Few variables

- Today
  - Many measurements
  - Large data sets
- Process the same
- Data have changed
  - p = 5 -> 500
  - n = 10 -> 1000



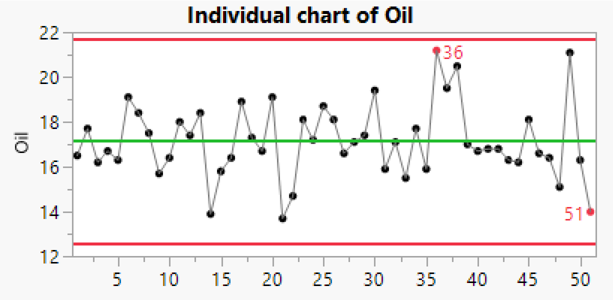
Process diagram

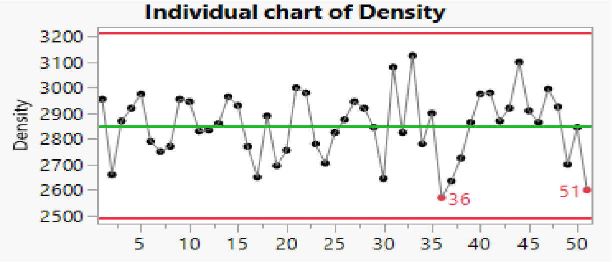
Traditional Statistical Process Control (SPC)

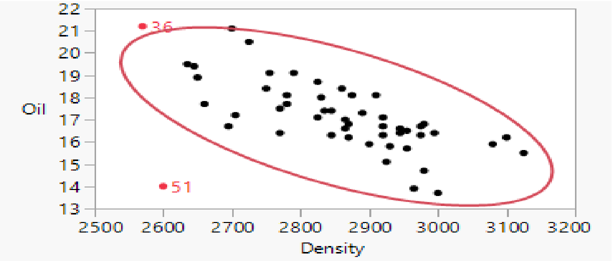
- SPC charts
  - Shewhart, CUSUM and EWMA

- Disadvantage
  - Charts a small number of variables
  - Examines them one at a time

- Most outliers remain undetected
  - No covariance information







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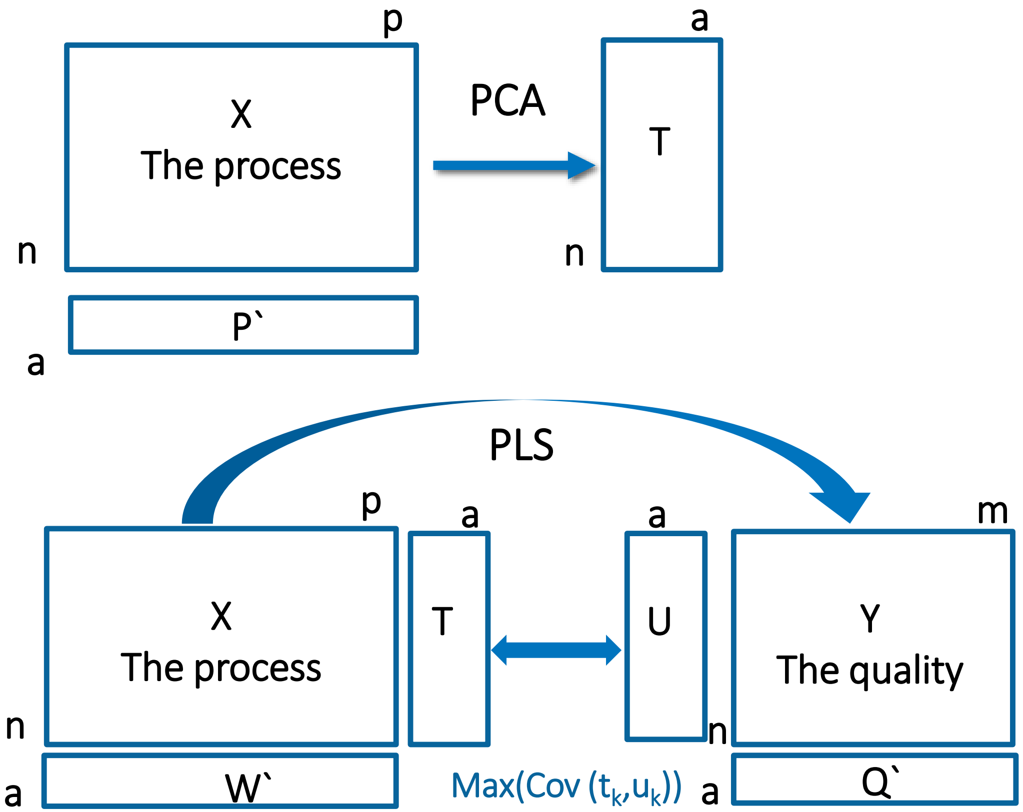
- Process Modelling and Diagnosis
  - Purpose
  - Data
- **Multivariate Statistical Process Control (MSPC)**
  - PCA / PLS
- **Process Application**
  - Low Density Polyethylene Process (LDPE)
  - Tennessee Eastman Process
- **Demos and Conclusions**

PCA and PLS Projection Methods

- **PCA finds the latent variables**
  $$X = TP^T + E \quad T = XP$$
  - Best explain the variance in X

a << p

- **PLS finds the latent variables**
  $$X = TP^T + E \quad T = XR$$
  $$Y = TQ^T + F$$
  - Best explain the variance in Y
  - Have the greatest relationship with Y



Multivariate Statistical Process Control (MSPC)

Projection methods

Build models

Historical process quality data

PCA and PLS	
Advantages	• Handles a large number of variables • Reduces dimensionality • Handles correlation
Monitoring processes	• Hotelling's T^2 • Squared prediction error (SPE) • Scores
Diagnosing processes	• Contribution plots

Apply models

New process data

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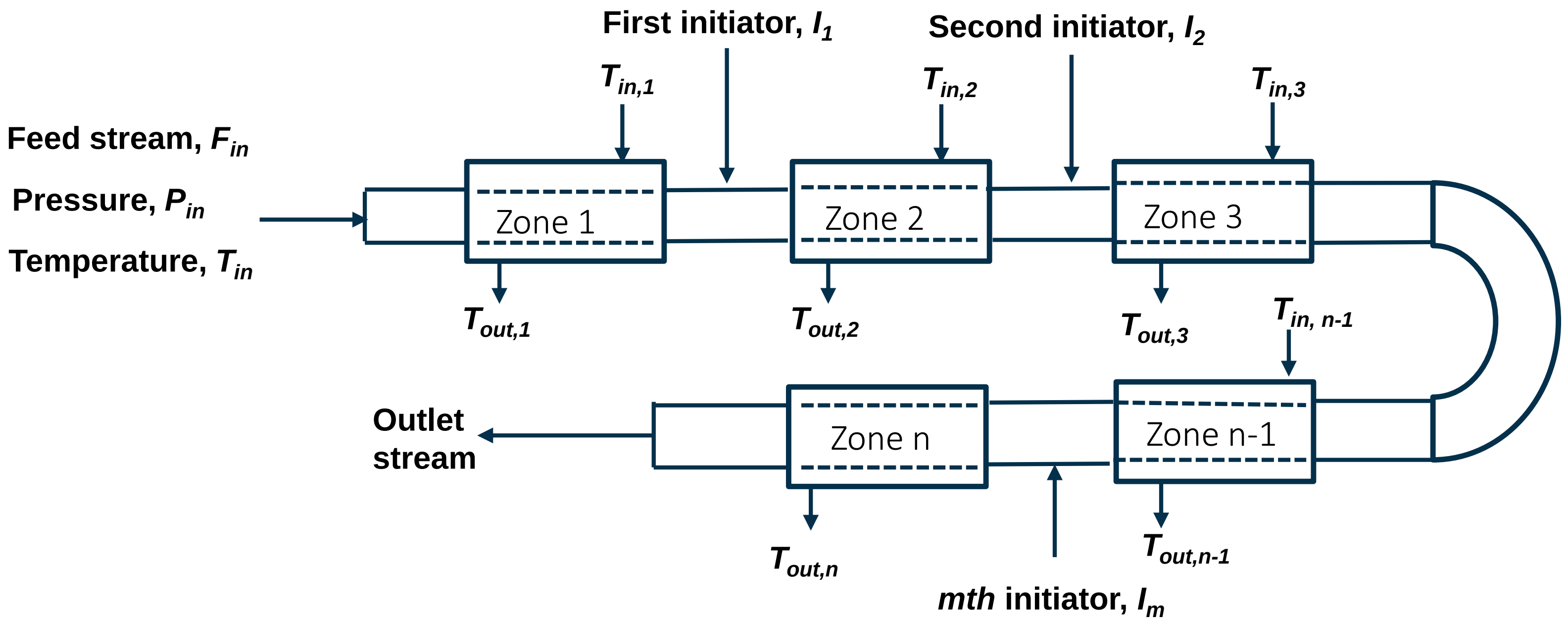
LDPE – Low-density polyethylene

LDPE is a thermoplastic made from petroleum. It was the first grade of polyethylene, produced in 1933 using a high pressure process via free radical polymerization. Its manufacture employs the same methods today.

LDPE is widely used for manufacture various containers, squeezable bottles, wash bottles, tubing, plastic parts for computer components. Its most common use is in plastic bags.

A High-pressure Tubular Reactor



Length of tubular reactor ranges from 500 to 1500m

Data Overview

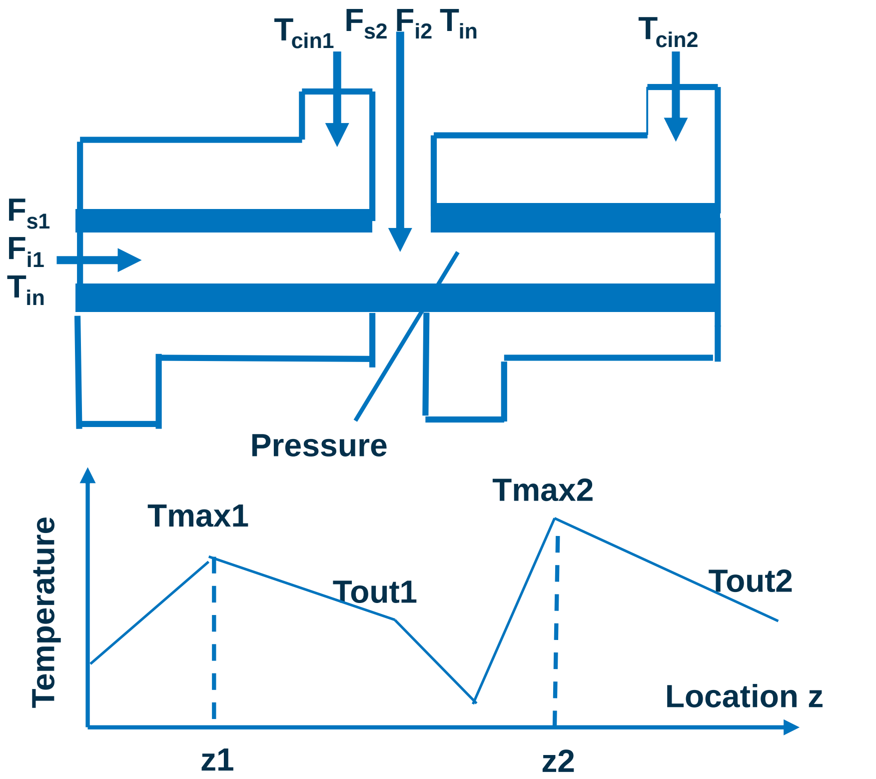
The simulated data based on MacGregor et al (1994)

	Tin	Tmax1	Tout1	Tmax2	Tout2	Tcin1	Tcin2	z1	z2	Fi1	Fi2	Fs1	Fs2	Press	Conv	Mn	Mw	LCB	SCB
42	207.5	295.24	227.01	284.93	242.97	116.21	117.86	0.03	0.577	0.4531	0.4636	669.35	244.55	3000	0.1326	27373	163729	0.795	26.04
43	207.13	297.62	228.51	283.09	243.39	116.11	118.25	0.028	0.581	0.4826	0.4357	655.02	245.5	3004	0.1329	27464	164820	0.793	26.07
44	205.09	294	233.02	281.96	243.82	117.31	118.49	0.032	0.587	0.4109	0.4214	658.35	249.55	3029	0.1309	27904	165132	0.761	25.92
45	206.47	295.67	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	665.86	250.06	3007	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
46	208.67	297.05	235.07	283.84	245.05	[illegible]	[illegible]	[illegible]	0.579	0.4612	0.4529	664.51	242.98	2991	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
47	204.13	295.43	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	658.65	243.65	2979	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
48	207.65	295.79	228.75	281.5	242.38	116.43	118.32	0.029	0.585	0.4595	0.4318	671.69	250.1	2976	0.1303	27485	163268	0.781	25.95
49	208.59	299.06	240.13	287.57	246.37	117.75	118.04	0.027	0.573	0.4753	0.503	663.16	246.91	3030	0.1351	26876	162292	0.814	26.42
50	209.24	297.47	228.42	281.15	236.85	116.15	117.1	0.027	0.588	0.4774	0.4377	676.67	246.38	3004	0.1314	27322	157795	0.777	26.03
51	207	295.72	233.06	280.57	241.19	117.09	118.04	0.03	0.596	0.459	0.459	666	246	3000	0.1307	27487	158666	0.77	25.94
52	207	295.72	233.06	278.86	[illegible]	117.09	118.13	0.03	0.605	0.459	0.459	666	246	3000	0.1299	27552	156977	0.76	25.87
53	207	295.72	233.06	276.79	[illegible]	117.09	118.24	0.03	[illegible]	0.459	0.459	666	246	3000	0.129	27632	155208	0.748	25.8
54	207	295.72	233.06	274.28	239.15	117.09	118.38	0.03	0.631	0.459	0.459	666	246	3000	0.1279	27732	153333	0.734	25.71

Process

Quality

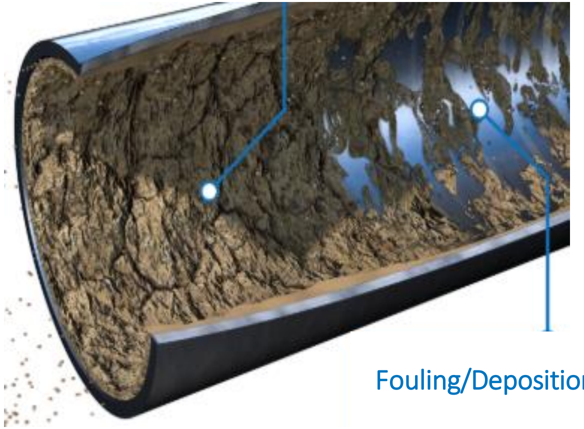
New



Two-zone LDPE reactor with a typical temperature profile

Common Problems

- **Common problems that affect LDPE process**
  - Impurity contamination **(affect temperature profiles)**
  - Change in initiator efficiencies
  - Fouling (deposition) of the reactor walls
  - Equipment, sensors, operators and lab analysis

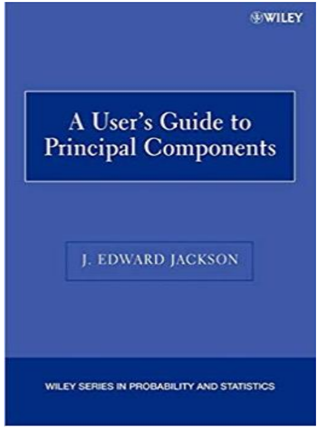


Fouling/Deposition

- **Affect polymer's quality**
- **Affect the behavior of the polymer in its final application**

Multivariate Process Control Procedure

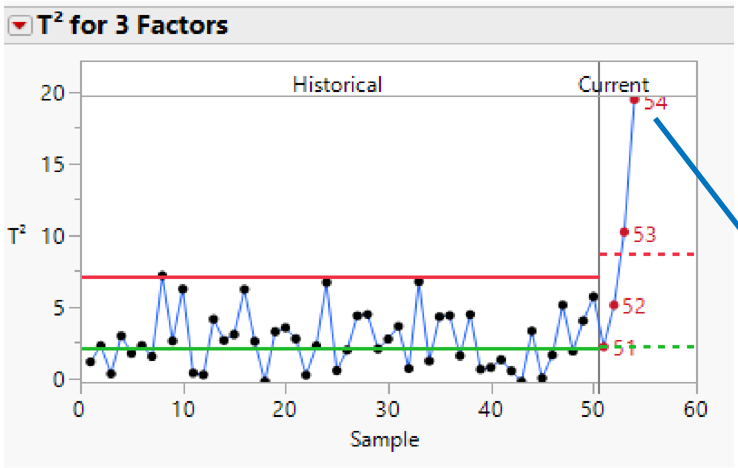
- **Four conditions (quotes from Jackson 1991):**
  - A single answer should be available to answer the question: “Is the process in control?”
  - An overall Type I error should be specified.
  - The procedure should take into accounts the relationships among the variables.
  - Procedures should be available to answer the question: “If the process is out-of-control, what is the problem?”
- **Let’s check model driven multivariate control chart**

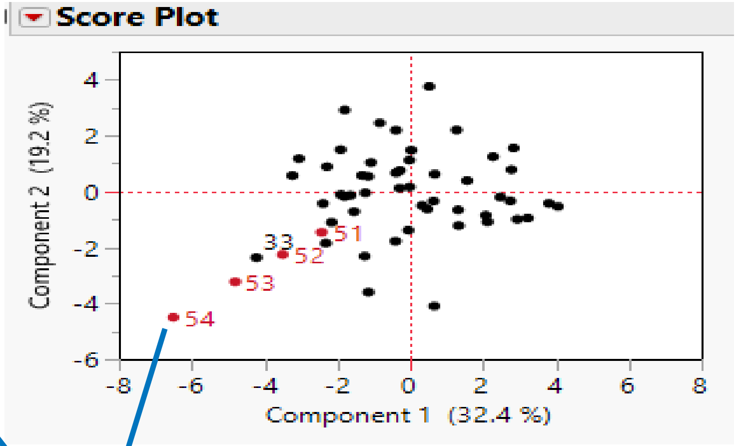


Demos

1. PLS modeling historical data
2. T2, SPE, Scores
   monitoring process
3. Contribution plots
   Diagnosing process

Monitoring the Process (T^2)





$$T_i^{\,2} = t^T \Lambda^{-1} t = \sum_k^a \left(\frac{t_k}{s_k}\right)^2 \sim \frac{a(n^2-1)}{n(n-a)} F_{a,n-a,\,\alpha}$$

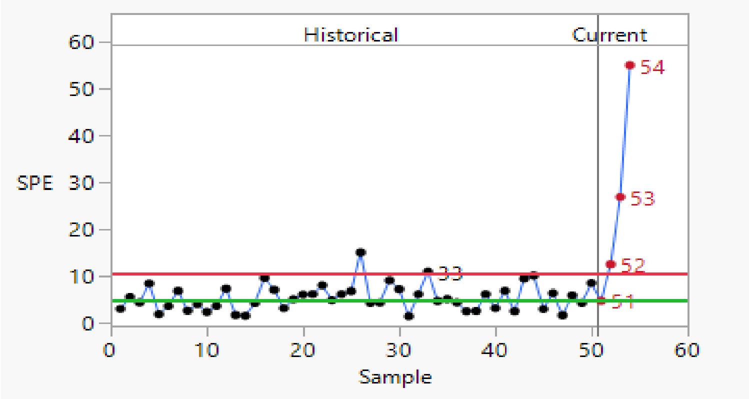
$$T_{54}^{\;\;2} = \left(\frac{-6.5}{1.97}\right)^2 + \left(\frac{-4.5}{1.52}\right)^2 + \left(\frac{-0.23}{1.29}\right)^2 = 19.7$$

- In the T^2 plot we can see that most of the observations are below the critical limits except for point 53 and 54.

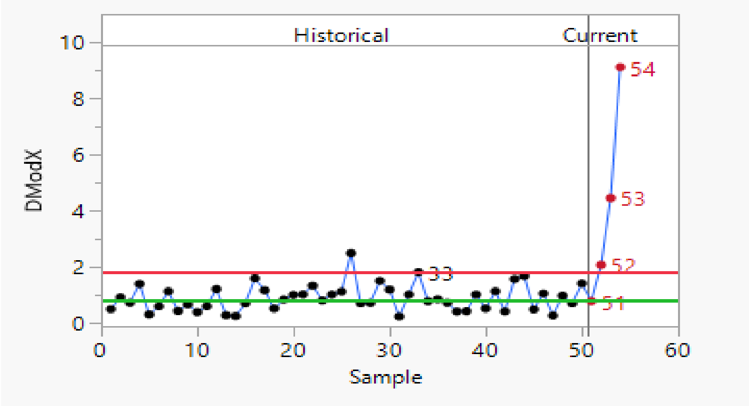
- Projecting the new data onto the model (t_1-t_2 plane) clearly indicates the process upset around point 52. Points 52, 53 and 54 progressively move outside the acceptance region.

Monitoring the Process (SPE and DModX)

Squared Prediction Error (SPE) Plot with 3 Factors



Normalized DModX Plot with 3 Factors



$$SPE_i = \boldsymbol{e_i}^{\boldsymbol{T}} \boldsymbol{e_i} = \sum_j^p \boldsymbol{e_{ij}^2} \sim \boldsymbol{g\chi^2_{h,\alpha}}$$

$$DModX_i = \frac{SPE_i/\boldsymbol{df_1}}{SPE/\boldsymbol{df_2}} \sim \boldsymbol{F_{h,nh,\,\alpha}}$$

- SPE is the sum of squared prediction error and DModX is a scaled version of SPE. Both measures the distance between the observations and the model plane.

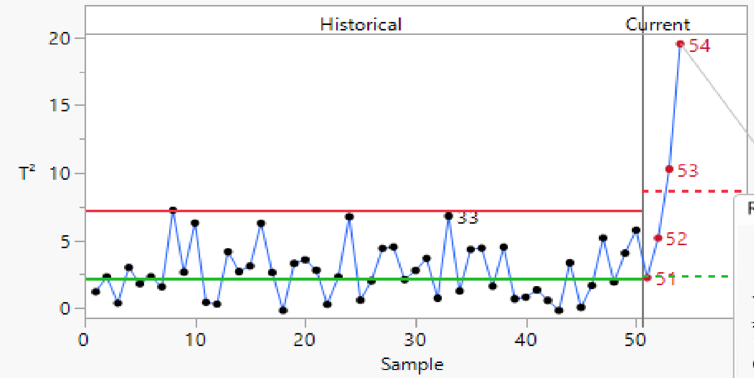
- In the SPE and DModX plots, we can see that most of the observations are below the critical limits except for the point 53 and 54.

Diagnosing the Process (T^2 Contribution Plots)

PLS Model Driven Multivariate Control Chart

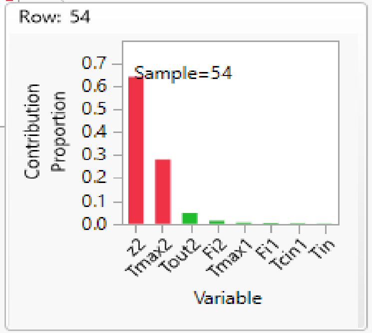
Monitor the Process

T^2 for 3 Factors



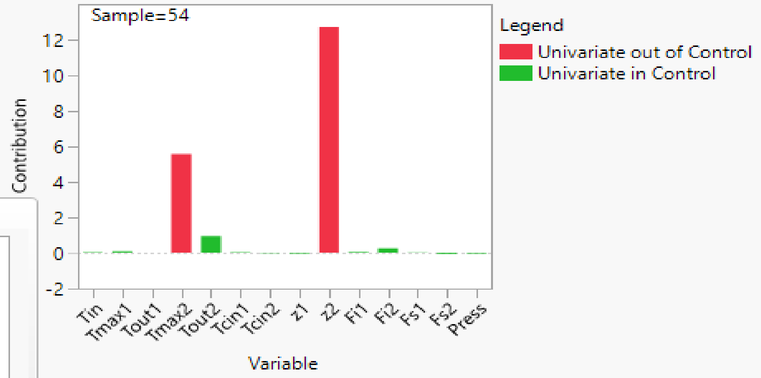
T^2 Limit Summaries

Data Points	Median	UCL	Out of Control Point	Alpha Level
Historical	2.383	7.430	1	0.05
Current	2.553	8.940	2	



Diagnose the Process

T^2 Contribution Plot for Selected Samples



$$T_i^2 = \sum_j^p Con(Ti^2, i, j)$$

$$Con(Ti^2, i, j) = \sum_k^A t_k\, s_k^{-2} p_{jk} x_{ij}$$

Identifying T^2 contributions of variables

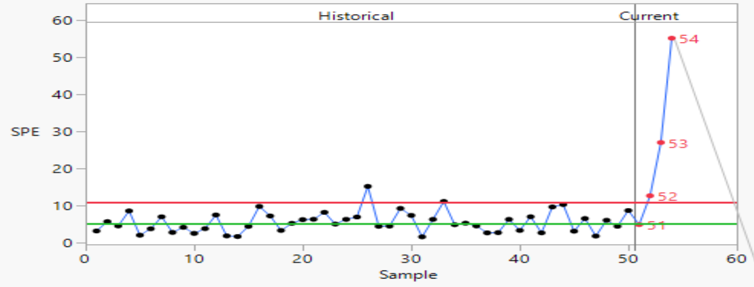
Major contributions come from Z_2 (position of the reactor where T_{max2} appears) and T_{max2} to the observation 54.

$Con(T_{54}^2, 54, Z_2) = (-6.506/3.88)*(-3.935) + (-4.5/2.298)*(-3.117) + (-0.232/1.665)*(-0.218) = 12.73$

Diagnosing the Process (SPE Contribution Plots)

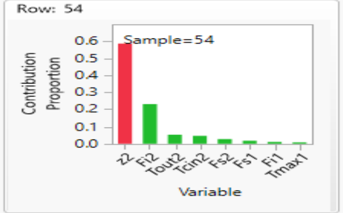
Monitor the Process

Squared Prediction Error (SPE) Plot with 3 Factors



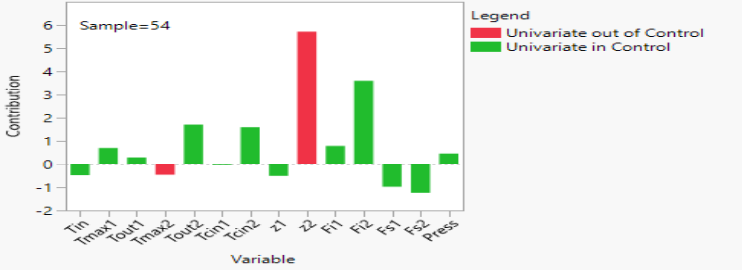
SPE Limit Summaries

Data Points	Median	UCL	Out of Control Point	Alpha Level
Historical	5.596	11.303	2	0.05
Current	5.596	11.303	3	

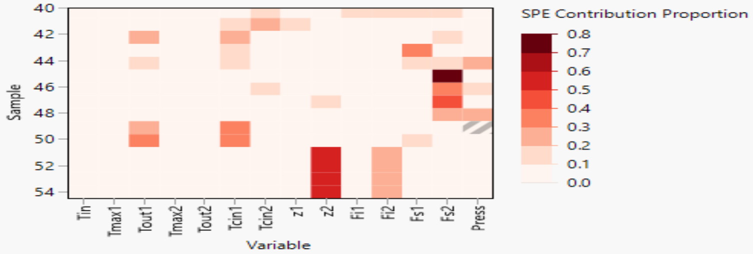


Diagnose the Process

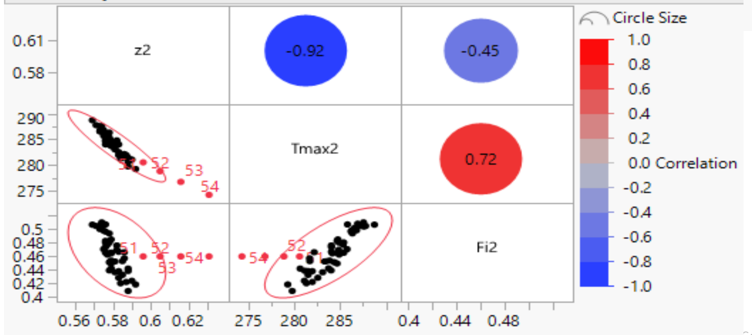
SPE Contribution Plot for Selected Samples



SPE Contribution Proportion Heat Map



Scatterplot Matrix

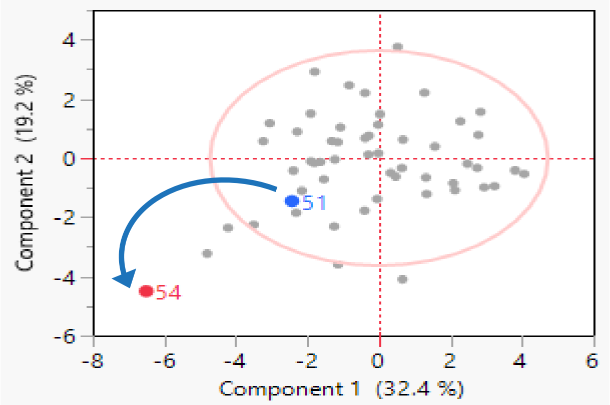


SPE contribution plots

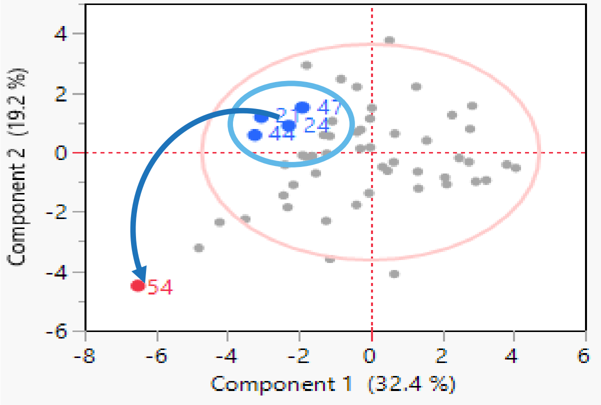
- Major contributions come from Z_2 (position of the reactor where T_{max2} appears) and F_{i2} (feed rate of the initiators to the second section).
- Hot spot position has moved further down the reactor and possibly the initiator efficiencies have dropped.
- Variable Z_2 ,T_{max2} and F_{i2} break the correlation structure.

Diagnosing the Process (Relative Score Contribution Plot)

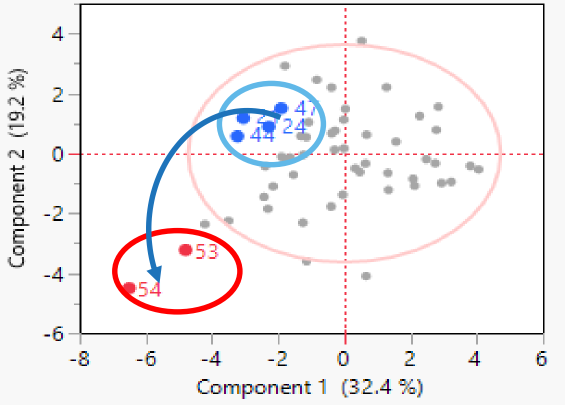
point-to-point

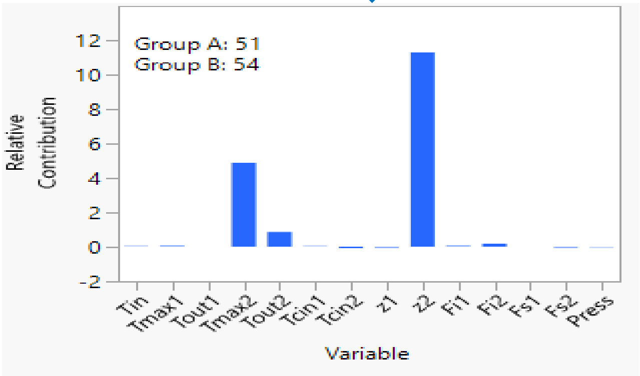


point-to-group



group-to-group



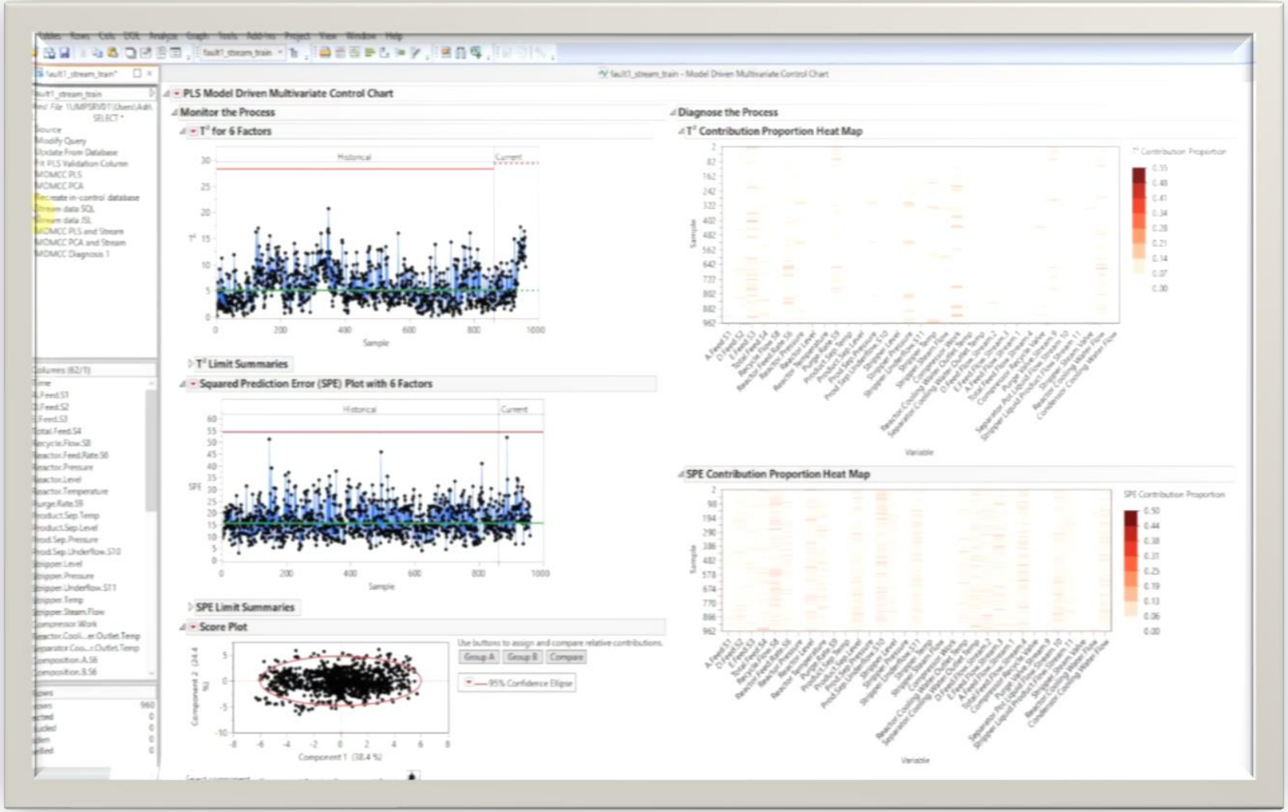


Identifying relative contributions of variables

- Major contributions to the difference between observation 51 and 54 come from Z_2 (position of the reactor where T_{max2} appears) and T_{max2}
- Hot spot position has moved further down the reactor and the hot-spot temperature T_{max2} has decreased.

Example-Tennessee Eastman Process

Process data streaming



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Conclusions

How the model driven multivariate control chart platform can help?

- MSPC (PCA / PLS)
  - Efficient
- Monitoring
  - Early
- Diagnosing
  - Easy
- Streaming
  - Effective

References

- Kourti, T. and MacGregor, J. F. (1995), "Process Analysis, Monitoring and Diagnosis, Using Multivariate Projection Methods", *Chemometrics and Intelligent Laboratory Systems*, 28, 3–21.
- **Contribution plots**: P Miller, RE Swanson, CE Heckler, "Contribution Plots: a Missing Link in Multivariate Quality Control", *Applied Mathematics and Computer Science*, *8* (4), 775-792, 1998.
- **Process monitoring**: John MacGregor and Theodora Kourti "Statistical Process Control of Multivariate Processes", *Control Engineering Practice*, **3**, p 403-414, 1995.
- Li, G., Qin, S.-Z., Ji, Y.-D., & Zhou, D.-H. "Total PLS Based Contribution Plots for Fault Diagnosis". *Acta Automatica Sinica*, *35*(6), 759–765, 2009.
- Downs, J. J., & Vogel, E. F. "A plant-wide industrial process control problem". *Computers & Chemical Engineering*, *17*(3), 245–255, 1993.

Thank you for your attention

Questions?

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