# Batch-invariant modelling of industrial batch reaction productivity

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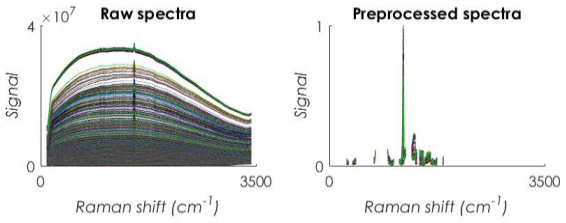
(Bio)chemical industrial batch reactions have to be ended at the correct time to prevent waste of source materials and decrease of product quality. Estimating the correct endpoint can be achieved by modelling the chemical productivity of the reaction. Chemical changes can be monitored in real-time using on-line spectroscopic measurements. However, such measurements can suffer from large batch-to-batch differences caused by variations in raw material, weather, customer wishes and operators.

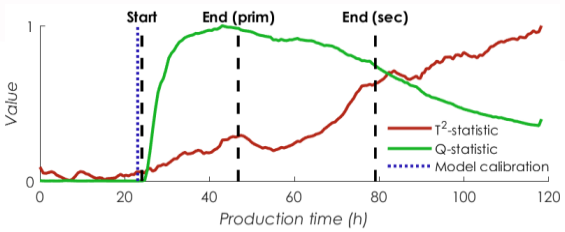
**This study presents a batch-invariant approach for detecting the end point of an example industrial batch reaction using spectroscopic Raman measurements.**

Batch differences are reduced by preprocessing the incoming spectra using baseline and scatter correction, wavelength selection and normalization, as illustrated below for one complete batch.

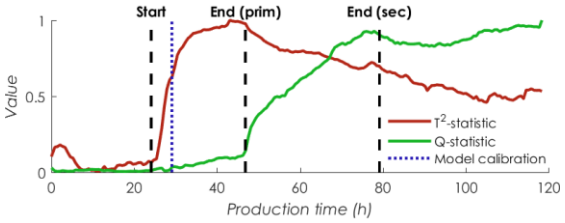



The reactor productivity is monitored by modelling the spectra using PCA and calculating the $T^2$- and Q-statistic for each spectrum. These statistics effectively represent the chemistry described by the model and the chemistry not described by the model, respectively.

The timing of the PCA model calibration determines which chemistry is represented in the statistics, as shown below. The example process has a primary and secondary reaction for most productions. Calibrating the model just before the start of the primary reaction results in the Q-statistic representing the primary product, as shown below. The spectra collected after calibration time are projected in the model as they are collected.

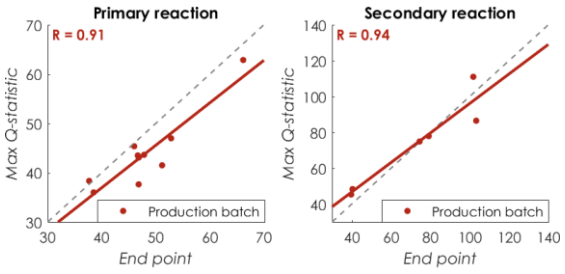



Calibrating the model between the starts of the primary and secondary reactions results in the $T^2$-statistic representing the primary reaction and the Q-statistic representing the secondary reaction, as shown below. In all cases, the point in time where the statistics level out mark the end of production for the respective products.




**These findings show that monitoring the Q-statistic allows for the detection of the end of a reaction that has not yet started at the time of PCA model calibration. This can be used to better time the termination of the process, improving production quality and efficiency.**

The above results are reproducible for other production batches, as is shown below.

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