

Data-Driven Causal Analysis and its application on a Large-scale Board Machine

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Abstract: In large-scale chemical processes, disturbances can easily propagate through the process units and thereby adversely affect the overall process performance. In recent years, causal analysis has played a key role in the diagnosis of plant-wide disturbances. Causal analysis enables to identify the propagation path of the disturbance and thereby disclose the root cause. Data-driven causal analysis utilizes historical process data in the form of time series and examines to what extent the time series influence each other. If directionality between time series can be inferred, it is taken as evidence for a cause-and-effect relationship. Data-driven causal analysis can efficiently complement knowledge-based causal analysis and provide valuable insights on process dynamics with minimal efforts.

The aim of this study is to apply several time and frequency domain data-driven causal analyses on an industrial case study of a paper board machine and to evaluate the effectiveness of each method. The analyses are applied on the drying section of a board machine due to its importance in the board making process and the high share of faults associated with this section. The outcome of each method is a causal model in the form of a directed graph describing the interactions among the variables in the process. The results of each method are discussed and methods are evaluated and compared using process knowledge. In addition, root cause analysis based on the frequency domain analysis is successfully applied.

Keywords: Causal model, Digraph, Fault diagnosis, Cross-correlation, Granger causality, Frequency domain, Board machine, Control loops.

1. INTRODUCTION

Causality, a physical phenomenon based on a cause-and-effect relationship between variables, is one of the prominent features of large-scale industrial systems (Pearl, 2000). Capturing causality between different plant variables is a vital tool in the diagnosis of faulty systems.

When faults occur in large-scale processes, they can easily propagate along the process units and cause the process to deviate from its desired operating conditions, thereby increasing the operation costs. Detection of the root cause of disturbance by human labour is usually very time consuming and expensive. The study of inter-dependencies between process variables enables to identify the root cause of the disturbance and its propagation path as early as possible with minimal efforts.

Typically, the outcome of a causal analysis is a causal model in the form of a directed graph (digraph) which qualitatively describes the influences among variables. Causal models have mainly been derived from process knowledge. (Yang et al., 2012) Modelling based on process knowledge can be based on mathematical equations (e.g., a set of differential equations) (Yang & Xiao, 2012) or it can be undertaken directly from Piping and Instrumentation diagrams (P&IDs) (Yang et al., 2012). Knowledge-based causal models capture quite precisely the causality among variables; however, they

provide only a qualitative representation of plant topology. Moreover, in many cases the dynamics of a physical system are unknown or unavailable, and even if it is known, insignificant information can disturb the modelling procedure and make it too complex (Yang & Xiao, 2012).

Data-driven causal analysis utilizes process historical data in the form of time series and measures to what extent the time series corresponding to specific variables influence each other. Its main advantage is that it does not require prior information on the interior system. Moreover, unlike knowledge-based analysis that produces only a qualitative model; data-based causal analysis produces a quantitative model due to its ability to estimate the strength interactions among variables.

Data-based methods can be classified into three types: time domain methods, frequency domain methods and information theory methods (Yang & Xiao, 2012). The time domain methods capture and explore the temporal aspects of measurements. Time domain methods include the cross-correlation method (Bauer & Thornhill, 2008) and the Granger Causality (GC) method (Bressler & Seth, 2011). The frequency domain methods are able to quantify the magnitude and direction of information flow in terms of *energy transfer* and to detect whether the influence between a pair of signals is along a direct or indirect path (Gigi & Tangirala, 2010). Information theory methods include

transfer entropy method (Schreiber, 2000) and utilization of Bayesian networks for estimating probabilities for fault occurrence (Yang & Xiao, 2006).

Bauer et al. (Bauer & Thornhill, 2008; Bauer et al., 2007) have successfully demonstrated how the cross-correlation and transfer entropy methods can be employed to identify the root cause of a plant-wide disturbance in industrial case studies. Yang et al. (Yang et al., 2012) applied both the cross-correlation and transfer entropy methods on an industrial case study in order to validate a knowledge-based causal model. In recent years, some remarkable developments to the data-based methods have been proposed. Guo et al. (Guo et al., 2008) introduced the *partial Granger causality* which is able to eliminate the influence of latent variables, thus leading to less spurious results. Ladroue et al. (Ladroue et al., 2009) extended the GC and the *partial Granger causality* to the *complex Granger causality* and the *partial complex Granger causality* respectively, which defined the GC between groups of time series. Feldmann and Bhattacharya (Feldmann & Bhattacharya, 2004) introduced the *predictability improvement* (PredI) method which is based on the concept of transfer entropy and is applicable to short time series.

However, each of the data-based methods suffers from several limitations and drawbacks (Yang & Xiao, 2012; Yang et al., 2010). The main challenges in the data-driven causal analysis are in establishing the statistical significance of the results and in distinguishing between direct and indirect interactions in multivariate (MV) processes. Yang et al. (Yang et al., 2012) claim that although both process knowledge and process data are used to capture causality between variables, neither of them can be solely used to find causality without validation.

The aim of this study is to evaluate the effectiveness of several time and frequency domain methods by applying causal analysis on an industrial large-scale system. For this purpose, a case study of a large-scale board machine is studied, with a particular focus on the interactions between the control loops in the drying section. Cause-and-effect analysis is applied using the cross-correlation method, Granger causality method and frequency domain methods.

This paper is organized as follows. Section 2 provides an overview of the data-base methods for capturing causality which were utilized in this study. Section 3 describes the process case study. In Section 4 the results of each causal analysis are given and in Section 5 the methods are compared and evaluated using process knowledge. Concluding remarks are given in Section 6.

2. CAUSAL INFERENCE BASED ON PROCESS DATA

Causal relationships between time series can be investigated from several points of view: time lags, energy transfer and information transfer (Yang & Xiao, 2012). This section presents the data-based methods which were employed in this study for causal inference.

2.1 Cross-correlation method

The cross-correlation function (CCF) describes statistical properties of two time series by quantifying their similarity

over time (Box et al., 1994). The CCF between two series, x and y , sampled at discrete times i when $i = 1 \dots N$ (N is the total number of samples) and a lag k is:

$$\phi_{xy}[k] = \begin{cases} \frac{1}{N-k} \sum_{i=1}^{N-k} \hat{x}_i \hat{y}_{i+k} & \text{if } k \geq 0 \\ \frac{1}{N+k} \sum_{i=1-k}^N \hat{x}_i \hat{y}_{i+k} & \text{if } k < 0 \end{cases} \quad (1)$$

where \hat{x} and \hat{y} are derived from x and y after mean centering and scaling to a unit standard deviation. The cross-correlation analysis recognizes cause-and-effect relationships by finding the maximum absolute value of the CCF of two time series. The sign of the lag at which the CCF gets its maximum absolute value is the estimated time delay. If the CCF gets its maximum absolute value for $k > 0$ then \hat{y} is shifted by k samples while if the CCF gets its absolute maximum value for $k < 0$ then the actual delay is from \hat{y} to \hat{x} . More explicitly, both the minimum and the maximum of ϕ_{xy} are recorded:

$$\phi^{min} = \min\{\phi_{xy}[k^{min}]\}, \phi^{max} = \max\{\phi_{xy}[k^{max}]\} \quad (2)$$

The time delay λ is defined as:

$$\lambda = \begin{cases} k^{max}, & \phi^{max} \geq -\phi^{min} \\ k^{min}, & \phi^{max} < -\phi^{min} \end{cases} \quad (3)$$

and the maximum correlation is:

$$\rho = \max\{\phi^{max}, |\phi^{min}|\} \quad (4)$$

Bauer and Thornhill (Bauer & Thornhill, 2008) introduced the directionality index, which measured the difference between the minimum and the maximum of ϕ_{xy} :

$$\psi = 2 \frac{|\phi^{max} + \phi^{min}|}{\phi^{max} + |\phi^{min}|} \quad (5)$$

In their study, Bauer and Thornhill (Bauer & Thornhill, 2008) have investigated the statistical significance of the correlation value and the directionality index and selected a threshold for significance for each of them depending on the total number of observations.

The cross-correlation method is a practical and efficient way for disturbance detection as well as validation for knowledge-based causal models (Yang et al., 2012; Bauer & Thornhill, 2008). However, the method has many shortcomings, such as being non-credible when dealing with non-linear systems or pure oscillations (Bauer & Thornhill, 2008). In addition, the cross-correlation method is based on pairwise analysis, thus it cannot distinguish between direct or indirect influences. For example, causality between A and C can be a combined result of the causal relations from A to B and from B to C; thus, all possible relationships should be analysed in order to establish a causal model or process knowledge should be used. (Yang et al., 2012)

2.2 Time domain Granger Causality

The concept of Granger causality (GC) was first introduced by Wiener (Wiener, 1956) and eventually formulated by Granger (Granger, 1969). The basic notion of GC is that if one time series affects another series then the knowledge of the former series should help to predict the future values of

the latter one (Granger, 1969). To illustrate bivariate GC analysis, consider two time series $X_1(t)$ and $X_2(t)$ and their corresponding autoregressive (AR) model:

$$\begin{aligned} (1) \quad X_1(t) &= \sum_{j=1}^p A_{11,j} X_1(t-j) + \sum_{j=1}^p A_{12,j} X_2(t-j) + \epsilon_1(t) \\ (2) \quad X_2(t) &= \sum_{j=1}^p A_{21,j} X_1(t-j) + \sum_{j=1}^p A_{22,j} X_2(t-j) + \epsilon_2(t) \end{aligned} \quad (6)$$

where p is the model order, and ϵ_1, ϵ_2 are the residuals for each series. Equation (6) is referred to as the unrestricted model (Bressler & Seth, 2011). The GC from X_2 to X_1 is defined as:

$$F_{x_2 \rightarrow x_1} = \ln \left[\frac{\text{var}(\epsilon'_1)}{\text{var}(\epsilon_1)} \right] \quad (7)$$

where ϵ'_1 is obtained from (6) by omitting all A_{12} (for all j) coefficients (Seth, 2010). The model after omitting all A_{12} coefficients is referred to as the restricted model (Bressler & Seth, 2011). The statistical significance of the GC can be determined via the F -statistic test (Greene, 2002):

$$F = \frac{\frac{RSS_r - RSS_{ur}}{p}}{\frac{RSS_{ur}}{T - 2p - 1}} \quad (8)$$

where RSS_r and RSS_{ur} are the residual sum of squares of the restricted and unrestricted models respectively, T is the total number of observations and p is the model order.

For multivariate (MV) processes, the MV GC, which is based on the expansion of a univariate AR model to a Multivariate Auto Regressive (MAR) model to include all measured variables (Guo et al., 2008) can be used. Then, one variable is assumed to cause a second variable if the variance of the residuals of the first variable significantly reduced by inclusion of the second variable in the MAR model (Seth, 2010).

The method requires that the time series are stochastic and Wide Sense Stationary (WSS). In addition, the model order should be chosen carefully. A suitable model order should produce residuals which are close to white noise (Bressler & Seth, 2011). Furthermore, since the method is based on AR models, it is only suitable for linear systems and its application to non-linear systems may not be appropriate (Bressler & Seth, 2011).

2.3 Frequency domain methods

The frequency domain methods can be seen as a decomposition of the energy transfer between pairs of time series at each frequency. The evaluation of directional interactions in the frequency domain is especially useful for a process with oscillatory behaviour (Faes et al., 2010).

The methods are applied by estimating the MAR model of the time series followed by Fourier transform into frequency domain. A MAR model is defined as:

$$\begin{bmatrix} x_1(t) \\ \vdots \\ x_N(t) \end{bmatrix} = \sum_{r=1}^p A_r \begin{bmatrix} x_1(t-r) \\ \vdots \\ x_N(t-r) \end{bmatrix} + \begin{bmatrix} \epsilon_1(t) \\ \vdots \\ \epsilon_N(t) \end{bmatrix} \quad (9)$$

where $X_t = (X_{1,t}, X_{2,t}, \dots, X_{N,t})$ is the vector of N process variables, $\epsilon_t = (\epsilon_{1,t}, \epsilon_{2,t}, \dots, \epsilon_{N,t})$ is N dimensional vector of

the MV noise terms, $\hat{A}_1, \hat{A}_2, \dots, \hat{A}_p$ are $N \times N$ matrices of the model coefficients and p is the model order. By applying the Z transform operation ($Z^{-i} = e^{-i2\pi f j}$) on (9), the equation is transformed into frequency domain:

$$\hat{X}(f) = \hat{H}(f) \hat{E}(f) \quad (10)$$

where $\hat{H}(f)$ is the transfer function of the model with the following relation to model coefficients:

$$\hat{H}(f) = (I - \hat{A}_r(f))^{-1} = \bar{A}^{-1} = (I - \sum_{r=1}^p \hat{A}_r Z^{-r})^{-1} \quad (11)$$

Kaminski and Blinowska (Kaminski & Blinowska, 1991) introduced the Directed Transfer Function (DTF) which is defined as (from variable j to i):

$$\gamma_{ij}^2(f) = \frac{|H_{ij}(f)|^2}{\sum_{j=1}^N |H_{ij}(f)|^2} \quad (12)$$

The DTF represents the signal power that spreads from variable j to variable i over all possible pathways. The DTF is constructed solely from the transfer function and does not depend on the noise covariance matrix.

In contrast, the Partial Directed Coherence (PDC), introduced by Baccala and Sameshima (Baccala & Sameshima, 2001) reveals only the power of the direct interactions between pairs of variables. The PDC from j to i is defined as:

$$\pi_{ij}(\omega) = \frac{\bar{A}_{ij}(\omega)}{\sqrt{\sum_{i=1}^N |\bar{A}_{ij}(\omega)|^2}} \quad (13)$$

The PDC is a function of $A_{ij}(r)$ alone and similarly to the DTF it does not depend on the noise covariance matrix. While DTF can be seen as a spectral measure of the total causal influence of one variable on the other, the PDC can be seen as a measure of the direct influence of one variable on the other. Gigi and Tangirala (Gigi & Tangirala, 2010) found that the total energy transfer is in fact composed of three components: direct energy transfer, indirect energy transfer and interference effect and were able to quantify each of those components. Moreover, Gigi and Tangirala (Gigi & Tangirala, 2010) have shown that the PDC cannot be seen as a quantitative measure of the direct energy transfer.

3. PROCESS DESCRIPTION

The process case study is a board machine (BM) which produces a three-layer liquid packaging boards and cup boards. Analysis is focused on the drying section of the BM due to its importance and effect on board quality (Jämsä-Jounela et al., 2013). Furthermore, due to the high interactions between the control loops in this section, faults can easily propagate through the units of this section. In the drying section, the remains of excess water in the web are evaporated to achieve the desirable moisture content in the board using steam-filled cylinders. The condensing steam in the cylinders releases latent heat which is used to evaporate the bound water. The condensate from the cylinders is collected by siphons to condensate tanks where steam and condensate are separated. Steam is then delivered back to the process and condensate is returned to a power

plant. The drying section is divided into five drying groups (DG) containing 74 drying cylinders and six steam groups (SG). Each SG has its own controllers to control steam pressures, steam pressure difference between steam and condensate headers and level of the condensate tanks. A scheme of the drying section and its control valves can be seen in Figure 1.

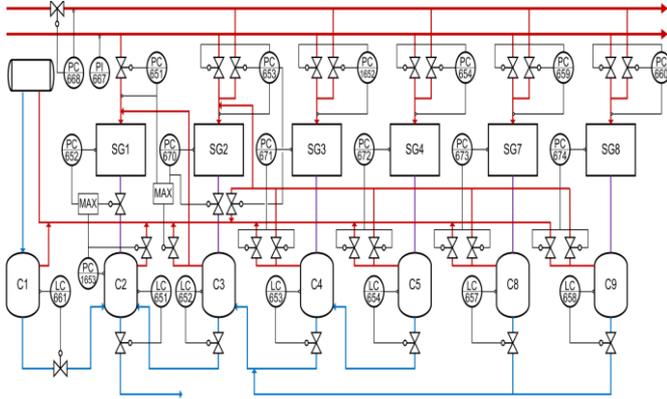


Fig. 1. Flow sheet of the drying section. Red lines indicate steam pipes, blue lines are condensate pipes and purple lines indicate mixed flow of steam and condensate

The stem pressure is controlled by two steam headers: 5 bar and 10 bar headers (at the top of Figure 1). PC651, PC653, PC 1652, PC654, PC659 and PC660 are pressure controllers that are used to control steam pressure in each SG using 5 and 10 bar steam. The pressure difference control between the steam headers and the condensate tanks is important for proper operation of the drying section since condensate removal with a siphon requires pressure difference. The pressure difference has to be high enough to enable efficient condensate removal from the cylinders but simultaneously not too high in order to prevent steam from blowing directly through the cylinders. This is achieved by manipulating the control valves in the steam outlet of the condensate tanks using controllers PC1653, PC0652, PC0670, PC0671, PC0672, PC0673 and PC0674. The level of the condensate tanks is controlled by regulating outlet flow control valves using controllers LC1653, LC0651, LC0652, LC0653, LC0654, LC0657 and LC0658.

4. RESULTS

The application of the cross-correlation, Granger causality and frequency domain methods on the basic control level of the drying section of the BM is demonstrated in this section.

First, visual inspection of the normalized time trends is performed. Then, measurements oscillating at same frequency are identified by examining the power spectra of the signals and their auto-covariance function (ACF). Then, cause-and-effect analysis is applied according the methods described in the previous section. The final outcome of each method is a causal model which can be evaluated using process knowledge. Process knowledge, in the form of a Piping and Instrumentation Diagram (P&ID) was utilized in several occasions in the modelling procedure in order to eliminate redundant links. Furthermore, the causal model

constructed based on the P&ID of the process was used to evaluate the accuracy of the data-based causal models.

4.1 Visual inspection of the time series

The time trends which were used for the analysis are the controlled variables (PVs) and controllers outputs (OPs).

The data analysed was sampled with a sampling period of 10 seconds. The time series were normalized by removing the mean values and scaling to a unit standard deviation. Figure 2 shows the normalized time trends of the PVs. Oscillating signals can be clearly seen in variables PC0653, PC0670, PC1652, PC0671, LC0653, LC0654 and PC0668.

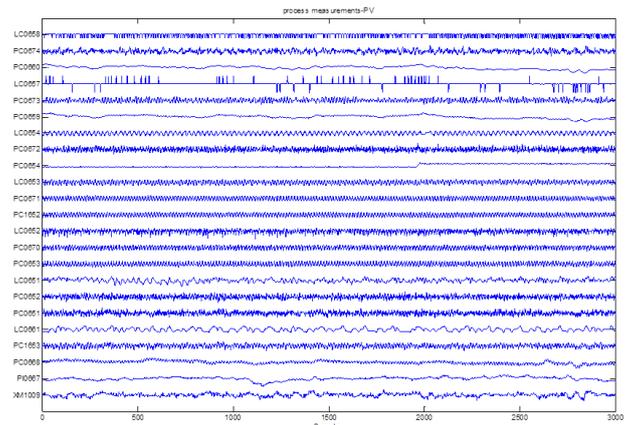


Fig. 2. Process measurements (PVs)

4.2 Oscillation analysis of the time series

Spectral analysis can detect measurements having a similar behaviour. Time series whose spectra are similar are usually subject to the same disturbance. Since the power spectra are invariant to the phase of a signal, they are insensitive to the time delays between the signals. (Bauer et al., 2005)

The power spectra of the process measurements (PVs) can be seen in Figure 3. The results show that the most prominent oscillation occurs at a frequency of 0.007 Hz (0.07 on the frequency axis) corresponding to $1/0.07 \approx 14$ samples per cycle. The loops oscillating at a common frequency are: PC0668, PC1653, PC0651, PC0652, PC0653, PC0670, LC0652, PC1652, PC0671, LC0653, PC0672 and PC0673. Thus, the disturbance is mainly affecting SG1, SG2 and SG3.

In addition to spectral analysis of the time series, the zero-crossings of the ACF were determined in order to characterize oscillations present in the data set. According to Bauer et al. (Bauer et al., 2005), it is more beneficial to utilize the ACF when analysing the zero-crossings rather than the time trends since it is much less noisy while retaining the same period of oscillation. Figure 4 shows the zero-crossings of the PVs. Similarly to the spectral analysis, the variables with a similar interval between the zero crossings are: PC1653, PC0652, PC0653, PC0670, LC0652, PC1652, PC0671, LC0653 and PC0673. The oscillation period as determined from the ACF and its zero crossings is 14

4.3 Frequency domain analysis

The frequency domain analysis was performed by evaluating the values of the PDC and the DTF between each pair of *PV*. The MAR model was estimated similarly as in the GC analysis. Some of the diagonal variance terms of the noise covariance matrix obtained from the MAR model differed by order of magnitude. According to Winterhalder (Winterhalder et al., 2005), false detection of influences from a low variance process to a process with a higher variance can occur in such cases. Thus, a renormalization of the PDC and the DTF using the variance terms (Baccala et al., 2007) was used to estimate the values of the PDC and the DTF. Consequently, a quantitative analysis of the causal influences was performed according to the components of energy transfer presented by Gigi and Tangirala (Gigi & Tangirala, 2010). Since the PDC measures the direct influence of one variable on another, it is more suitable than the DTF for constructing the causal model. Hence, the causal model was constructed by evaluating the PDC values among the *PVs* (Figure 7). The threshold for the statistical significance of the PDC values was determined using the direct causal Fourier transform (CFTd) surrogates as introduced by Faes et al. (Faes et al., 2010). The threshold for significance for each PDC value at each frequency was set at the 95th percentile of the empirical distribution of the PDC value computed over 100 sets of multivariate surrogate series.

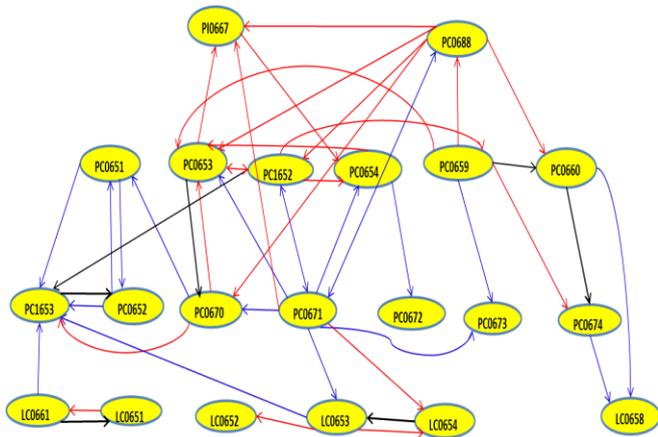


Fig. 7. Causal digraph based on the max PDC values (red arcs correspond to 0.2-0.4 PDC values, blue arcs correspond to 0.4-0.6 PDC values and the black arcs correspond to PDC values higher than 0.6)

5. COMPARISON BETWEEN THE METHODS

Each of the methods applied was able to contribute valuable information for estimating the causal influences between the control loops. The cross-correlation method offers a model-free causal analysis and requires the least computational effort. Most importantly, it enables to estimate the time delays between time series which is highly beneficial when investigating the propagation path of a fault. However, the method produced a considerable number of spurious results and process knowledge had to be used in order to eliminate redundant links. This is mainly due to the oscillating behaviour of the series which makes it difficult to determine

which of the series is lagging behind, thus leading to many ambiguous results. Furthermore, due to the high connectivity between the controllers, the consistency check (Yang et al., 2010) in this case turned out to be very tedious and time consuming.

The GC analysis produced more reliable results than the cross-correlation method and most of the identified interactions corresponded to the ones identified from process knowledge. Yet, several indirect links were erroneously identified as direct ones. Thus, also in this analysis process knowledge was found to be vital for eliminating ambiguous links. A recent improvement to the GC method is the partial Granger causality which is able to eliminate the influence of exogenous inputs/ latent variables and is therefore can result in less spurious links (Guo et al., 2008).

The PDC can be seen as the frequency domain representation of the GC; hence, it complements the GC time domain analysis. Furthermore, since this case study deals with oscillating signals, it is only natural to provide a frequency domain representation of the causal interactions. Unlike the two previous methods, the outcome of the analysis is not a causal matrix but a matrix layout plot showing the values of PDC/DTF at each frequency for each pair of variables, thus, the analysis is more time consuming than the GC and cross-correlation analyses. Similarly to the GC analysis, the spectral analysis produced several redundant links and therefore both the CFTd surrogates and PDC max values had to be used in order to determine the statistical threshold for the results. The main contribution of the frequency domain analysis with respect to other methods is in dealing with plant-wide oscillations due to its ability to quantify each of the components of the total energy transfer at each frequency (Gigi & Tangirala, 2010).

6. SUMMARY AND CONCLUSIONS

This study presented the main time and frequency domain data-based methods for detecting causal inter-dependencies between time series and demonstrated their utilization using a case study of a drying section of a large-scale board machine.

Each of the methods has its own advantages, drawbacks and limitations. Consequently, each of the methods produced a slightly different causal digraph. However, all the methods were able to detect the most powerful interactions among the control loops. Most of the spurious results were obtained due to the strong indirect interactions that were erroneously identified as direct. Therefore, the process flow diagram was essential in order to identify redundant links. Furthermore, one should remember that the data-based methods identify interactions according to their level of influence since when a fault propagates along a certain path; it may stop at some point due to signal attenuation (Yang et al., 2010). Ergo, several nodes corresponding to several controllers do not appear in the data-based causal models (e.g., controller LC0657).

The GC method and frequency analysis were found to be more appropriate than the cross-correlation analysis for this case study, mainly since these analyses were performed under a MV framework, thus they result in less redundant links in the causal map. Moreover, when dealing with oscillatory

signals, frequency domain methods should be preferred over time domain methods.

To conclude, none of the methods alone is powerful enough in detecting cause-and-effect relationships. Therefore, when dealing with large-scale industrial systems, one should try several methods to obtain useful results and make a good use of process knowledge if it is available. In addition, it should be taken into consideration that the time and frequency domain methods assume linear dependencies among variables, which is far from true in most industrial processes. Therefore, in the future it is recommended to use non-linear methods as well. For instance, the transfer entropy method can be employed to supplement the linear methods.

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