Improving root cause analysis by detecting and removing transient changes in oscillatory time series with application to a 1,3-Butadiene process

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ABSTRACT

Oscillations occurring in industrial process plants often reflect the presence of severe disturbances affecting process operations. Accurate detection and root-cause analysis of oscillations is of great interest for the economic viability of the process operation. Standard oscillation detection and root cause analysis methods require a large enough number of data samples. Unrelated transient changes superimposed on the oscillation pattern reduce the number of useful data samples. The present paper proposes simple heuristic methods to effectively detect and remove two types of transient changes from oscillatory signals, namely step changes and spikes. The proposed methods are used to pre-process oscillatory time series. The accuracy gained when using auto-correlation function method for oscillation detection (Thornhill et al., 2003) and transfer entropy method for oscillation propagation (Bauer et al., 2007) is experimentally evaluated. The methods are carried out on a 1,3-Butadiene production process where several measurements showed an established oscillation occurring after a production level change.

Keywords: Plant-wide disturbances; oscillations; pre-processing; transient removal; fault detection, chemical process.

1. INTRODUCTION

Disturbances occurring in industrial process systems can travel through the interconnected process equipment and appear in several measurements in the process resulting in what is often termed 'plant-wide disturbances' (Thornhill and Horch, 2007). Oscillatory disturbances are a common type of plant-wide disturbances affecting industrial process systems. The detection and the diagnosis of these oscillatory disturbances are of great importance as these disturbances can increase the level of process variability and, ultimately, decrease the profit of the process operation (Shunta, 1995). In Horch (2007) the author defines oscillations as "periodic variations that are not completely hidden in noise". Several methods for oscillation detection are available in the literature and listed in Thornhill and Horch (2007). Among oscillation detection methods with successful industrial implementation (Bauer, et al., 2016) we can cite methods based on spectral PCA analysis (Thornhill, et al., 2006), methods based on the regularity of the integral absolute error (IAE) (Hägglund, 2005; Forsman & Stattin, 1999), methods based on the decay ratio of the auto-correlation function (Miao & Seborg, 1999), methods based on zero-crossings of the auto-correlation functions (Thornhill, et al., 2003) and methods based on wavelet analysis (Matsuo, et al., 2004).

Methods for the isolation of the root cause of an oscillatory process disturbance include surrogate testing (Thornhill, 2005, Choudhury et al., 2007), bi-spectra and related bi-coherence (Choudhury et al., 2004), harmonics (Zang and Howell, 2005) and spectral envelope method (Jiang et al., 2007). A method using the spectral envelope is proposed in Jiang et al., (2007). Yuan and Qin, (2014) use Granger causality in the spectral domain to isolate the root cause of oscillatory disturbances while in Bauer et al. (2007), transfer entropy, a metric of causality based on information theory introduced in Schreiber (2000) is adapted for the root cause analysis of oscillatory as well as non-oscillatory process disturbances.

The authors in Jelali and Huang (2009) claim that oscillation detection methods can nowadays be considered as a largely solved research topic. In industrial practice, however, the presence of transient disturbances in the oscillatory signals can lead to a decrease of the accuracy of standard oscillation detection methods (Jelali and Huang, 2009), (Zhou, et al., 2017) and therefore reduce their industrial acceptance.

In Cecílio et al. (2014), a transient disturbance is defined as "a short deviation of a measurement from its previous and subsequent trend. In addition, this deviation should seldom repeat within the time horizon of analysis. After the occurrence of a transient disturbance, the measurement may return to its previous trend or follow a different trend". **Figure 1** exemplifies two types of transient disturbances affecting an oscillatory signal and shows that their presence can mislead a visual inspection of oscillations.

Detection of transients affecting oscillatory signals is also a topic of investigation in power systems (Cai et al. 2017). In the areas of power systems protection and power quality assessment, methods based on time–frequency domain analysis such as wavelet transform (Liu et al. 2014, Costa 2014 and Huang et al. 2002) are proposed for transient detection. Transient disturbance detection in power systems differs nevertheless from the problem studied in the present work. The topic here is the detection and the root cause analysis of oscillatory disturbances affected by transients. In power systems protection and power quality assessment, the objective is the detection of transients, while the oscillatory components reflect the nominal behaviour of power, voltage or current signals in an AC power system. In Cecílio, et al. (2014), a method based on nearest neighbours is proposed to detect transients and in Cecílio, et al., (2016) a method based on nearest neighbour imputation is used to remove transients.

Common industrial practice is either to exclude from the analysis time intervals exhibiting transients or to completely drop out signals with transients (Tikkala, et al., (2014)). However, in order to allow accurate oscillation detection, the oscillation should persist during eight cycles at minimum and excluding time intervals with transients can hinder that (Thornhill, et al., 2003). The same argument holds for root cause analysis methods: for the transfer entropy method, a minimum number of 2000 samples are recommended in Bauer et al.(2007). A typical example is the start of an oscillation during an intermediate phase of the process operation such as a grade transition, a production level change or a start-up. Pre-processing methods that are able to remove transients from univariate oscillatory time series are therefore needed to fully exploit the available process data when applying oscillation detection and root cause analysis methods. The problem is also different from outlier detection (Liu et al., 2004), which aims at removing single points.

The empirical mode decomposition (EMD) method proposed in Srinivasan and Rengaswamy (2007) allows the detection and the quantification of multiple oscillation modes by iteratively applying it on an extracted non-constant mean. This approach inherently removes the non-constant mean (low-frequency oscillation mode) from the signal. Multivariate empirical mode decomposition (MEMD) proposed by Aftab et al.(2018) extends the EMD method to plant wide oscillation detection and benefits from the same advantage i.e. the ability to deal with the slowly varying trends. Alternatively, the direct cosine transform (DCT) introduced in Li et al. (2010), isolates different frequency components, e.g., multiple oscillations, of a time series and detects the oscillations by checking the regularity of zero-crossings of the isolated components. Likewise, the DCT method is able to handle slowly varying trends by isolating them (low-frequency component) and discarding them based on the low regularity of the corresponding component zero crossing.

On the other hand, transient changes like spikes and steps affecting the oscillating time series are not discussed in Srinivasan and Rengaswamy (2007), Li et al. (2010) and in Aftab et al.(2018). The particularity of these transients is a clear localization in the time domain but no precise localization the frequency domain. This aspect motivates investigating time domain approaches for the pre-processing of oscillating time series affected by such transients.

The present work extends the analysis of the transient detection and removal methods introduced in Zhou, et al. (2017) where the authors proposed heuristic methods to detect and to remove transients from oscillatory signals by applying it in conjunction with oscillation and transfer entropy method to study the effects. In addition to this expansion, the procedure is improved and formulated precisely in mathematical terms. The methods are here used as a pre-processing step for oscillation detection and root cause analysis methods in an offline context. In this work, the performance is evaluated on simulated data as well as on an industrial case study.

The remainder of the paper is organized as follows. The autocorrelation function (ACF) oscillation detection method and transfer entropy based causal analysis are briefly introduced In Section 2. In Section 3, the proposed methods for steps and spikes detection and removal are described in detail. In Section 4, a sensitivity analysis to the tuning parameters is done and recommendations for default parameter settings are provided. The proposed methods are tested first in simulation in Section 5 then applied on a real industrial dataset collected from a 1,3-Butadiene process to demonstrate the improvement both in oscillation detection and root cause analysis in Section 6. Finally, Section 7 concludes the paper.

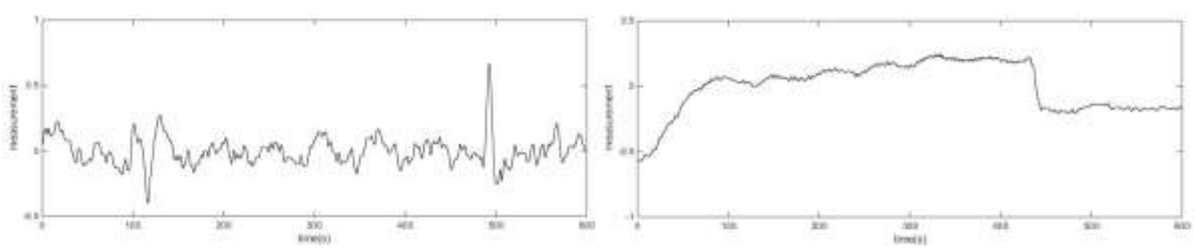

Figure 1. *Examples of transients affecting oscillatory signals: left side: transient spikes, right side: transient step.*

2. OSCILLATION DETECTION AND USING AUTO-COVARIANCE FUNCTION (ACF) AND CAUSAL ANALYSIS USING TRANSFER ENTROPY

The ACF method (Thornhill, et al., 2003) is a method for oscillation detection. This method determines the regularity of the zero crossings of the auto-covariance function. The ACF of an oscillating signal is itself oscillatory with the same period as the oscillation in the time trend. The advantage of using the ACF for oscillation detection is that the impact of noise is reduced because white noise has an ACF that is theoretically zero for lags greater than zero. The zero crossings of a periodic oscillation are regularly spaced while for a signal that is not oscillating, the zero crossings of the ACF happen at random times. The zero crossings intervals are therefore similar in the first case and dissimilar in the second. The standard deviation of the intervals is used as an indication of the regularity of the oscillation and a clustering algorithm determines which measurements belong to the same group of oscillations.

Transfer entropy is one possible metric to quantify the influence or causality of one process variable on another process variable proposed in (Bauer et al, 2007) for plant disturbance analysis. This statistical method evaluates the predictability of a variable from another variable based on Probability Density Functions (PDF). The causality measure used to quantify the extent of the influence of a variable **x** on another variable **y** is derived from Transfer Entropy $TE\ (\mathbf{x}|\mathbf{y})$ (Schreiber, 2000). The latter is derived from entropy. Entropy is a measure of uncertainty of a random variable summing a weighed logarithm of the PDF (Shannon and Weaver, 1948). Transfer entropy is calculated from joint PDF of two variables and provides a measure for the dependencies between those variables. The causality measure $TE\ (\mathbf{x},\mathbf{y})$ is derived by comparing the influence of **x** on **y** with the influence of **y** on **x**: $TE\ (\mathbf{x},\mathbf{y}) = TE\ (\mathbf{x}|\mathbf{y}) - TE\ (\mathbf{y}|\mathbf{x})$. A large value of $TE\ (\mathbf{x},\mathbf{y})$ indicates therefore a strong causality from **x** to **y**.

3. DETECTION AND REMOVAL OF TRANSIENT DISTURBANCES

This section describes the proposed approach to detect and remove transient disturbances from oscillatory signals. Following the definition given in Cecílio et al., (Nearest neighbors method for detecting transient disturbances in process and electromechanical systems, 2014), two types of transient disturbances are considered in the present work. Step changes are defined by a fast signal variation followed by a deviation to a value significantly different from the original one and no return of the signal to its original value within a short time interval. Spike changes are, on the other hand, defined by a fast signal variation followed by a deviation to a value significantly different from the original one, and a return of the signal to its original value within a short time interval. In industrial data, it is possible that spike and step follow each other and appear to occur at the same time. Also, spikes can occur in quick succession. Generally, steps are considered more significant as they are persistent and usually have a larger effect on process performance. The proposed algorithm is able to deal with these occurrences by adjusting its parameters. The data used to develop parameter guidelines in the following sections, however, does not include the simultaneous occurrence of steps and spikes.

The proposed approach uses as prior information an estimated value of the signal oscillation frequency obtained from a standard method for oscillation detection (ACF, Thornhill, et al., 2003) with no pre-processing. Note that alternative oscillation detection methods can be used to get an estimate of the signal oscillation frequency.

3.1 Step and Spike Detection Algorithm

The detection algorithms are based on an increase in the rate of change The detection algorithm of steps and spikes are similar because a step is a large change in one direction while a spike is a large change in one direction followed by a change in another direction. The key challenge is to identify large changes by setting appropriate levels and parameters. The parameters here are scaled – where appropriate – to the oscillation period T_p that was detected in a first analysis.

The time trends is defined as:

$$\underline{x} = [x_1, \cdots, x_N] \tag{1}$$

with time index n and N the number of samples of the selected time period. In the first step, any linear time trend for the selected time period is subtracted:

$$\underline{x'} = \underline{x} - \underline{x}^{linear} \tag{2}$$

where $x_n^{linear} = b_0 + b_1 n$ is the linear regression of $\underline{x}$ with linear regression coefficients computed form $\underline{x}$.

Similarly, parabolic time trend can be removed by using a quadratic polynomial regression model.

To eliminate high frequency components a moving average filter is applied with window length $2M$+1:

$$x_n'' = \frac{1}{2M+1} \sum_{k=n-M}^{n+M} x_{n+k}{}' \tag{3}$$

where $M = \left\lceil \frac{T_p}{\alpha} \right\rceil^{ceil}$ with smoothing level α. For both step and spike detection the rate of change is important. To approximate differentiation, the difference vector is computed:

$$d_n = x_n'' - x''_{n-1} \; for\, n = 2...N \tag{4}$$

3.1.1 Rate of change detection

The mean μ_d and standard deviation σ_d of difference vector are computed over the selected time series N to define the threshold for change detection. Change detection occurs for the points that exceed the threshold

$$d^{change}: |d_n - \mu_d| > \beta\sigma_d \tag{5}$$

with deviation threshold factor β. To differentiate between fast and moderate changes, two different threshold factors, which replace β are introduced, namely β^{fast} and β^{mod}. This results in d^{fast} and d^{mod}. Moderate changes may be required to be considered for spike detection because the spike can occur over a number of samples, which are not necessarily consecutive.

Most steps and spikes do not occur over one or two samples but over several samples. Therefore fast or moderately changing points need to be grouped into intervals. The start of an interval is defined as sample n_k^{start} and end point of interval as n_k^{end}, the sample after the last detected change. The duration of the interval is defined $n_k^{end} - n_k^{start} + 1$. There will be *K* intervals indexed from $1 \ldots k$ for the sample period of *N* samples.

3.1.2 Consolidation of step and spike intervals

The grouping of large changes into intervals needs to be done particularly carefully as it has a significant effect on the detection and is different for steps and spikes.

In steps, only consecutive samples of fast changing samples are added into one interval.

For spikes, the shift from a sharp increase to decrease of variable x'' can result in a short period of little change. It is therefore useful to define a threshold below which the samples belong to the same interval. The threshold is scaled to the oscillation period as T_p/δ where δ is the adjacency level factor. The samples in between two fast changing intervals that are close together are also added to the interval. After consolidating the intervals in this way, moderately changing are added to the interval if they within the proximity defined by T_p/δ of existing intervals. No new intervals are defined by moderately changing peaks.

3.1.3 Definition of pre- and post-interval levels

To establish whether the increase in the rate of change is a step or a spike the amplitude levels before and after the detected change have to be evaluated. These intervals are referred to as 'pre' and 'post' events and are of length T_p/γ where γ is the adjacency factor and T_p the estimated oscillation period. If there is a sufficiently large difference between pre- and post-levels then the interval is defined as a step. If the levels are sufficiently similar then the interval is defined as a spike.

The *K* pre-intervals are defined as:

$$\underline{x}_k^{pre} = \left[x_{n_{k,pre}^{start}}'' \cdots x_{n_{k,pre}^{end}}''\right] \tag{6}$$

with mean μ_k^{pre} and standard deviation σ_k^{pre} of $\underline{x}_k^{pre}$ where $n_{k,pre}^{start} = n_k^{start} - \frac{T_p}{\gamma}$ and $n_{k,pre}^{end} = n_k^{start}$ and adjacency level γ. Conversely,

$$\underline{\mathrm{x}}_{\mathrm{k}}^{\mathrm{post}} = \left[\mathrm{x}_{\mathrm{n}_{\mathrm{k,post}}^{\mathrm{start}}}{}'' \cdots \mathrm{x}_{\mathrm{k}_{\mathrm{k,post}}^{\mathrm{end}}}{}''\right] \tag{7}$$

with corresponding mean μ_k^{post} and standard deviation σ_k^{post}.

3.1.4 Threshold for significance

Arguably the most important step is to set thresholds what levels of change in amplitude account for both step and spike. The threshold for each interval is defined by the standard deviation of the periods before and after the change event, 'pre' and 'post as follows:

$$\Delta_{\mathrm{k}} = \epsilon \cdot \max\{\sigma_{\mathrm{k}}^{\mathrm{pre}}, \sigma_{\mathrm{k}}^{\mathrm{post}}\} \tag{8}$$

Where ϵ is the deviation level factor, which is different for steps ϵ^{step} and spikes ϵ^{spike}, resulting in Δ_k^{step} and Δ_k^{spike}.

A <u>step</u> is detected if the difference of the measurement at the beginning and end of the interval is larger than the threshold:

$$\left|x_{n_k^{end}} - x_{n_k^{start}}\right| > \Delta_k^{step} \tag{9}$$

A second condition is that the difference between the mean of the pre- and post transient level must be larger than the same threshold:

$$\left|\mu_k^{pre} - \mu_k^{post}\right| > \Delta_k^{step} \tag{10}$$

A <u>spike</u> is detected if the difference of the measurement at the beginning and end of the interval is <u>smaller</u> than the threshold:

$$\left|x_{n_k^{end}} - x_{n_k^{start}}\right| < \Delta_k^{spike} \tag{11}$$

A second condition for the spike is that the difference between the mean of the pre- and post transient level must be smaller than the same threshold:

$$\left|\mu_k^{pre} - \mu_k^{post}\right| < \Delta_k^{spike} \,. \tag{12}$$

3.1.5 Graphical explanation

Figure 2 shows an exemplary data trend that includes a step and gives the key variables of the previous section. The top panel shows the time trend with linear trend removed and after filtering. The step is detected between samples 17 and 20 which are marked as n_k^{start} and n_k^{end} respectively. The periods before and after the interval are eight samples long, marked as grey dots and are labeled 'pre' and 'post'. The mean value of the pre and post periods μ_k^{pre} and μ_k^{post} are used to differentiate between steps and spikes. The bottom panel shows the difference vector d_n for the selected time trend.

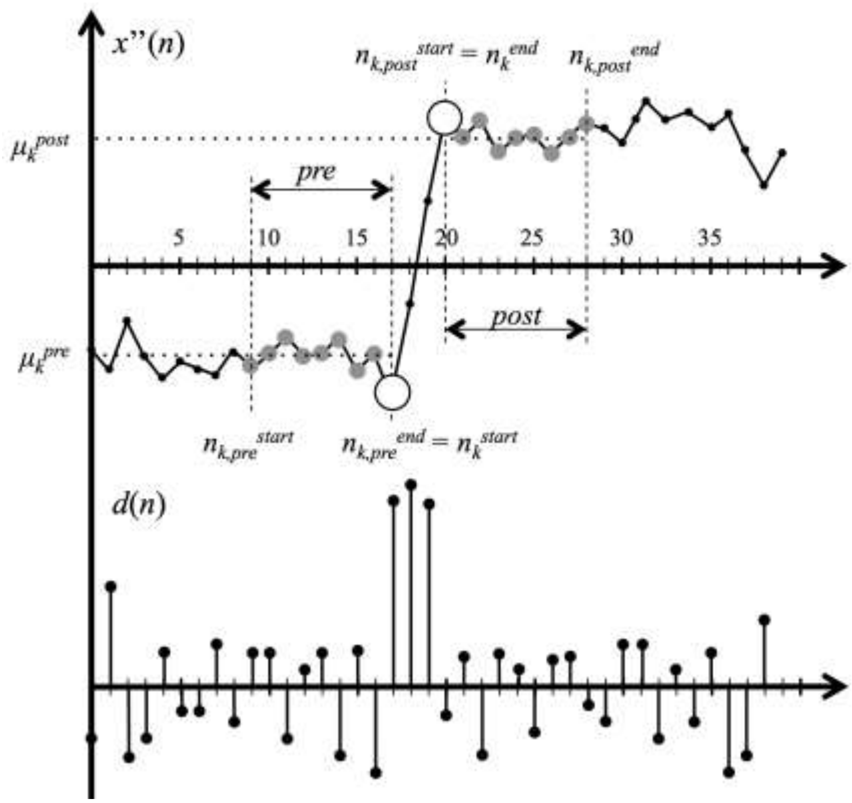

Figure 2. *Graphical representation of an exemplary time trend, linear trend and mean removed and filtered. Bottom panel shows the difference vector* d.

<u>3.2 Step and Spike Removal Algorithm</u>

As the aim of this work is to improve the use of oscillation detection using autocorrelation functions (ACF), it is important to note that the method of ACF requires a level of stationarity as a preliminary. The step removal algorithm aims to improve the stationarity by replacing spikes and steps.

The step removal method consists of three stages illustrated by **Figure 3**. First, the mean and linear trends are removed from the signal as defined in the previous section detailing the detection. Thus, the algorithm starts with vector x'. From this signal, a baseline containing steps and slow drifts is computed using a median filter with filter length T_p:

$$b_n = median(x_{n-T_p/2} \dots x_{n+T_p/2})$$

The median is defined as the value in the middle if the data set is sorted in ascending or descending order. This baseline is subtracted to remove steps and slow drifts from the signal.

$$y_n = x'_n - b_n$$

Note that median filters are traditionally used to remove outliers (Tukey, 1977). Applying a median filter with a window length equal to the oscillation period T_p to a zero mean periodic signal leads to an identically null filtered signal. The reason is that a median value evaluated over a complete cycle of a periodic signal is equal to its mean value. It follows that the periodic part of the signal is removed. Therefore, the baseline only contains the steps and slow drifts of the original signal. Subtracting the baseline from the signal reveals oscillations and other fine deviations other than steps or slow drifts.

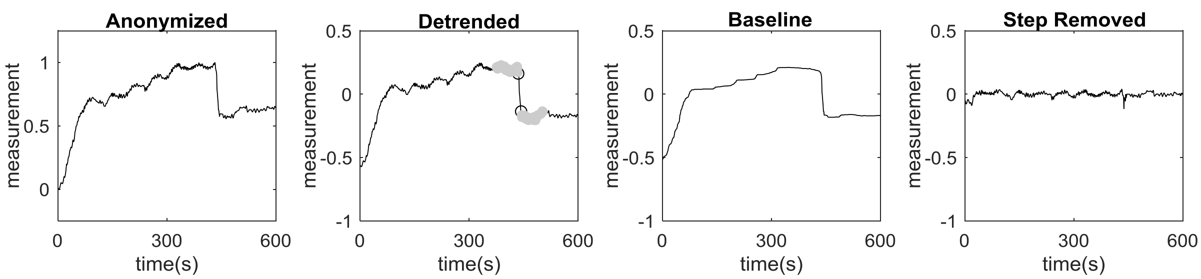

Figure 3. *Step removal method. Pre-transient and post-transient areas are marked in thick grey lines.*

The spike removal algorithm follows the same procedure as the step removal, that is, mean and the linear function are subtracted from the time trend and a median filter is applied. Then, time intervals where a spike is detected are replaced by an averaged value of sample points taken over the pre- and post-intervals where no spike occurs. The start and end of the spike intervals were stored in n_k^{start} and n_k^{end}. This method requires the signal to be stationary, i.e. without steps or drifts, in order to ensure that transient free cycles of the time series are similar and that their averaged values are a good estimate of the transient time intervals. The spike removal method is illustrated in **Figure 4**.

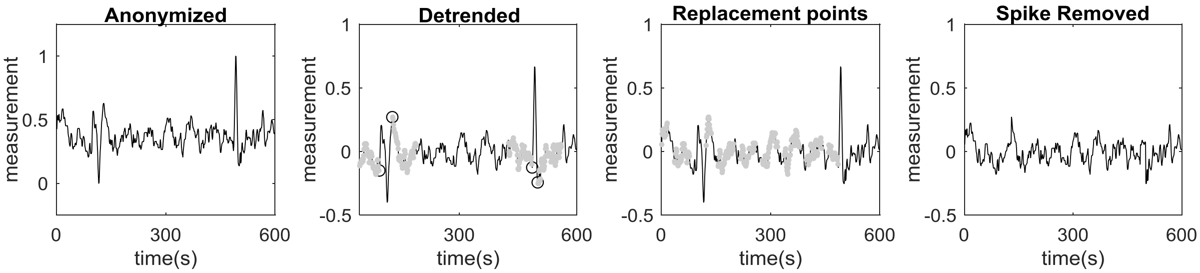

Figure 4. *Spike removal method. Two spikes are occurring where the second spike rises and falls quickly. The first spike is less pronounced and somewhat masked by the oscillation.*

4. PARAMETER SETTINGS

The objective of the spike and step removal is to improve other detection methods, such as oscillation detection. These methods do not work well in the presence of spikes and steps. A measurement for the correct identification of oscillations is therefore introduced to measure the success of the spike and step removal. The parameters of the step and spike removal algorithms are optimised so that oscillations are detected successfully.

This section analyses the sensitivity of the proposed methods to their respective tuning parameters. It also provides suggestions for selecting default parameters. A set of experiments is performed on a dataset collected from a real-world industrial process. The dataset consists of measurements generated by pressure, flow and temperature sensors. Through visual inspection, 219 signals are found to be oscillatory, nine signals include steps and 39 include spikes. The F_1 score (Rijsbergen & J., 1979) is used to evaluate the performance of the proposed detection method. The F_1 score is a metric used to evaluate the performance of binary classification methods and is defined as follows:

$$F_1 = 2 \times \frac{P \times R}{P + R}$$

with precision P defined as

$$P = \frac{N_C}{N_O}$$

where N_C is the number of correctly detected oscillatory measurements and N_O is the number of all measurements detected as oscillatory. Recall R is defined as

$$R = \frac{N_C}{N_A}$$

where N_A is the number of actual measurements that show an oscillation.

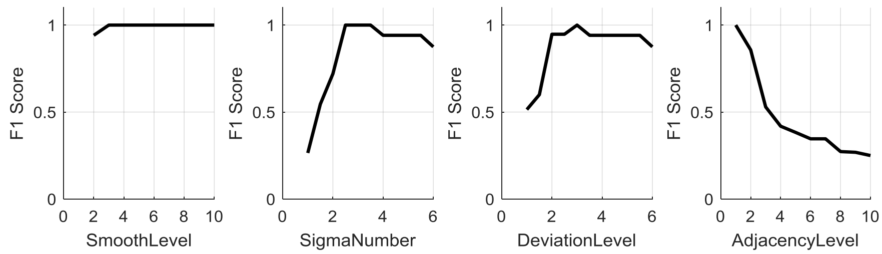

Figure 5. F_1 score evaluated for various values of the step detection parameters. Parameters are dimensionless values.

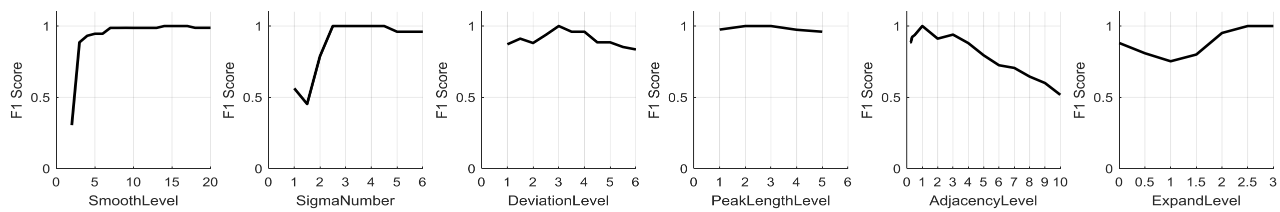

Figure 6. F_1 Score evaluated for various values of the spike detection parameters. Parameters are dimensionless values.

Figure 5 and **Figure 6** illustrate respectively the effect of the value of the parameters used in the step and in the spike detection methods based on their influence on the F_1 score value. During each test, a single parameter is varied while the others are set to their recommended values. After running the step and the spike detection method with all possible combinations of parameters, two sets of recommended default parameter settings are provided in **Table 1**. The spike and step removal is considered successful when it leads to the correct detection of oscillations. As there are 39 spikes and nine steps in the data sets, this means that all of them have to be correctly identified. In addition, only those occurrences of steps and spikes must be detected and no others. If this is the case, then the F_1 score will be equal to one.

Table 1: *Recommended parameter settings for step and spike detection methods.*

Parameter	**Description**	**Recommended value step detection**	**Recommended value spike detection**
α	Smoothing level of moving average filter, factor influencing the window length of the mean filter	10	15
$\beta^{fast}, \beta^{mod}$	Deviation threshold factor to detect fast and moderate changes (moderate changes for spikes only)	3, n.a.	3, 2.5
γ	Adjacency level factor to define length of pre- and post transients	1	1
δ	Adjacency level factor to define acceptable length between intervals, for spikes only	n.a.	2
$\epsilon^{step}, \epsilon^{spike}$	Deviation level to define detection threshold	3	3

5. TEST EXPERIMENT ON SIMULATED DATASET

This section describes the results of the proposed transient detection and removal methods on simulated data. Seven datasets are generated corresponding to different scenarios of transients and disturbances (oscillatory signal/ oscillatory signal with white noise and/or with a baseline drift). In **Figure 7**, from left to right, the columns depict the raw signal, the signal after step removal, the signal after step removal rescaled for better visualization and the signal after spike removal. If step and spike are both present in a signal, a step removal is performed first, then a spike removal follows. In **Figure 7** dataset 'Data1' is a sinusoidal signal with a step. After step removal and rescaling (row one, column three) a "residual" spike can be observed. This "residual" spike is present because the step magnitude is significantly greater than the oscillation magnitude. The step removal is then corrected by a spike removal (row one, column four). Dataset 'Data2' is a sinusoidal signal with a step and white noise. From **Figure 7** (row two, column three), we can see the proposed transient detection and removal methods work well despite the presence of noise. Dataset 'Data3' is a sinusoidal signal with two consecutive steps and white noise. The transient detection and removal method are able to remove both steps (row three, column four). Dataset 'Data4' is a sinusoidal signal with a baseline drift and a spike. As no step is present in the signal, the step detection and removal methods have no effect on the signal (row four, column three). The spike detection and removal methods completely remove the spike (row four, column four) despite the presence of the drift. Dataset ‘Data5’ is a sinusoidal signal with a drift, two consecutive spikes and white noise. Both spikes are removed by the proposed transient detection and removal methods despite the presence of noise and baseline drift.

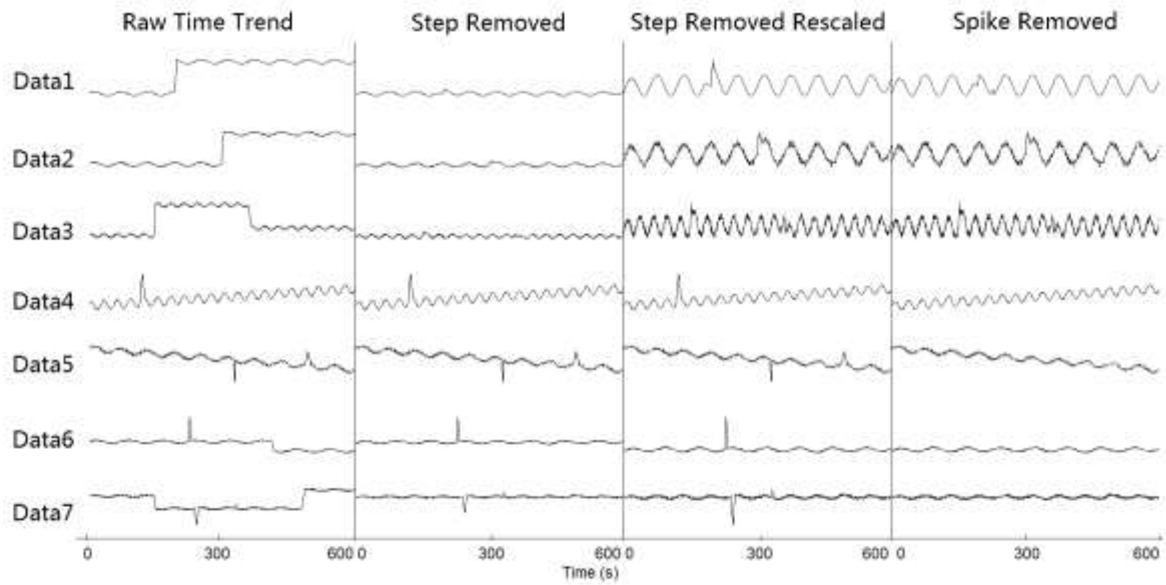

Figure 7. *Proposed transient removal methods are applied to simulated oscillatory signals including steps and spikes.*

Dataset ‘Data6’ is a sinusoidal signal with a spike followed by a step. The step is first removed (row six, column two). Then the spike is removed in (row six, column four). Dataset ‘Data7’ is a sinusoidal signal with two steps and spikes for which all the transients are removed by the proposed method (row seven, column four). Datasets ‘Data6’ and ‘Data7’ illustrate the ability of the proposed method to remove combinations of transients affecting an oscillatory signal.

6. INDUSTRIAL CASE STUDY

The advantage of using the proposed transient detection and removal is evaluated in this section. The increase in accuracy of both the Auto-Correlation Function (ACF) and the transfer entropy methods is quantified. The analysis is conducted on a 1,3-Butadiene purification section of a chemical plant located in Germany.

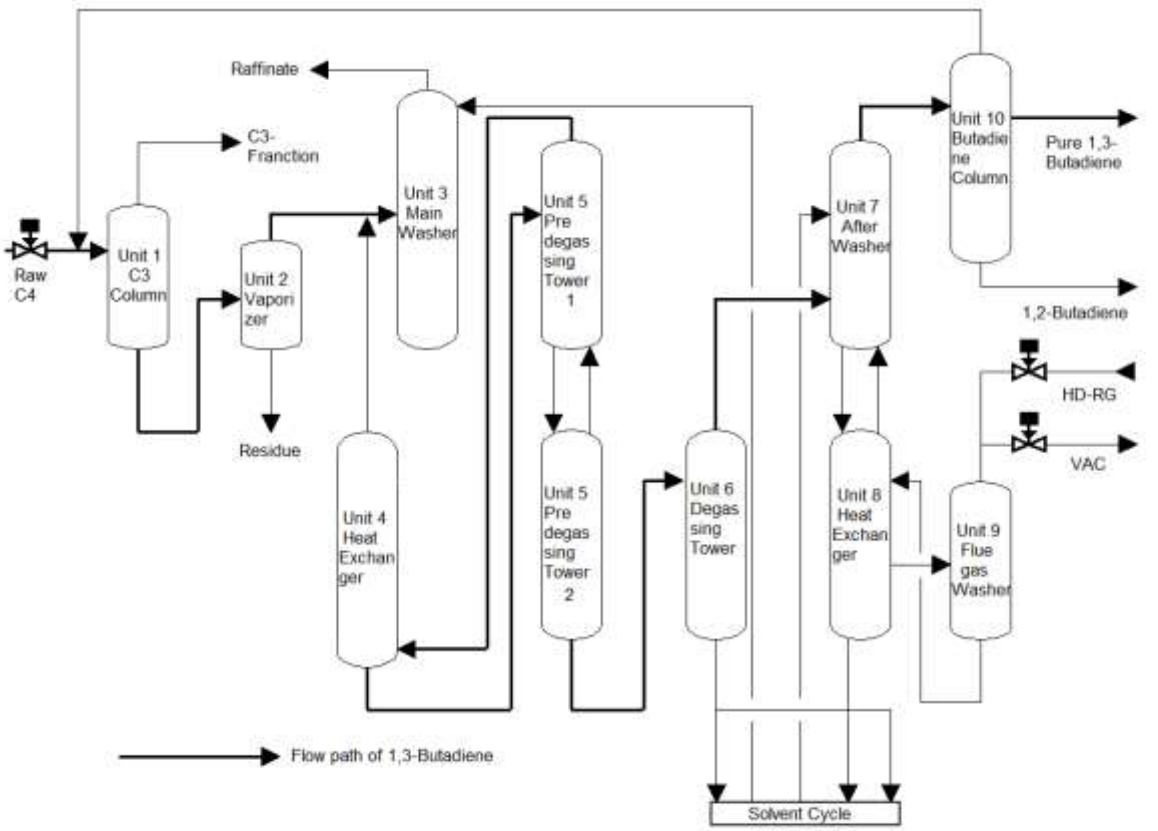

__Figure 8__. Simplified process schematic of a 1,3-Butadiene process.

An overview of the simplified process schematic of the 1,3-Butadiene process is provided in **Figure 8**. The process input consists of a flow of raw C4. Pure 1,3-Butadiene is obtained after separation of impurities, e.g. C3 fraction, raffinate, and 1,2-butadiene via two conventional and two extractive distillation units (White, 2007). The process data is presented in an Excel file with a one-minute sampling time. Some examples of collected process data are provided in **Figure 9**.

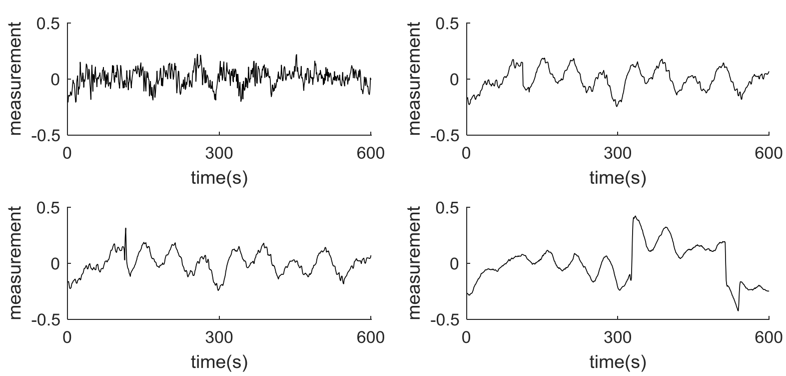

***Figure 9.** Examples of oscillatory process variables.*

The analysed dataset contains 670 signals in total. Forty eight signals are discarded from the analysis due to high compression rate. Through visual inspection, 219 process variables are considered as oscillatory and 403 as non-oscillatory through visual inspection. The 219 oscillatory signals consist of 115 flow measurements, 43 level measurements, 11 pressure measurements, 43 temperature measurements and 7 quality measurements. The 219 oscillatory signals exhibit a similar oscillation with a time period close to 60 minutes and originate from various plant units, suggesting that the oscillations might result from the propagation of the same root cause. Process units affected by the oscillatory plant-wide disturbance are listed in **Table 2**.

Table 2. *Process units affected by the plant wide oscillatory disturbance.*

Unit index (refer to Fig. 8)	1	2	3	4	5	6	7	8	10	other units
Number of oscillatory signals	25	8	37	17	36	37	17	2	20	20

6.1 Improvement of oscillation detection with transient removal

Description of the experimental tests

The improvement gained when using the proposed transient removal methods is demonstrated by comparing the performance of the ACF method (Thornhill, et al., 2003) in two conditions, with and without applying transient removal.

The ACF method is first applied with a broad band pass filter. Filter cut-off frequencies are set to values significantly distant from the estimated value of the oscillation frequency $2\pi/T_p$ ensuring that no spurious oscillations are generated by the filter (Thornhill, et al., 2006). The result (Error! Reference source not found.**4**) indicates missed and misclassified oscillation of signals with transients. Next, the ACF method is used with a narrow band-pass filter to show that transient disturbances cannot be removed no matter how the filter is configured. Furthermore, the performance of oscillation detection is degraded because spurious oscillations are generated due to the filter settings. Finally, when transient removal is applied to the signals prior to using the ACF method, the result shows that all oscillatory signals are properly detected and clustered.

More specifically, the cut-off frequencies of the broad band-pass filter are set to $[17\ 120]$ minutes ($[1.39\ 9.80] \times 10^{-4}$Hz) and the bandwidth ($8.42 \times 10^{-4}$Hz) satisfies the requirement of minimum band width (2.24×10^{-4}Hz) of the ACF method (Thornhill, et al., 2006): $\mathrm{bandwidth} > \mathrm{f_{filtercentre}}/2.5$. The cut-off frequencies of the narrow band-pass filter are $[35\ 67]$ minutes ($[2.49\ 4.75] \times 10^{-4}\mathrm{Hz}$) and the bandwidth of the narrow filter ($2.27 \times 10^{-4}\mathrm{Hz}$) satisfies the requirement of minimum bandwidth ($1.45 \times 10^{-4}\mathrm{Hz}$). The lower cut-off frequency ($67\ \mathrm{min}, 2.49 \times 10^{-4}\mathrm{Hz}$) of the narrow band-pass filter is relatively close to the oscillation frequency ($60\ \mathrm{min}, 2.78 \times 10^{-4}\mathrm{Hz}$). This leads to generation of spurious oscillations that adds to the 60 min oscillation present in the signal (Thornhill, et al., 2006). Finally, the proposed approach to remove transient disturbances is used prior to applying the ACF method with filter settings identical to the broad band-pass filter ($[17\ 120]\mathrm{min}, [1.39\ 9.80] \times 10^{-4}\mathrm{Hz}$).

6.2.2 Case study results

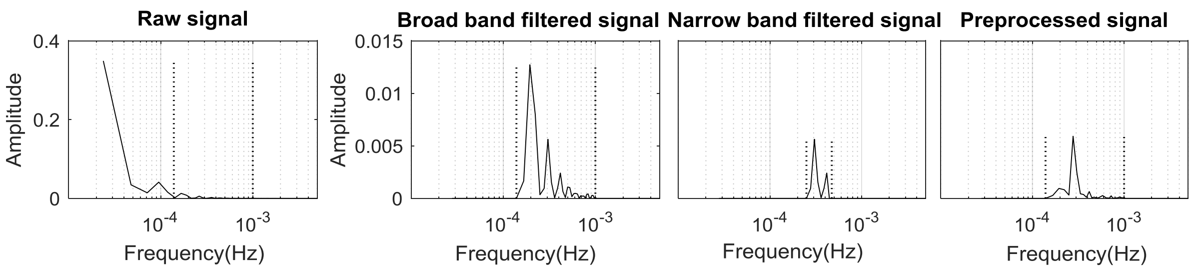

Figure 10. *Power spectrum of the measurement used by the step detection and removal methods, before transient removal (first three panels) and after transient removal (fourth panel).*

In **Table 3**, the number of oscillatory measurements detected at the actual frequency of $60\ \mathrm{min}, 1.66\ 10^{-4}\mathrm{Hz}$, the number of oscillatory measurements detected at an incorrect frequency, as well as the undetected oscillations and the false positives (false alarms) based on a visual inspection of the dataset are provided.

If transients are not removed before applying the ACF method, six signals are misclassified, i.e. their oscillation time period is wrongly estimated and therefore they are grouped into a wrong oscillation cluster. Performance improvements of the ACF method with transient removal compared to the ACF method without transient removal (both with broad band-pass filter) in term of correctly detected oscillatory signals is 7.4% (15 signals) and 24.4% (10 signals) in term of false alarms. Note that a misclassification also affects the root cause analysis as root cause analysis is performed within each cluster and therefore the obtained diagnostic can be misled. Visual inspection of the misclassified and missed oscillatory signals shows that they exhibit transient changes. This means that transient changes can affect clustering. The reason why transient changes can affect oscillation detection is revealed in **Figure 10**, which shows that some spectral components of the transient being relatively close to the oscillation frequency cannot be removed by linear filtering as illustrated by the narrow-filtered signal power spectrum (third panel).

Alternatively, the power spectrum of the signal after applying the proposed approach shows an effective removal of the spectral components close to the oscillatory frequency (fourth panel).

Table 3. *Influence of transient removal on the performance of the ACF method.*

	Filter	**Correctly detected**	**Misclassified**	**Missed**	**False alarms**
Without transient removal	Broad	204	6	9	41
Without transient removal	Narrow	209	10	0	159
With transient removal	Broad	219	0	0	31

6.2 Improvement of root cause analysis with transient removal

Description of the experimental tests

The improvement gained by using the proposed transient removal methods is demonstrated by comparing the outcome of a root cause analysis using the transfer entropy method on raw oscillatory signals and on oscillatory signals with transient removal. The root cause analysis using the transfer entropy method is applied to each unit of the 1,3-Butadiene process described in Section 6.1. For each unit, the oscillatory signals detected using the ACF method as described in Section 4.2. Three root cause analysis are conducted at the unit level. First on the vaporiser unit, then on the pre-degassing towers unit and finally on the steam distribution unit.

Case study results

Root cause analysis on vaporiser unit. Oscillating process variables detected by the ACF method in Section 6.2 and belonging to the vaporiser unit are displayed on a simplified process schematic in ***Figure 11***. The oscillatory process variables are marked in dark circles while the non- oscillatory process variables are marked in grey circles. Note that the oscillatory process variables are connected to each other through the process flow.

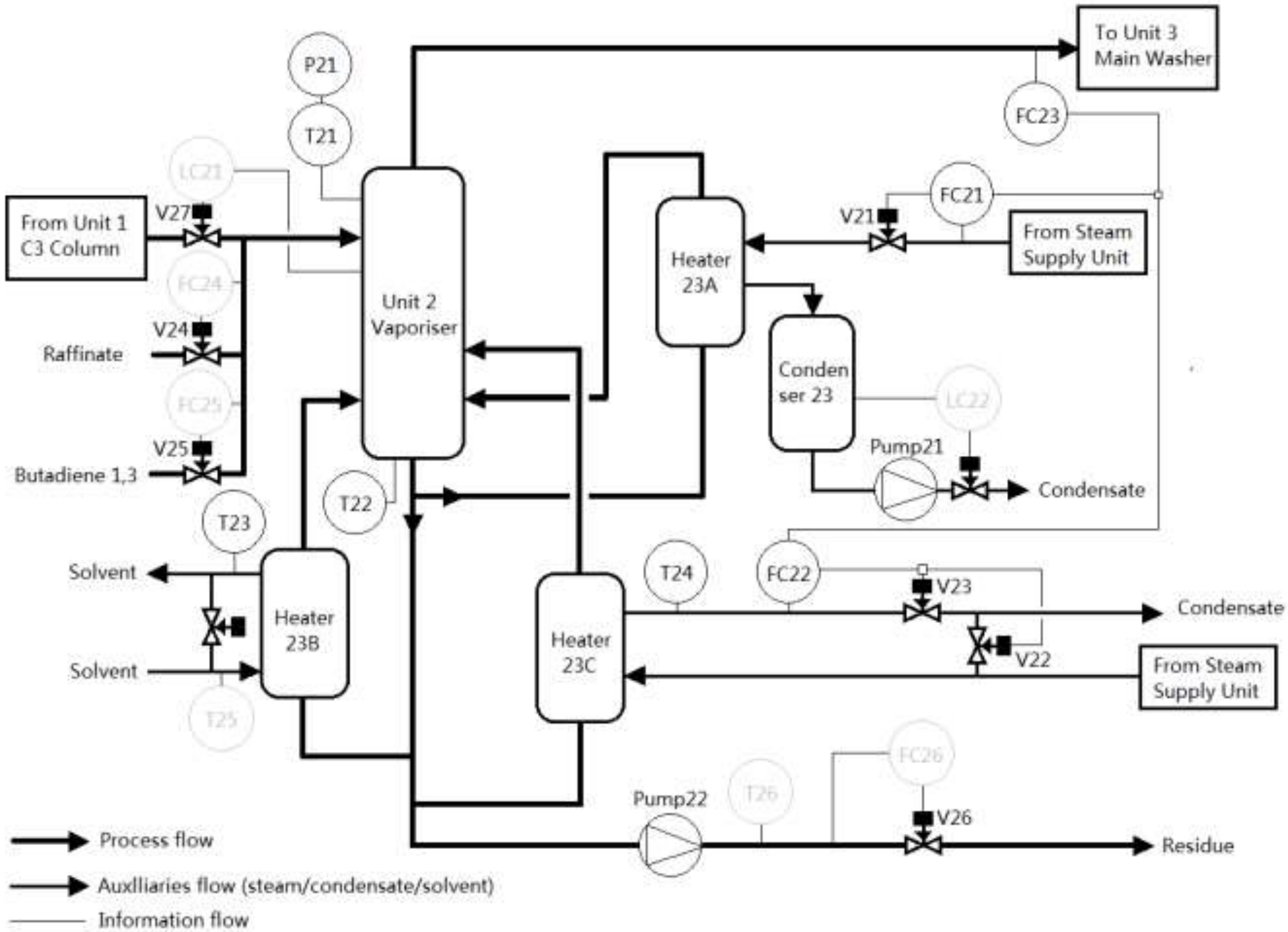

Figure 11. *Simplified process schematic of the vaporiser unit indicating the location of detected oscillatory measurements (dark circles), non-oscillatory measurements are marked in grey circles.*

The time trends of the oscillatory signals belonging to the vaporiser unit are shown in **Figure 12**. **Figure 14** shows the oscillatory signals after applying transient removal. Transfer entropy is computed pairwise between a given oscillatory measurement and all the other oscillatory measurements belonging to the vaporiser unit. Trends in **Figure 12** and **Figure 14** are sorted according to the value of the computed transfer entropy. Finally, propagation paths are obtained in the form of causality maps. Causality maps are constructed by connecting the measurements with directed lines if a significant causal relationship is detected by the pairwise computed transfer entropy and if there exists a physical connection between this pair of measurements. The causality map obtained on measurements without applying transient removal is shown in **Figure 13**, while the causality map obtained on measurements on which transient removal is applied is shown in **Figure 15**.

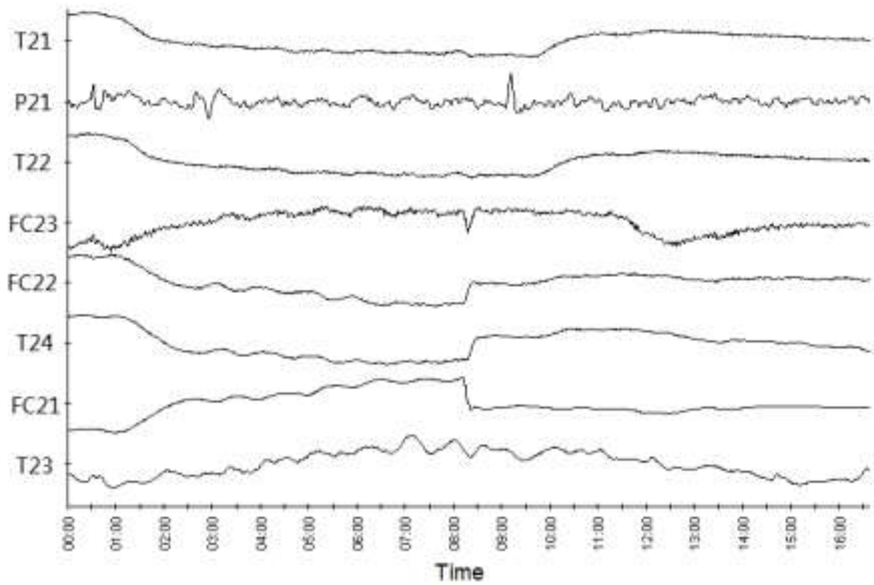

Figure 12. *Time trends of oscillatory measurements detected in the vaporiser unit without transient removal and sorted according to the transfer entropy criteria.*

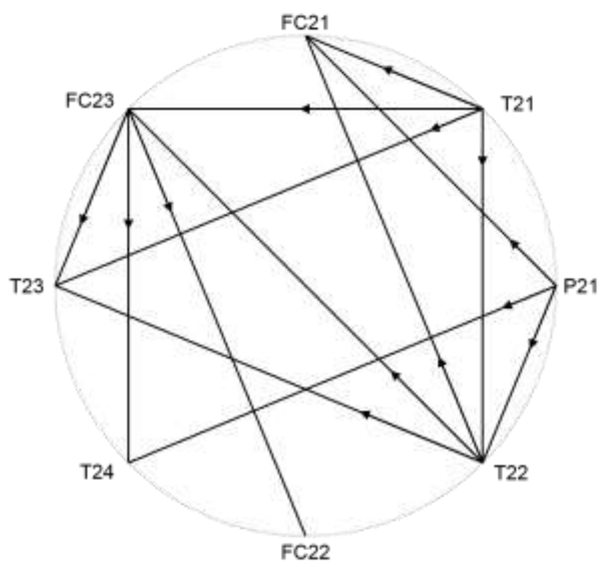

Figure 13. *Causality map of the oscillatory measurements detected in the vaporiser unit obtained without transient removal.*

From **Figure 13** and **Figure 15**, the root cause analysis of the oscillatory disturbance affecting the vaporiser unit when using raw time trends, i.e. without transient removal, points towards the temperature and the pressure measured at the top of the vaporiser column as being the closest to the root cause of the oscillation. The causality map in **Figure 15** and the process schematic in **Figure 11** suggest that the oscillatory disturbance originates from temperature T21 and pressure P21 since the measurements located upstream of T21 and P21 i.e. LC21, FC24 and FC25 are not oscillatory. The oscillatory disturbance is transmitted first to T22 and FC23 then to T23, T24 FC32 and FC22. The root cause analysis conducted on the raw time trends suggests therefore that the oscillatory disturbance originates from within the vaporiser.

On the other hand, the root cause analysis of the oscillatory disturbance affecting the vaporiser unit when using the proposed transient removal method, points towards two flow measurements both originating from the steam supply unit FC21 and FC22.

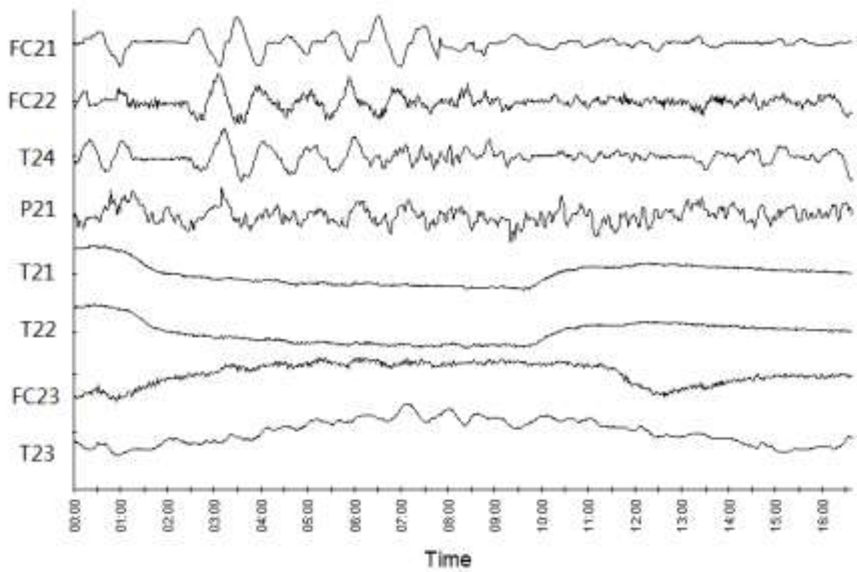

Figure 14. *Time trends of oscillatory measurements detected in the vaporiser unit after transient removal and sorted according to the transfer entropy criteria.*

The causality map of the reconstructed data and the process schematic suggests that the oscillation originate from the steam supply FC21 and FC22, propagates to the central vaporiser column where it affects the top-side column pressure P21 and temperature T21 and further to the flow FC23. Additionally, the oscillation travels to the bottom-temperature T22 and further affects the solvent temperature T23. The root cause analysis conducted on the pre-processed oscillatory signal using the proposed transient removal method suggests therefore that the oscillatory disturbance originates from the steam supply unit i.e. not from the process itself but rather from the auxiliary system.

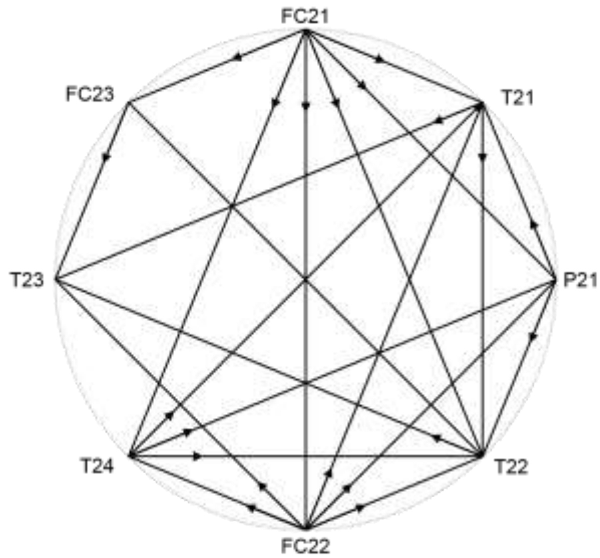

Figure 15. *Causality map of the oscillatory measurements detected in the vaporiser unit obtained after transient removal.*

Root cause analysis on pre-degassing unit

Oscillating process variables detected by the ACF method in Section 6.2 and belonging to the pre-degassing unit are displayed on a simplified process schematic in **Figure 16**. The oscillatory process variables are marked in dark circles while the non- oscillatory process variables are marked in grey circles.

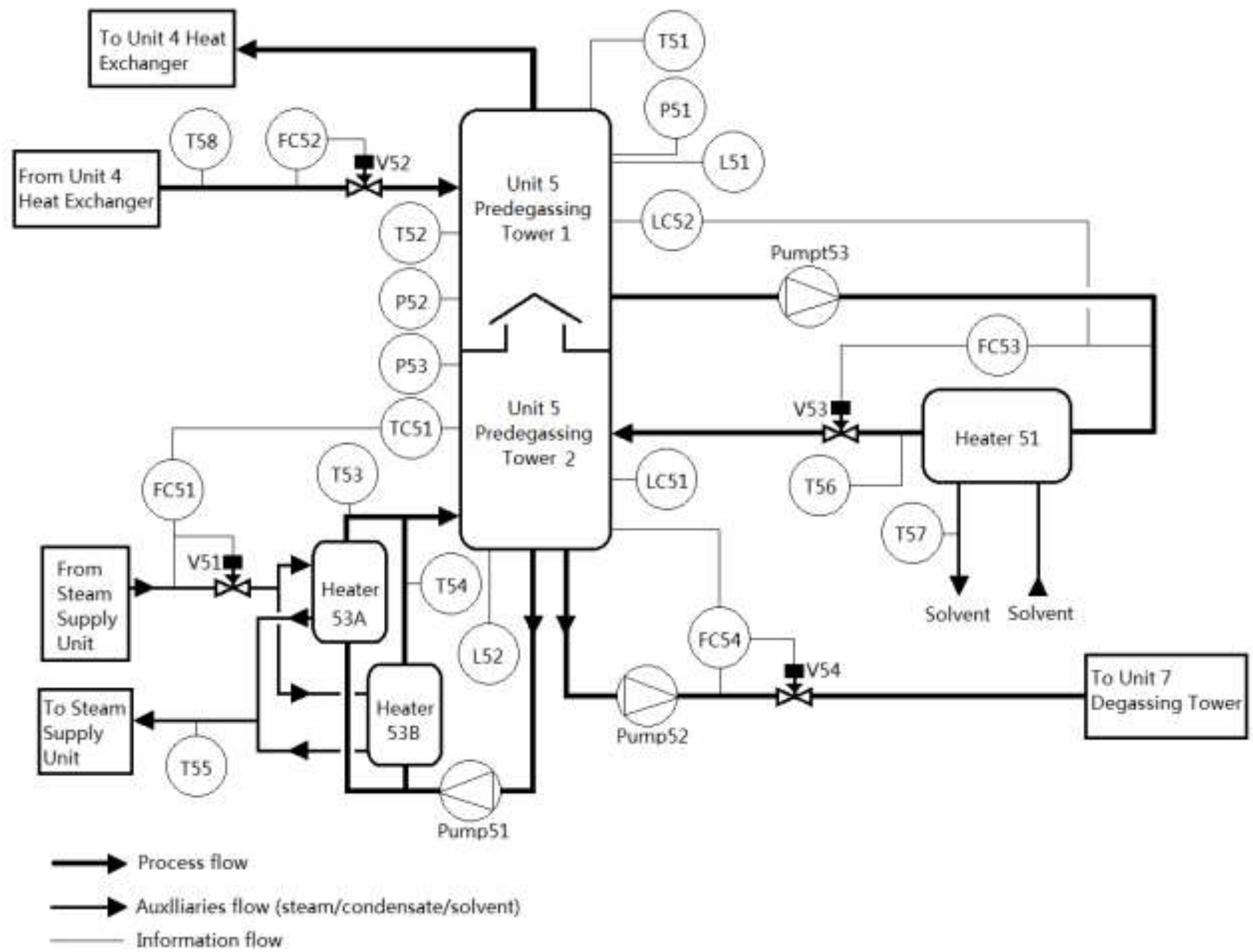

Figure 16. *Simplified process schematic of the pre-degassing unit indicating the location of detected oscillatory measurements (dark circles), non-oscillatory measurements are marked in grey circles.*

The time trends of the oscillatory signal belonging to the pre-degassing unit are shown in **Figure 17**. **Figure 19** shows the same oscillatory signals after applying the proposed transient removal method. Trends are again sorted according to the value of the computed transfer entropy. The causality map resulting from the analysis of oscillatory measurements without transient removal is shown in **Figure 18**, the causality map resulting from the analysis of oscillatory measurements on which transient removal is applied after transient removal is shown in **Figure 20**.

From **Figure 18** and **Figure 20**, the root cause analysis of the oscillatory disturbance affecting the pre-degassing unit using oscillatory measurements without transient removal suggests that either the steam supply FC51, the temperature T56 (together with the solvent temperature T57), or the C4 flow FC52 (together with temperature T58) could all potentially be the closest measurements to the root cause of the oscillatory disturbance. This result is consistent with the analysis conducted on the vaporiser unit that pointed to the steam supply unit as a potential location of the root cause of the oscillatory disturbance. The C4 flow FC52 originates from the heat exchanger unit (Unit4 in **Figure 8**). A closer look at the measurements of the process variables related to the solvent reveals that the solvent source is not oscillatory, meaning that it cannot be the root cause of the oscillatory disturbance under investigation.

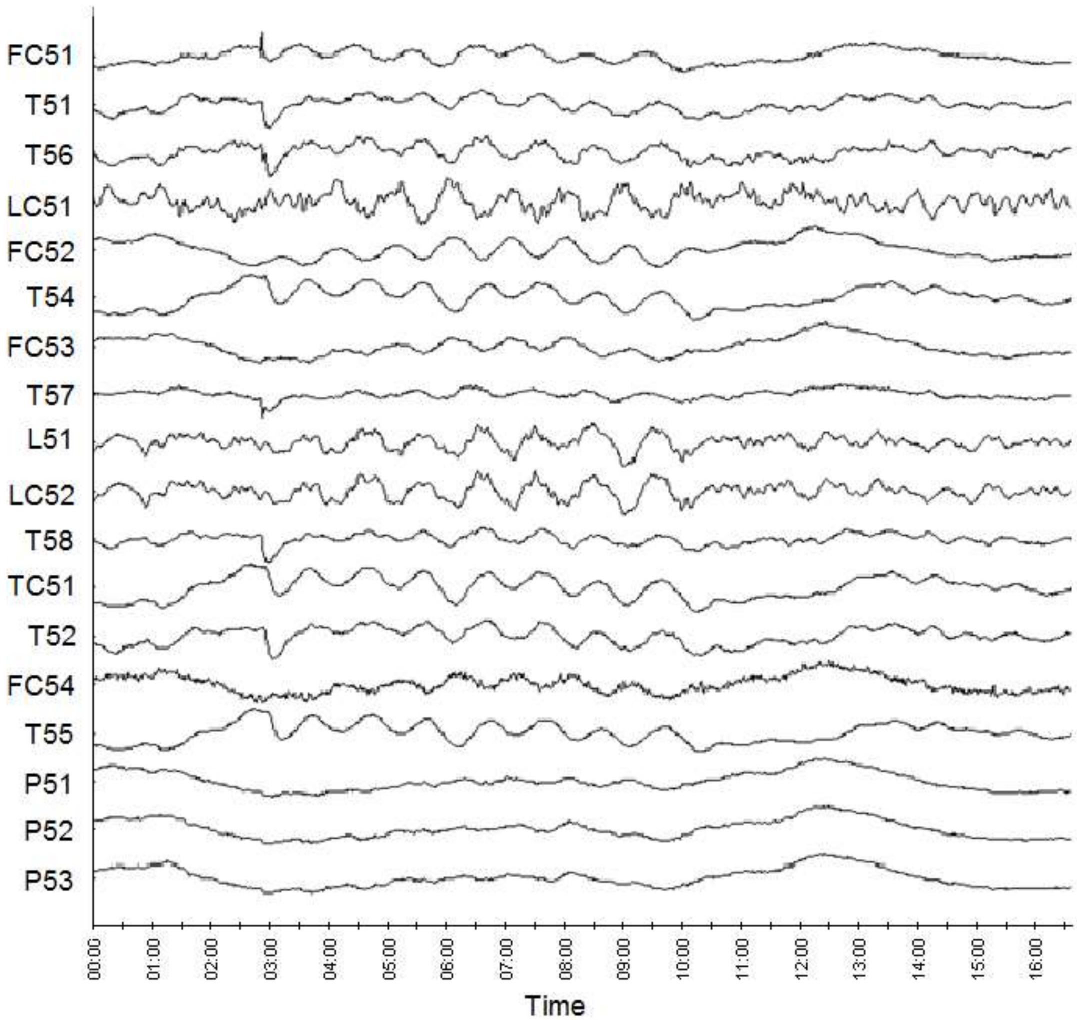

Figure 17. *Time trends of oscillatory measurements detected in the pre-degassing unit without transient removal and sorted according to the transfer entropy criteria.*

The root cause analysis of the oscillatory disturbance affecting the pre-degassing unit when using the proposed transient removal method suggests conclusions similar to the root cause analysis conduction on raw oscillatory signals with a slight difference that a significant causal relationship between the steam supply FC51 and the temperature T56 is revealed.

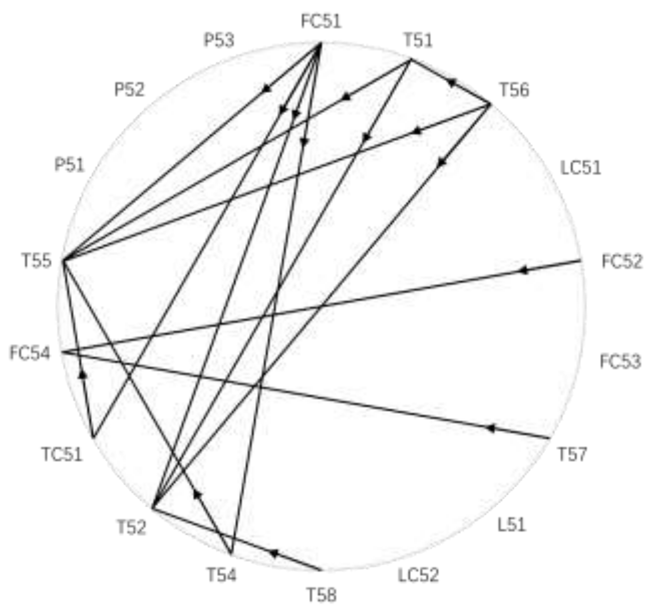

Figure 18. *Causality map of the oscillatory measurements detected in the pre-degassing unit obtained without transient removal.*

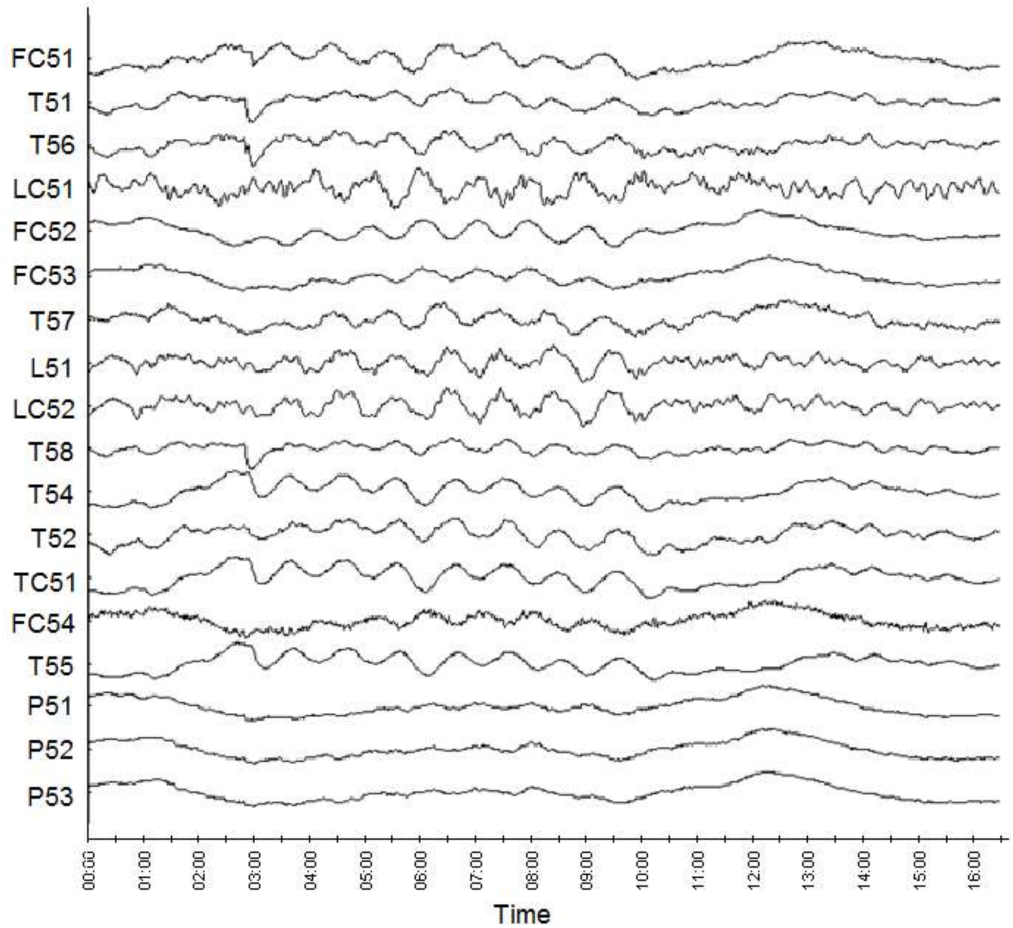

Figure 19. *Time trends of oscillatory measurements belonging to the pre-degassing unit after transient removal and sorted according to the transfer entropy criteria.*

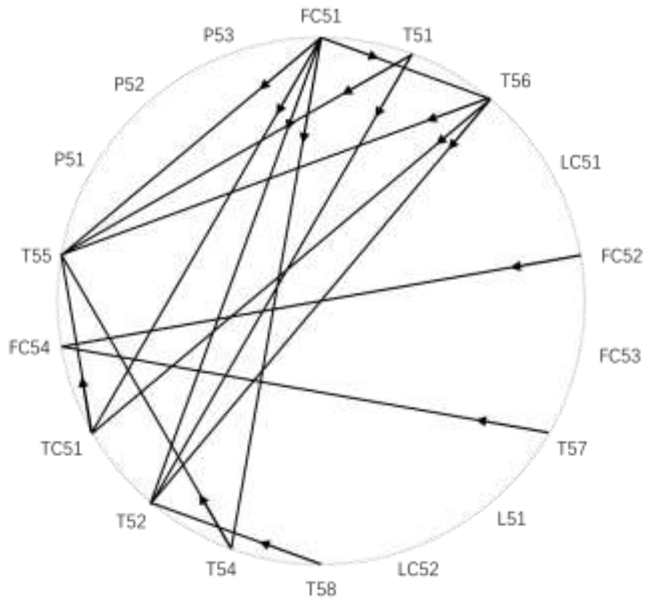

Figure 20. Causality map of the oscillatory measurements detected the pre-degassing unit obtained after transient removal.

In summary, both root cause analysis conducted on the pre-degassing oscillatory signals with and without transient removal suggest that the oscillatory disturbance originates from the steam supply unit.

Root cause analysis on steam supply unit

The analysis conducted on two of the 1,3-Butadiene process units pointed to the steam supply unit as a possible location for the root cause of the oscillatory disturbance affecting 219 process variables. It is important to note that auxiliary systems, because of their plant wide connectivity, can propagate disturbances across multiple units of a process. The oscillatory measurements collected from the steam supply unit are displayed on a simplified process schematic in **Figure 21**. Again, the oscillatory measurements are marked in dark circles, the non-oscillatory measurements are marked in grey circles.

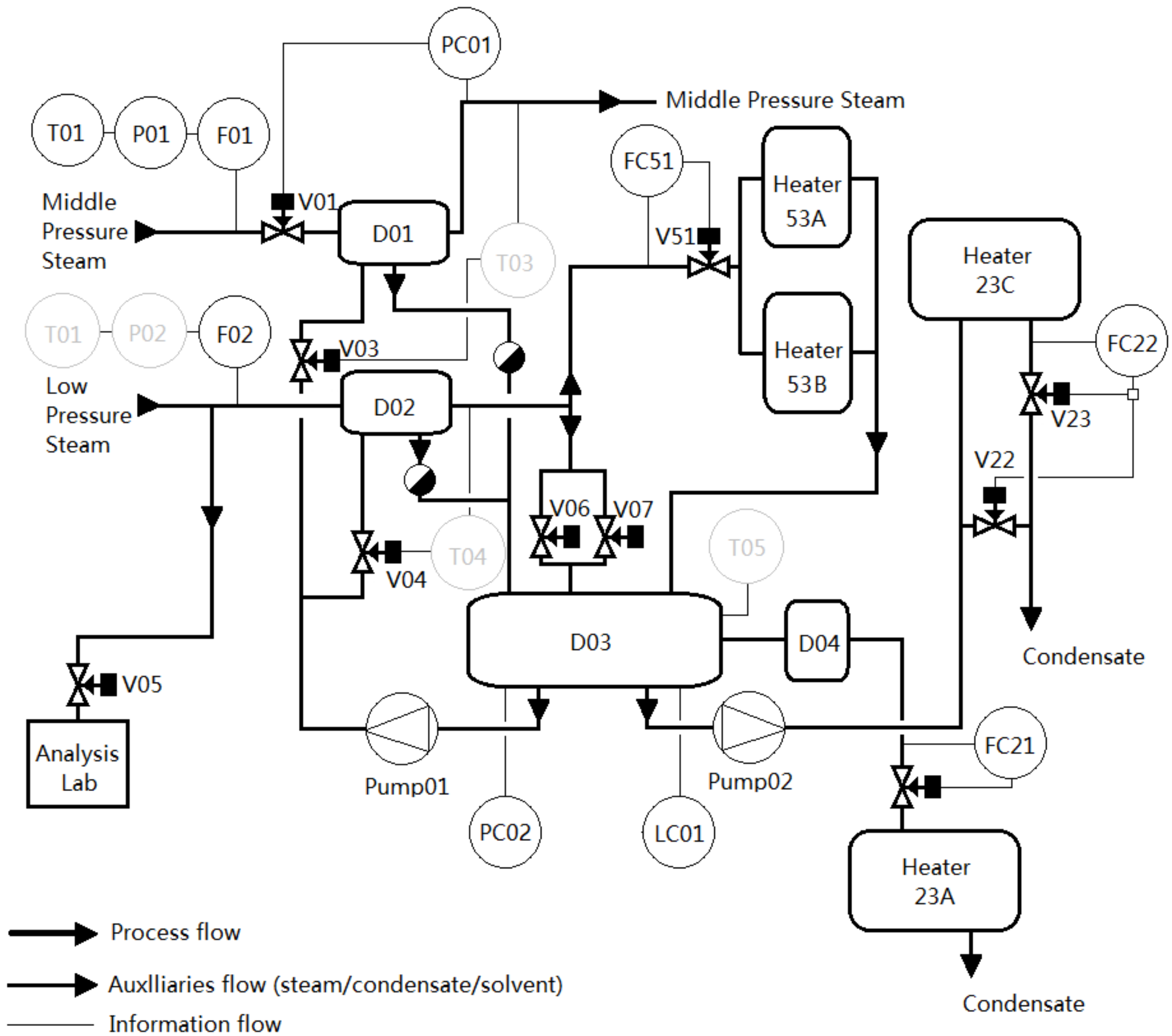

Figure 21. *Simplified process schematic of steam unit indicating the location of detected oscillatory measurements (dark circles), non-oscillatory measurements are marked in grey circles. "D" stands for "Steam processing column".*

The time trends of the oscillatory signal belonging to the steam supply unit are shown in **Figure 22**. **Figure 24** shows the oscillatory signal after applying the proposed transient removal method. The causality map obtained on measurements without applying transient removal is shown in **Figure 23**, while the causality map obtained on measurements on which transient removal is applied is shown in **Figure 25**.

From **Figure 23** and **Figure 25** the root cause analysis of the oscillatory disturbance affecting the steam supply unit using oscillatory measurements without transient removal suggests that the steam pressures P01, PC01 and PC02 are the closest to the root cause, pointing towards the middle pressure steam header.

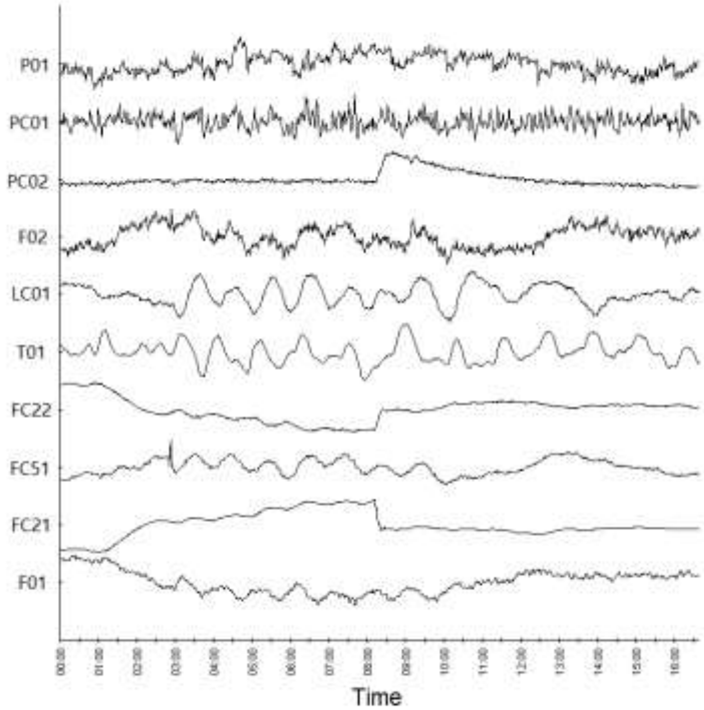

Figure 22. *Time trends of oscillatory measurements detected in the steam unit without transient removal and sorted according to the transfer entropy criteria.*

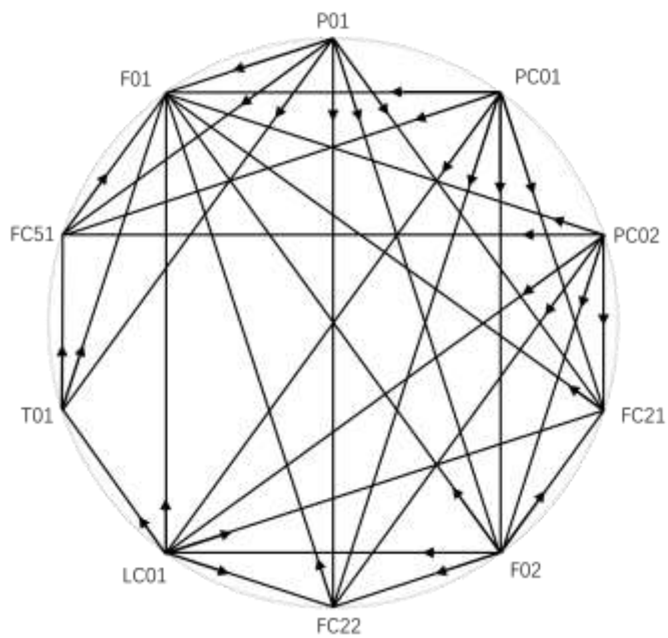

Figure 23. *Causality map of the oscillatory measurements detected in the steam unit obtained without transient removal.*

The root cause analysis of the oscillatory disturbance affecting the steam supply unit when using the proposed transient removal method suggests conclusions similar to the root cause analysis conduction on raw oscillatory signals.

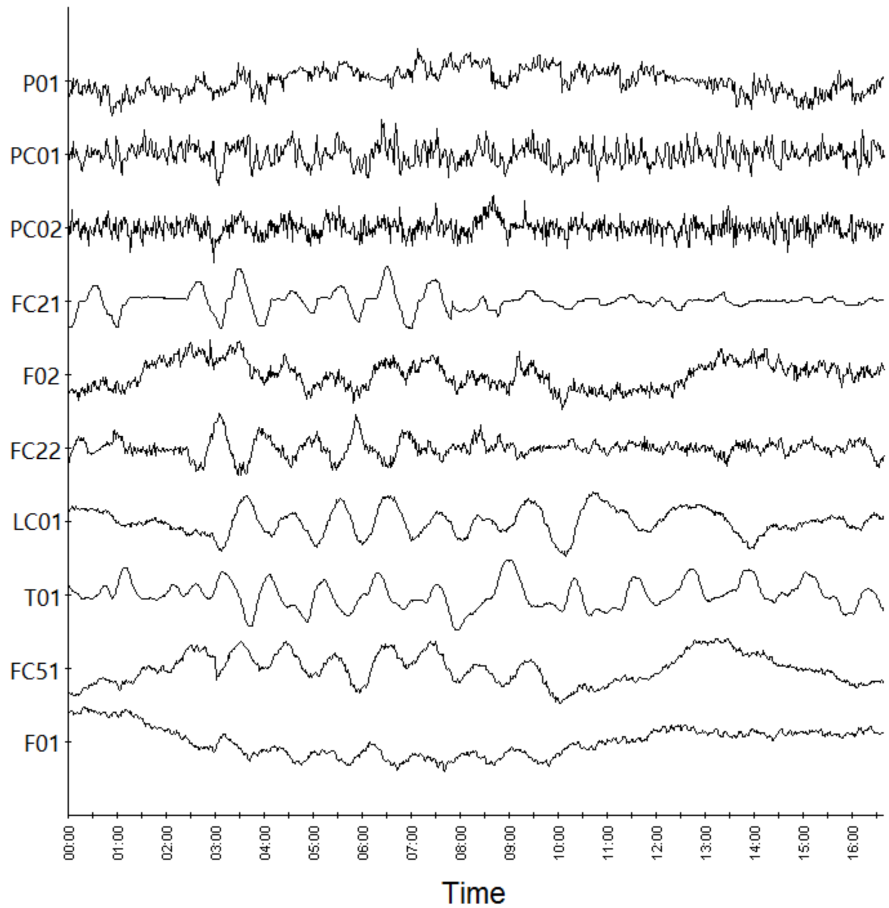

Figure 24. *Time trends of oscillatory measurements detected in the steam distribution unit after transient removal and sorted according to the transfer entropy criteria.*

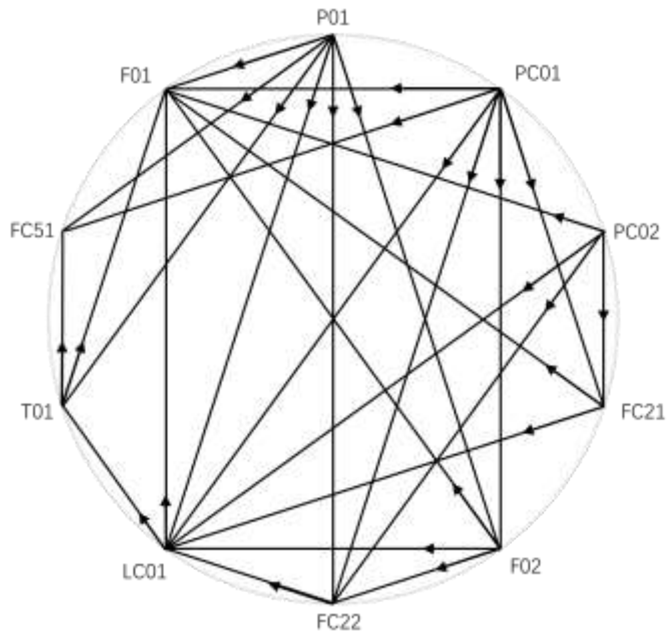

Figure 25. *Causality map of the oscillatory measurements detected in the steam unit after transient removal.*

In summary as for the case of the pre-degassing unit, root cause analysis conducted on the pre-degassing oscillatory signals with and without transient removal suggest the same root cause: the middle pressure steam header.

Conclusion on root cause analysis

The root cause analysis of the oscillation disturbance conducted on three units of the 1,3-Butadiene process pointed towards the middle pressure steam header as the source from which originates a plant wide disturbance affecting 219 of the 1,3-Butadiene process variables. For two of the unit level root cause analysis (pre-degassing unit and steam supply unit), the proposed transient detection and removal method did not modify the results obtained by the transfer entropy causal analysis. In one of the unit level root cause analysis (vaporiser unit), the proposed transient detection and removal method modified the results obtained by the transfer entropy causal analysis. It is important to emphasize that the result obtained after applying the proposed transient detection and removal method, the transfer entropy causal analysis pointed to a root cause and a propagation path that agree with the analysis conducted on the two other unit i.e. from middle pressure steam header to unit steam supply to process units. The fault propagation paths after transient removal revealed a more complete picture.

7. CONCLUSION

In this paper we proposed simple heuristic methods to detect and remove transients from oscillatory time series. Such methods are instrumental in improving the accuracy of oscillation detection and oscillation causal analysis methods. Two types of transients are considered: steps and spikes. In the proposed step detection method, the oscillatory signal is first de-trended and smoothed then, fast signal variations are detected and the amount of deviation before and after the detected fast signal change is evaluated. In the proposed spike detection method, after de-trending and smoothing, in order to capture different type of spikes with fast/slow rising and falling edges, the signal first derivative is evaluated and compared to two thresholds corresponding to a fast and a slow variation of the signal. Pairs of peaks of opposite signs that are close enough in time are grouped to form a transient time interval and the amount of deviation before and after the detected transient time interval is evaluated. In the step removal method, the mean and linear trend are removed from the signal, a baseline containing steps and slow drifts is computed using a median filter and subtracted from the signal. In the spike removal method, time intervals where a spike is detected are replaced with an averaged value of sample points taken from the time intervals where no spike occurs.

The proposed heuristic methods to detect and remove transients were used to pre-process process measurements prior to applying the auto-covariance function oscillation detection method and the transfer entropy causality analysis method. Validation of the two methods on a dataset collected from a 1,3-Butadiene process plant affected by a plant wide oscillatory disturbance demonstrated their ability to significantly improve the performance of the ACF in term of missed and misclassified oscillations reduction and of the root cause analysis using the transfer entropy method when transient changes are present in the process data.

There are still limitations to this approach and the parameter guidelines are based on the assumption that there is no simultaneous occurrence of spikes and steps, or spikes and steps lying in close proximity. In addition, the use of a single estimated oscillation period to compute a baseline in the step and spike removal algorithm (Section 3.2) limits the applicability of the proposed method to oscillations with single or multiple integer frequencies. These cases should be investigated in future work. It also has to be noted that this way of dealing with spikes and steps is recommended for detection methods that require stationarity. Removing steps and spikes in this manner for system identification, for example, will be counter-productive.

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