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# Optimization of Chemical Batch Processes within a Systematic Retrofit Framework including Evaluation of Historical Process Data

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Batch processes are widely used in industry. Notably for specialty chemicals or pharmaceutical processes batch mode is often applied. When investigating industrial batch processes with the goal to optimize the process performance by retrofitting, a standard batch has to be defined in order to have a base case as starting point.
Due to the necessity of process control abundant historical data exist for industrial batch processes. Is there an effective way to treat the vast amount of historical data with a reasonable expenditure of time in order to improve the description of the standard batch? A case study was investigated in order to answer this question and it was found that with a statistical evaluation of historical data interesting process performance trends can be revealed.

## 1. Introduction

Industrial chemical batch processes are popular in specific product areas as they are flexible with respect to reaction time and to the kind and quantity of products that are processed. In industrial batch process plants a lot of parameters are constantly measured and stored in compressed databases. The compressed data has been shown to accurately represent the original data (Singhal and Seborg, 2005) and can therefore be used to describe the real process performance.
The compressed and stored data of a batch process is abundant and often not clearly arranged. Several studies on the effective analysis of batch process data have been carried out (Chiang et al., 2006; Mitchell et al., 2008). The evaluation of batch process data can be generally a demanding and time consuming task and therefore a registered recipe is often considered to represent a standard batch, i.e. the average performance of the batch process. In certain cases the recipe describes the standard batch accurately but in other cases the real process performance deviates from the recipe. To investigate whether the real process performance matches the recipe the historical process data has to be consulted.
Retrofitting can be understood as technical and structural changes in the process layout to meet new requirements or to improve process performance. Especially the impact of

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additional vessel sizes as retrofit option has been widely investigated in literature (Espuña et al., 1989; Fletcher et al., 1991). Later studies focused on a systematic indicator based methodology where retrofit alternatives were proposed by analyzing the whole flowsheet and applying heuristics (Uerdingen et al., 2003; Simon et al.; 2008; Carvalho et al., 2009). Particularly for retrofit methodologies that target the integral process behaviour the definition of the standard batch which represents the base case is crucial.

Because the knowledge about the standard batch is such an important starting point for retrofitting purposes, it was investigated whether a reasonable data treatment could highlight the real process performance. It will be shown how the data treatment results can be used to define the standard batch of an industrial batch production facility. In a next step the impact of the standard batch definition on the results of an indicator based retrofit methodology will be observed.

## 2. Methodology

### 2.1. Definition of the standard batch

In this study the focus was on the unit occupancy and batch times of a batch process, but the methodology can be applied to every other process variable. The process data was extracted and for every batch number registered it was investigated whether all relevant steps in the recipe were available. If a step was missing, the whole batch was removed from the dataset. Furthermore, if the unit occupancy time deviated more than two standard deviations from the mean unit occupancy time, the batch was considered to be an outlier and removed from the dataset. This was done in order to assess the general process performance without considering batches where substantial problems delayed the batch time.

The collected data was evaluated by a statistical analysis. The batch and unit occupancy times of the units were calculated as mean values with standard deviation. At first the average batch was defined and then also the golden batch. The golden batch represented the best achievable performance, and was described by the 10 % fastest batches. Special attention was paid at the bottleneck units which were the units with the biggest unit occupancy time per batch. These bottleneck units define the cycle time of the batch and are crucial for process improvement.

In a next step the process performance over time was investigated. The data for the batches was evenly divided into data subsets called clusters. In order to be able to observe time-dependent trends, the batches of a cluster have to be subsequent batches in time. All clusters were statistically evaluated in the same way as the whole dataset before.

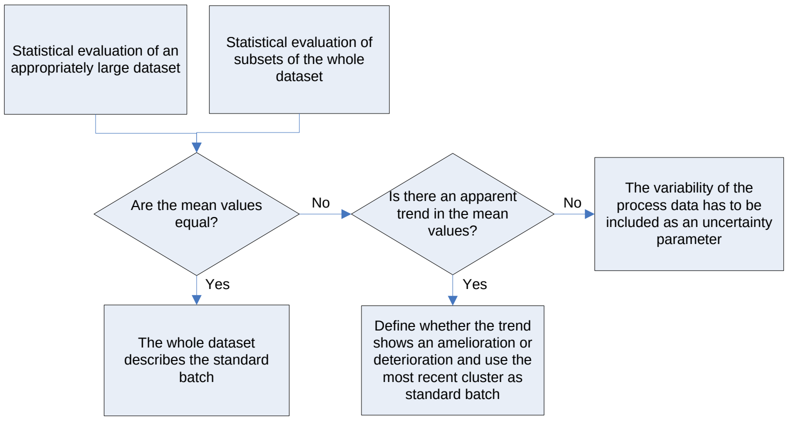


*Figure 1: Flowchart for standard batch selection based on historical data treatment results.*

Then the results for the average batch were compared to the results of the clusters in order to define the standard batch. Figure 1 presents a schematic overview for the selection strategy. When the results of the clusters corresponded to the average results, the average batch can be used as the standard batch. This would be a hint to a very constant process performance. Generally it will often occur for batch processes that the cluster results deviate from the average batch. In that case it has to be investigated whether the clusters vary randomly or whether an apparent trend can be observed. When no trend can be seen in the cluster results the deviations should be included in the average batch in order to describe uncertainties in the process performance. On the other hand, if a clear trend can be observed the most recent clusters should be used to describe the actual standard batch of the process.
The defined standard batch found by the procedure shown in Figure 1 is then used as base case in a systematic indicator based retrofit methodology. The results will be compared to the evaluation where the average batch was used to define the base case.

### 2.2. Indicator based retrofit methodology

The first step of the retrofit methodology was the path flow decomposition procedure of the considered flowsheet (Uerdingen et al., 2003). The path flow rates as mass per batch were based on the standard batch. Every path flow of the standard batch was then assessed individually by a set of indicators shortly described in the following paragraph.
The reaction quality indicator (RQ) measures the effect of the considered component path on the reactions occurring along the path. The accumulation factor (AF) is a hint to unwanted substance build-up in recycle flows, and is therefore only applied to cycle flows. The energy cost (EC) and the waste cost (WC) represent the allocated process costs related to utility consumption and waste treatment to the component path flows. The material value added (MVA) indicator represents the value of a path flow. A positive MVA indicates that the stream is valuable (mostly product streams). Negative MVA values indicate costs.
Based on the indicators calculated for the standard batch, specific heuristics reveal retrofit actions for improving the process performance. The evaluation of the heuristics

will result in a set of technical and structural process retrofit alternatives (Simon et al., 2008). For the base case and retrofit alternatives different objective functions were calculated in order to quantify the economic and environmental impact of the retrofit alternative.

## 3. Case study

A mono product batch process facility was investigated. The process starts in a reactor (R) where the reaction product is formed. In a next step the product is purified first in a crystallization unit (C) and then separated from the mother liquor in a filter (F). Finally the residual moisture content of the product is removed in a drier (D). The process data over 3 months was investigated which resulted in the treatment of 207 batches.

## 4. Results and Discussion

For 171 out of 207 batches all relevant historical data was stored. From them 23 were identified as outliers resulting in 148 batches representing the average batch.

*Table 1: Mean unit occupancy and batch times for the average and golden batches and the identification of the bottleneck unit considering all batches in the dataset.*

| unit | occupancy time average batch | | occupancy time golden batch | | bottleneck unit |
|---|---|---|---|---|---|
| | *mean* | *rel. stdev* | *mean* | *rel. stdev* | *frequency* |
| R | 6.4 | 10% | 5.7 | 8% | 7% |
| C | 6.8 | 8% | 6.1 | 6% | 16% |
| F | 7.3 | 6% | 7.3 | 4% | 69% |
| D | 6.7 | 10% | 6.3 | 6% | 7% |
| batch time | 25.5 | 5% | 23.6 | 1% | |

Table 1 shows the mean unit occupancy times of reactor (R), crystallizer (C), filter (F) and drier (D) of the average and the golden batch. Also the batch times and the relative standard deviation were given. The last column in Table 1 gives an overview of the frequency a unit of a batch was the bottleneck. The filter had the biggest average unit occupancy time for both the average and the golden batch. Moreover, the frequency of the bottleneck unit showed that in 69% of all batches the filter had the biggest unit occupancy times. Interestingly the unit occupancy time of the filter is the same for the average and the golden batch. This can be explained by the fact that in industry special focus is given to the bottleneck unit and therefore it was achieved to keep the filter's occupancy time constant. The other units were processed faster for the golden batch compared to the average batch. Even though a reduction in unit occupancy time of those units does not influence the cycle time, a reduction in unit occupancy time can have a beneficial impact, e.g. reduced energy consumption. Another interesting finding is that in 16% of all batches the crystallizer was the bottleneck unit. Therefore it may be worth to target at constant performance of C in order not to become the bottleneck unit in some batches. The relative standard deviations provide information about the uniformity of the process performance. For instance, the batch time of the average batch had a relative standard deviation of 5 % which is 76.5 min. Depending on the application the standard batch is used for, this deviation in time may not be negligible.

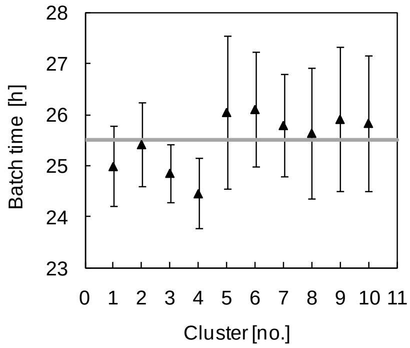


*Figure 2: Evaluation of the batch time of chronologically subsequent batch clusters compared to the average batch time (continuous line). The bars indicate the standard deviation for each cluster.*

The batches of each dataset were divided into 10 chronologically subsequent clusters, 8 clusters consisting of 15 batches and 2 of 14 batches. All clusters were statistically evaluated. The average batch time of each cluster and the standard deviation are shown in Figure 2. In order for the clusters to be compared to the average batch, the batch time of the average batch is indicated as solid line. As can be clearly seen in Figure 2 the average process performance in clusters 1-4 is superior compared to the average batch, while in clusters 5-10 the performance was worse. Additionally the standard deviation bars indicated that the process performance was more stable during clusters 1-4. The reasons for the two different performance regions should be discussed with the process engineers and operators of the industrial plant.

*Table 2: Mean unit occupancy and batch times for clusters 1-4 and clusters 5-10.*

| | average cluster 1-4 | | average cluster 5-10 | |
|---|---|---|---|---|
| | *mean* | *rel. stdev* | *mean* | *rel. stdev* |
| R, occupancy time | 6.3 | 8% | 6.4 | 11% |
| C, occupancy time | 6.7 | 6% | 6.8 | 9% |
| F, occupancy time | 7.1 | 5% | 7.4 | 6% |
| D, occupancy time | 6.4 | 5% | 7.0 | 11% |
| batch time | 24.9 | 3% | 25.9 | 5% |

As a consequence of the cluster trends, clusters 1-4 and clusters 5-10 were combined and evaluated as two datasets. The average unit occupancy and batch times of those two datasets are listed in Table 2. Comparing clusters 1-4 to the golden batch (see Table 1) it can be observed that only the filter unit occupancy time is smaller. As this is in most of the cases the bottleneck this finding is of special importance as it shows that there is a potential to further reduce the occupancy time of F. Comparing clusters 5-10 to the average batch it can be observed that the drier has a higher occupancy time in those clusters. All other units are close to the average batch and also the standard deviations are comparable. This finding can be a hint that in clusters 5-10 there was a problem in the drier that delayed the batch time.

## 5. Conclusions and Outlook

The data treatment of industrial process data with basic statistical tools revealed the real process performance over time, which would have been masked if only the average batch had been considered. For the process manager the data treatment highlighted hotspots where problems or irregularities occurred. The reasons for these specific hotspots were further investigated by the process experts. Then the detected hotspots helped the process manager to identify technical and/or organizational improvement potential that was not obvious on first sight.

Another aspect of the procedure is that it enables a more precise definition of a process base case which is of high importance for retrofit related research, where the goal is to improve the process performance based on the analysis of the base case. The next step is to apply the newly defined standard batches in the indicator based retrofit methodology in order to determine how these affect the outcome, i.e., the proposed retrofitting actions and their estimated multi-objective gain.

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