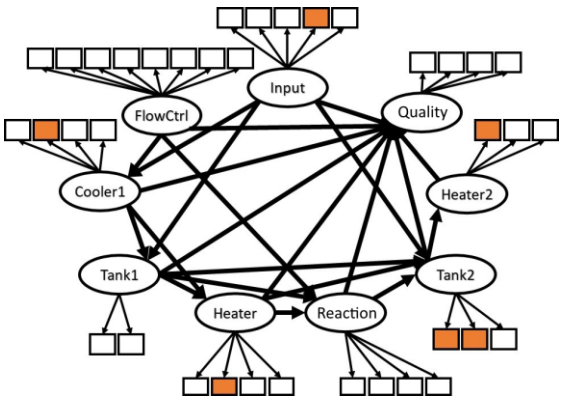
Understanding chemical production processes through PLS path modelling

Geert van Kollenburg[1], Jeroen Jansen[1]

There is a consistent societal and political push for industrial processes to reduce resource consumption. This reduction needs to be attained within economically viable settings for the producers. One example of optimizing both resource consumption and cost reduction optimization is the maximization of catalyst lifetime.

In this study, Partial Least Squares Path Modelling (PLS-PM) was used to evaluate relationships between various parts of a production process to detect and identify whether changes occurring during the production process affected the catalyst lifetime.

PLS-PM is an approach to structural equation modelling, which allows for the quantification of statistical relations between groups of observed variables. By grouping production data, such as temperatures, pressures and flowrates, based on where in the process where they are measured, PLS-PM can be used to find statistically relations between those parts of the process (as shown below).



An important aspect of path modelling is that expert knowledge can be incorporated into the model specification. For example, the relationships in the model were specified by process operators and engineers.

As we had multiple data sets related to varying catalyst lifetime, we were able to find correlations between step-to-step relations and catalyst lifetime. The correlations for the significant relations are shown below. These relations are now further investigated and are monitored in real-time to optimize and increase process control.

Relation from	Relation to	Correlation to cost
Cooler	Input	0.50
Tank1	Cooler	0.55
Heater	Cooler	-0.56
Tank2	Heater	0.83
Product	Heater	0.70

Next to the found relations shown above, the study confirmed that running the plant on lower capacity increased the yield per unit of catalyst. While this decreases production speed it may be beneficial on the long run.

From the results shown above, the following can be concluded:

- **PLS-PM can identify important relations between different steps in production processes.**
- **The relations between process variables can be predictive for production quality and/or efficiency.**
- **Historical process data becomes extremely valuable by incorporation of expert knowledge.**
- **Process operators can easily be involved in the statistical modelling, making communication of analysis results easier.**

Future work will focus on improving path modelling methodology so that it can be used in a wide range of research fields. Applications will range from the analysis of milk derivatives production to predicting pollution pathways in river water.

Radboud University

Nouryon

1. Radboud University, Nijmegen