DOCTORAL THESIS

Adapting Experimental and Monitoring Methods for Continuous Processes under Feedback Control

Challenges, Examples, and Tools

Francesca Capaci

Quality Technology and Management

LULEÅ UNIVERSITY OF TECHNOLOGY

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ABSTRACT

Continuous production covers a significant part of today's industrial manufacturing. Consumer goods purchased on a frequent basis, such as food, drugs, and cosmetics, and capital goods such as iron, chemicals, oil, and ore come through continuous processes. Statistical process control (SPC) and design of experiments (DoE) play important roles as quality control and product and process improvement methods. SPC reduces product and process variation by eliminating assignable causes, while DoE shows how products and processes may be improved through systematic experimentation and analysis. Special issues emerge when applying these methods to continuous process settings, such as the need to simultaneously analyze massive time series of autocorrelated and cross-correlated data. Another important characteristic of most continuous processes is that they operate under engineering process control (EPC), as in the case of feedback controllers. Feedback controllers transform processes into closed-loop systems and thereby increase the process and analysis complexity and application of SPC and DoE methods that need to be adapted accordingly. For example, the quality characteristics or process variables to be monitored in a control chart or the experimental factors in an experiment need to be chosen considering the presence of feedback controllers.

The main objective of this thesis is to suggest adapted strategies for applying experimental and monitoring methods (namely, DoE and SPC) to continuous processes under feedback control. Specifically, this research aims to [1] identify, explore, and describe the potential challenges when applying SPC and DoE to continuous processes; [2] propose and illustrate new or adapted SPC and DoE methods to address some of the issues raised by the presence of feedback controllers; and [3] suggest potential simulation tools that may be instrumental in SPC and DoE methods development.

The results are summarized in five appended papers. Through a literature review, *Paper A* outlines the SPC and DoE implementation challenges for managers, researchers, and practitioners. For example, the problems due to process transitions, the multivariate nature of data, serial correlation, and the presence of EPC are discussed. *Paper B* describes the issues and potential strategies in designing and analyzing experiments on processes operating under closed-loop control. Two simulated examples in the Tennessee Eastman (TE) process simulator show the benefits of using DoE methods to improve these industrial processes. *Paper C* provides guidelines on how to use the revised TE process simulator under a decentralized control strategy as a testbed for SPC and DoE methods development in continuous processes. *Papers D* and *E* discuss the concurrent use of SPC in processes under feedback control. *Paper D* further illustrates how step and ramp disturbances manifest themselves in single-input single-output processes controlled by variations in the proportional-integral-derivative control and discusses the implications for process monitoring. *Paper E* describes a two-step monitoring procedure for multivariate processes and explains the process and controller performance when out-of-control process conditions occur.

Keywords: Continuous process; Statistical process control; Design of experiments; Engineering process control; Quality improvement; Simulation tools.

CONTENTS

APPENDED PAPERS

This doctoral thesis summarizes and discusses the following five appended papers.

A[1] **Capaci, F.,** Vanhatalo, E., Bergquist, B., and Kulahci, M. (2017). Managerial Implications for Improving Continuous Production Processes. *Conference Proceedings, 24th International Annual EurOMA Conference: Inspiring Operations Management,* July 1-5, 2017, Edinburgh (Scotland).

B[2] **Capaci, F.,** Bergquist, B., Kulahci, M., and Vanhatalo, E. (2017). Exploring the Use of Design of Experiments in Industrial Processes Operating under Closed-Loop Control. *Quality and Reliability Engineering International,* 33 (7): 1601-1614. DOI: 10.1002/qre.2128.

C[3] **Capaci, F.,** Vanhatalo, E., Kulahci, M., and Bergquist, B. (2019). The Revised Tennessee Eastman Process Simulator as Testbed for SPC and DoE Methods. *Quality Engineering,* 31(2): 212-229. DOI: 10.1080/08982112.2018.1461905

D **Capaci, F.,** Vanhatalo, E., Palazoglu, A., Bergquist, B., and Kulahci, M. (2019). On Monitoring Industrial Processes under Feedback Control. *To Be Submitted for Publication.*

E[4] **Capaci, F.** (2019). A Two-Step Monitoring Procedure for Knowledge Discovery in Industrial Processes under Feedback Control. *Submitted for Publication.*

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[1] Paper A was presented by Francesca Capaci on July 4, 2017, at the *24th International Annual EurOMA Conference: Inspiring Operations Management* in Edinburgh, Scotland.

[2] An early version of paper B was presented by Francesca Capaci on September 13, 2016, at the 16th *International Annual Conference of the European Network for Business and Industrial Statistics (ENBIS-16)* in Sheffield, United Kingdom.

[3] An early version of paper C was presented by Francesca Capaci on September 7, 2015, at the 15th *International Annual Conference of the European Network for Business and Industrial Statistics (ENBIS-15)* in Prague, Czech Republic.

[4] Paper E is the development of a research idea presented by Francesca Capaci on June 21, 2016, at the *4th International Conference on the Interface Between Statistics and Engineering (ICISE-2016)* in Palermo, Italy.

THESIS STRUCTURE

This thesis is organized in four parts: theoretical foundations, empirical work and findings, future research, and appended papers. Figure I illustrates the chapters included in parts I–III. The type and order of the appended papers are given in part IV.

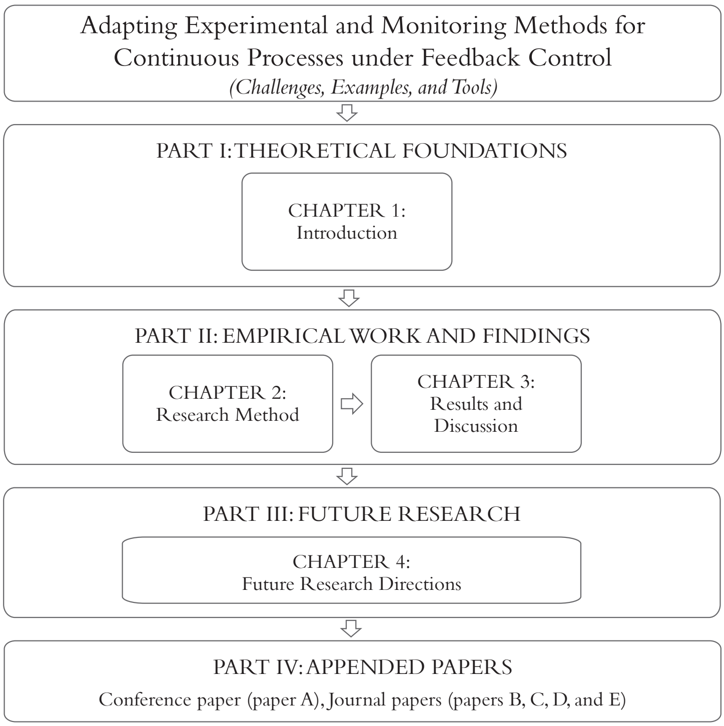

Figure I. Structure of thesis showing its four parts; the chapters are in parts I–III, and the papers appended are in part IV. The type and order of the appended papers are also shown.

Chapter 1 (*Introduction*) provides an introduction and theoretical foundation to the research area. The problem statement, research objective, and scope are outlined. The chapter also briefly describes the authors' contributions to the appended papers. Chapter 2 (*Research Method*) summarizes the method chosen for the research. Chapter 3 (*Results*) outlines the main results and discusses the main contributions, implications, and limitations of the research. Chapter 4 (*Future Research Directions*) presents new ideas and the future research questions that emerged during the research process.

PART I: THEORETICAL FOUNDATIONS

"He who loves practice without theory is
like the sailor who boards ship without a rudder and
compass and never knows where he may cast."
Leonardo da Vinci

1. INTRODUCTION

This chapter provides an introduction and theoretical foundation to the research area. The problem statement, research objective, and scope are outlined. The chapter also briefly describes the authors' contributions to the appended papers.

1.1. Statistical process control and design of experiments for quality control and improvement

Statistical process control (SPC) and design of experiments (DoE) are two well-established methodologies including statistical and analytical tools to analyze quality problems and improve process performance. A manufacturing process uses a combination of resources, such as tools, operations, machines, energy, information, and people, to transform a set of inputs, mainly raw material, into a finished product(s) (see Figure 1.1). Process inputs are upstream controllable process variables, such as temperature, pressure, and feed rate, whereas the process and finished product(s) can be associated with one or more observable and measurable response variables. The response variables can be process or product quality characteristics and process variables. Changing the (controllable) inputs may induce a related change in response variable(s). Typically, other inputs called noise factors also affect the response variable(s), but they are impossible, difficult, or too expensive to change or control; that is, they are uncontrollable (Goh, 2002; Montgomery, 2012a). Figure 1.1 illustrates the general model of a process, highlighting how SPC and DoE interact with process inputs and response variables for quality control and improvement.

SPC allows for process monitoring by means of control charts. In a control chart, a process variable or quality characteristic is plotted against time and compared with the control limits. One purpose of using control charts is to separate the common from assignable causes of variation (Woodall, 2000; Montgomery, 2012b). The common causes of variation represent the inherent, embedded variation in a process, whereas assignable causes represent the unwanted process variation that usually arises from external disturbances (Mohammed et al., 2008; Woodall, 2000).

A control chart has two distinct phases (see, for example, Bersimis et al., 2007; Jones-Farmer et al., 2014). In Phase I, the control chart is used retrospectively on a historical dataset to check whether the process can be considered under control; that is, whether the process operates with only the common causes of variation (Jones-Farmer et al., 2014). Once the in-control process condition has been established, the control limits for the process variable or quality characteristic of interest can be used for Phase II (Jensen et al., 2006; Vining, 2009). In Phase II, the control chart is used prospectively on new collected values to monitor deviations from the in-control condition (Wells et al., 2012). Whenever new collected values of the monitored variable fall outside the control limits, the control chart issues an out-of-control signal (Jensen et al., 2006). In this case, corrective action on the process may be needed to uncover and remove the assignable causes and reduce unwanted process variation (Jensen et al., 2006; Montgomery, 2012b).

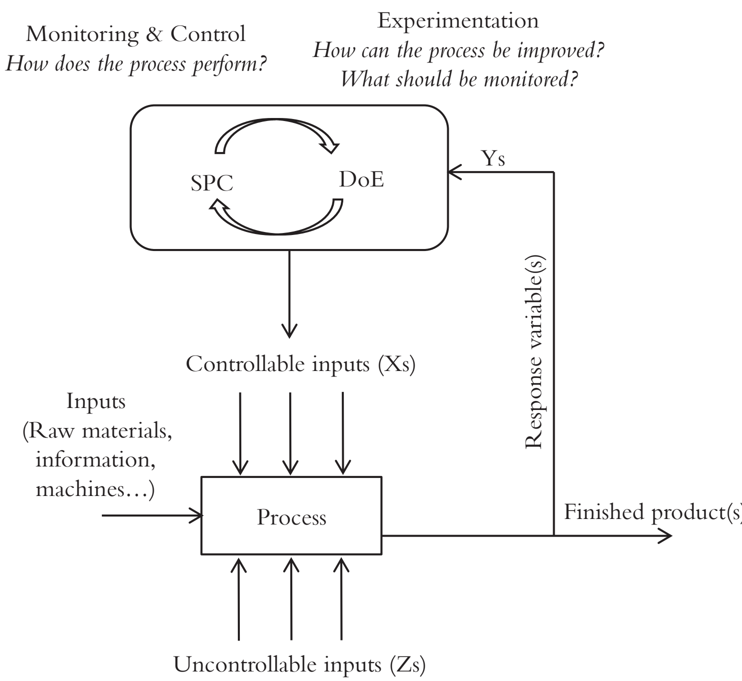

Figure 1.1. General model of a process highlighting how SPC and DoE interact with process inputs and response variables. Adapted from Montgomery (2012a).

A designed experiment allows for systematically changing the controllable process inputs to study their effects on the response variable(s) (Mason et al., 2003; Box et al., 2005; Antony et al., 2011; Montgomery, 2012a). Factorial and fractional factorial designs are two major types of designed experiments in which the experimental factors (that is, all or a subset of controllable process inputs) are varied together in such manner that all or a subset of factor-level combinations are tested.

DoE mainly uses offline quality improvement tools to find the potential causal relationships between the process inputs and response variable(s). Knowledge of the crucial process inputs is essential to understand and characterize a process and improve its performance by steering it toward a target value and/or reducing the process variability (Montgomery, 2012a). When the key factors are identified and the nature of relationship between the factors and response variable(s) established, an online process control chart for process monitoring can be routinely employed to promptly adjust the process whenever unforeseen events drive the process toward out-of-control situations.

1.2. Continuous processes

Reid and Sanders (2012) classify production processes into two fundamental categories of operations: intermittent and repetitive operations. Depending on the product volume and degree of product customization, the intermittent operations can be further divided into project and batch processes and repetitive operations can be divided into line and continuous processes (*ibid.*). Figure 1.2 presents the product-process matrix for production processes, and their main characteristics and management challenges.

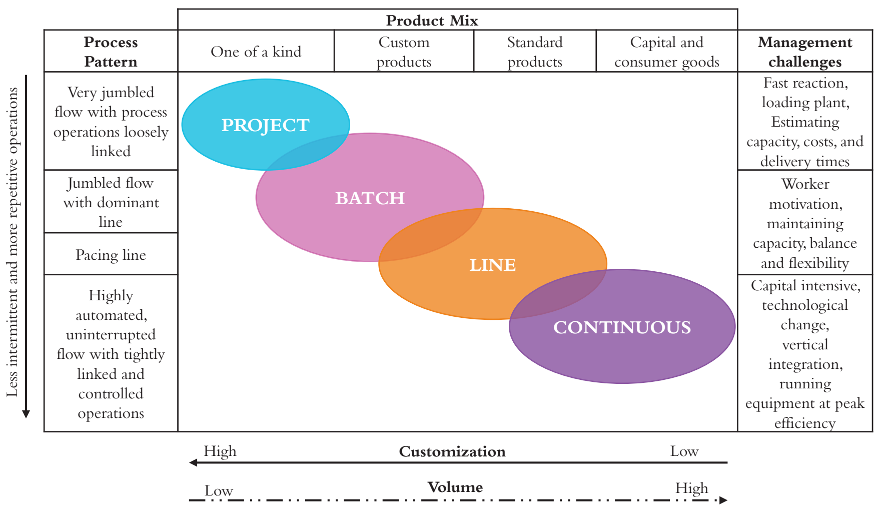

Figure 1.2. Product-process matrix for production processes, and their main characteristics and management challenges. Adapted from Reid and Sanders (2012).

New achievements in information and communication technologies are now leading to Industry 4.0, the new industrial revolution. Among others, the key technologies and features of this ongoing revolution include faster sensing technology, Internet of Things (IoT), cloud services, embedded systems, robotics, real-time analysis and decision-making, and connectivity (Santos et al., 2017). Industry 4.0 has the potential to disrupt the entire traditional approaches to manufacturing processes, posing new significant challenges at, among others, the scientific, technological, managerial, and organizational levels (Zhou et al., 2015; Santos et al., 2017). Thus, researchers are working on refining the product-process matrix (Ariss and Zhang, 2002; Schroeder and Ahmad, 2002; Bello-Pintado et al., 2019). Wagner et al. (2017) argue that the full impact of this revolution on production processes is not clearly defined as yet. Nevertheless, the ongoing challenges include implementation of digital manufacturing, big data analysis and processing, the management of cooperation between different systems, and enhanced knowledge management (Zhou et al., 2015; Wagner et al., 2017; Preuveneers and Ilie-Zudor, 2017).

Continuous and batch productions represent the main process technologies in the process industry, which is responsible for about 25% of production worldwide and involves industries such as pulp and paper, oil and gas, food and beverage, steel, mining, and material (Lager et al., 2013). A common misconception is that "process industry" and "continuous processes" are interchangeable terms, although in fact they differ in meaning (Abdulmalek et al., 2006). This study uses the definitions of the American Production and Inventory Control Society (APICS dictionary, 2019) as follows. They define the process industry as

> *"a production that adds value by mixing, separating, forming and/or performing chemical reactions by either batch or continuous mode,"*

and a continuous process as

> *"a production system in which the productive equipment is organized and sequenced according to the steps involved to produce the product. The material flow is continuous during the production process. The routing of the jobs is fixed and setups are seldom changed."*

Continuous processes differ from other types of manufacturing processes in three main features: types of incoming materials, transformation processes, and outgoing materials (Lager, 2010). The incoming materials in continuous processes are usually raw materials, often stemming directly from natural resources and showing inherent characteristics that may vary substantially (Fransoo and Rutten, 1994; Abdulmalek et al., 2006; Kvarnström and Oghazi, 2008). The transformation process includes several operational units, such as tanks, reactors, mixing units working in a continuous flow, and the relationship between process inputs and response variables that might not be immediately clear (Hild et al., 2001; Vanhatalo, 2009; Lee, S. L. et al., 2015). Finally, the outgoing materials (often also incoming materials) are non-discrete products; for example, liquids, pulp, slurries, gases, and powders that evaporate, expand, contract, settle out, absorb moisture, or dry out (Dennis and Meredith, 2000; Frishammar et al., 2012; Lyons et al., 2013). The nature of the handled materials makes these processes more sensitive to stoppages and interruptions owing to the loss in production quality and long lead times for startups (Duchesne et al., 2002; Abdulmalek et al., 2006; Lager, 2010; Krajewski et al., 2013).

1.3. The need for engineering process control

The dimensions and characteristics of continuous processes often make it unavoidable to implement engineering process control (EPC) to stabilize the quality characteristics and process variables (Lyons et al., 2013; Lee, S. L. et al., 2015; Peterson et al., 2019). One of the most common control structures used in industry is feedback control (Akram et al., 2012; Saif, 2019). Feedback controllers transform processes from open-loop into closed-loop systems[5], thus increasing the process complexity.

Figure 1.3 provides a schematic representation of an (a) open-loop and (b) closed-loop system. Ogata (2010, p. 7) defines an open-loop system as one

> *"where the output* (i.e., the response variable) *is neither measured nor fed back for comparison with the desired target,"*

and a closed-loop system as one

> *"that maintains a prescribed relationship between the output* (i.e, the response variable) *and the desired target by comparing them and using the difference as a means of control."*

[5] In control theory, a "system" is a combination of components acting together and performing a certain objective (Ogata, 2010). In the DoE and SPC literature, a "process" is a system with a set of inputs and outputs (Montgomery, 2012a; Montgomery, 2012b). In this thesis, the terms "process" and "system" are used interchangeably.

In an open-loop system, a fixed operating condition corresponds to the desired target of the response variable, and the accuracy of the system depends on calibration (Ogata, 2010). Conversely, in a closed-loop system, an automatic controller continuously compares the controlled (response) variables to a set-point value (i.e, the target value) and adjusts the measured deviation, regulating a manipulated variable, that is, a (controllable) process input (*ibid.*). The required adjustments can be determined because the causal relationship between the manipulated and controlled variables is often already established and known (Dorf and Bishop, 2011; Romagnoli and Palazoglu, 2012).

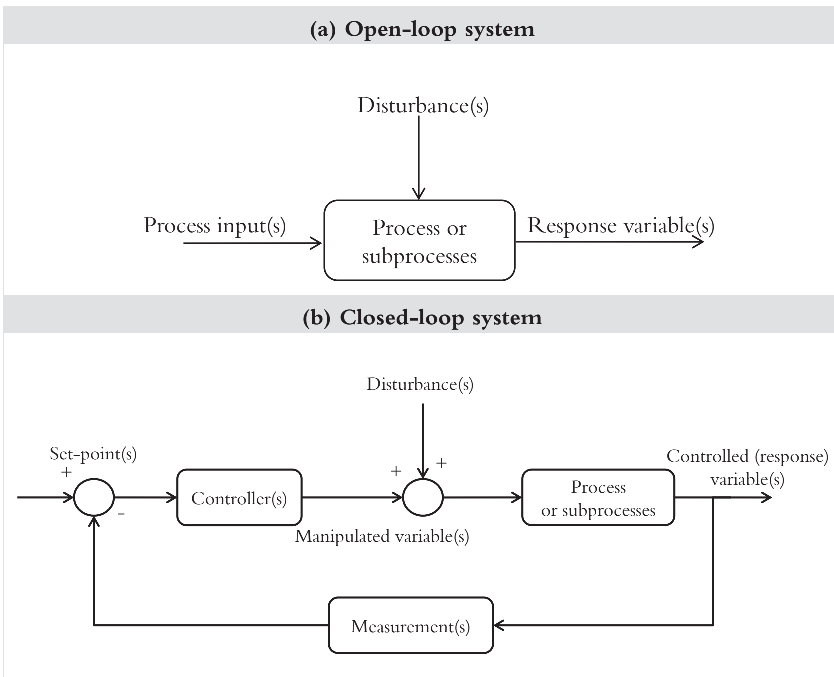

Figure 1.3. Schematic representation of an (a) open-loop and (b) closed-loop system

1.4. Monitoring and experimental challenges in processes under feedback control

For decades, management improvement programs such as Total Quality Management and Six Sigma have been promoting the use of statistical improvement methods such as SPC and DoE to improve process and product quality (Bergquist and Albing, 2006; Bergman and Klefsjö, 2010). Although these methods are well established in the statistics and quality engineering literature, their application has been found to be relatively sparse in industry (Tanco et al., 2010; Bergquist, 2015b; Lundkvist et al., 2018). The use of SPC and DoE in industrial applications in discrete manufacturing production environments faces barriers such as lack of theoretical knowledge, change management, practical problems, and lack of resources for internal training (Tanco et al., 2009; Žmuk, 2015a; 2015b). In addition to these barriers, the implementation of SPC and DoE methods in continuous processes is further complicated by the need to promote and adapt the use of such methods to continuous production environments (Bergquist, 2015b).

The need to run continuous processes under feedback control represents one of these challenges, as explained in the two following sub-sections.

1.4.1. SPC challenges in processes under feedback control

Feedback controllers make a process insensitive to disturbances and maintain crucial quality characteristics or process variables around their target values or set-points (Romagnoli and Palazoglu, 2012). The control action stems from upstream process inputs (or manipulated variables) transferring the short-term variability from controlled responses to manipulated variables (MacGregor and Harris, 1990; Hild et al., 2001; Akram et al., 2012).

The concurrent use of SPC and EPC has been widely recognized in the literature (see, for example, Box and MacGregor, 1976; Faltin and Tucker, 1991; Box and Kramer, 1992; Box and Luceño, 1997; Del Castillo, 2002; Del Castillo, 2006; Woodall and Del Castillo, 2014). Statistical process control charts should be applied to engineering controlled processes to detect and remove assignable causes of variation rather than compensating for them. Thus, an overall process improvement can be achieved by using the complementary capabilities of SPC and EPC to reduce the long-term and short-term process variability (MacGregor, 1992; Tsung, 2001). In line with these views, Box and Luceño (1997) suggest SPC for process monitoring and EPC for process adjustments.

When a process involves EPC, monitoring only the controlled variable may be ineffective owing to the controllers' potential masking of process disturbances (Wang and Tsung, 2007; Reynolds Jr and Park, 2010). The SPC literature outlines two approaches to monitor processes under EPC. The first recommends monitoring the difference between the controlled variable and set-point value, or the control error (Montgomery et al., 1994; Keats et al., 1996; Montgomery et al., 2000). The second approach is to monitor the manipulated variable (Faltin et al., 1993; Montgomery et al., 1994). Sometimes, monitoring the control error or manipulated variable alone might be ineffective (Tsung and Tsui, 2003). Therefore, a combined approach of jointly monitoring the control error and manipulated variable (or the controlled and manipulated variables) using a bivariate control chart has also been proposed (Tsung, 1999; Tsung et al., 1999; Jiang, 2004; Siddiqui et al., 2015; Du and Zhang, 2016). The combined approach increases the chances of the control chart issuing an out-of-control signal when either the controller fails to compensate for the disturbance completely or the manipulated variable deviates from its normal operating condition.

The combined approach of monitoring the controlled and manipulated variables in the same multivariate chart(s) can also be extended to multivariate processes (Tsung et al., 1999; Tsung, 2000; John and Singhal, 2019). In multivariate processes (with multiple inputs and response variables), several response variables usually need to be maintained at their target values and several manipulated variables may have to be adjusted. Consequently, the concurrent use of SPC and EPC becomes further complicated in multivariate processes (Faltin et al., 1993; Akram et al., 2012). The complexity of the problem mainly arises from the need to simultaneously monitor a large number of variables and understand the information dispersion among process variables due to engineering control (Yoon and MacGregor, 2001; Akram et al., 2012).

1.4.2. DoE challenges in processes under feedback control

Conventional applications of DoE methods implicitly assume open-loop operations. In this configuration, the potential effects of changes in process inputs on the response variables can be observed directly (Hild et al., 2001; Goh, 2002; Montgomery, 2012a). Under closed-loop operations, variables that might be interesting responses are usually maintained around desired target values (i.e., set-points). The potential effects of changes in process inputs are displaced from response variables to other process streams. Thus, the relationships between process inputs and response variables might be difficult to understand (Lee, S. L. et al., 2015). Closed-loop operations require a different experimental strategy based on further research to better understand the experimental results (Hild et al., 2001; Vanhatalo and Bergquist, 2007; Vanhatalo, 2009).

The response surface methodology (RSM) (Box and Wilson, 1951) and evolutionary operations (EVOP) (Box, 1957) are sequential in nature and hence appealing strategies in experiments involving continuous processes. However, the application of RSM and EVOP may have to be adjusted for closed-loop operations because, for example, the variables to be optimized might not be immediately clear.

1.5. Problem statement, scope, and research objective

As with other types of manufacturing processes, one of the major concerns with continuous processes is the inherent variation exhibited during production. SPC and DoE methods can play important roles in quality control and product and process improvement strategies. The conventional SPC and DoE methods and applications assume open-loop operations. However, continuous processes often operate under EPC as in the case of feedback controllers (Lee, S. L. et al., 2015; Peterson et al., 2019). The presence of feedback controllers challenges the conventional open-loop assumption of SPC and DoE methods.

Despite the abundant literature on the concurrent use of SPC and EPC, more research is needed to develop an integrated framework simultaneously studying controller and process performance to better understand the process disturbances in out-of-control conditions (Siddiqui et al., 2015). Moreover, how DoE can contribute to improving industrial processes operating under feedback control is not clearly defined in the literature (Vanhatalo, 2009). How closed-loop operations affect experimental procedures, analyses, and results is an open research question. To gain access to processes allowing for full-scale SPC and DoE methods development is challenging. SPC method development requires datasets with given characteristics, such as sampling time, sample size, and occurrence of specific faults, while DoE method development in full-scale industrial plants is costly and time-consuming.

The main objective of this thesis is to suggest adapted strategies for applying experimental and monitoring methods (namely, DoE and SPC) to continuous processes under feedback control. Specifically, this research aims

I. to identify, explore, and describe the potential challenges when applying SPC and DoE to continuous processes,

II. to propose and illustrate new or adapted SPC and DoE methods to address some of the issues raised by one of the identified challenges, the presence of feedback controllers, and
III. to suggest potential simulation tools that may be instrumental in SPC and DoE methods development.

This research is framed into the quality engineering field and builds on a framework broader than from an exclusive statistical standpoint. The study does not focus on theoretical development of the applied SPC and DoE analysis methods per se, but instead develops the suggested solutions and methods considering the adapted methods and analysis procedures to apply SPC and DoE and improve continuous processes under feedback control. Besides academics and researchers in the quality engineering field, this study is directed to quality managers, industrial practitioners, and engineers interested in quality control and improvement of continuous processes. By illustrating the potential SPC and DoE challenges in continuous processes, this study can reinforce or broaden the knowledge of SPC and DoE methods development needs. Moreover, implementation of the adapted SPC and DoE methods is expected to contribute to improving the continuous processes under closed-loop control. Finally, the promotion of simulators to test new or adapted SPC and DoE methods is expected to provide tools and aids supporting the development of these methods.

1.6. Additional SPC and DoE challenges in continuous processes

Beyond the challenges due to the presence of feedback controllers, the literature highlights those that may arise when applying SPC and DoE methods to continuous processes. For a broader perspective of the research field, the following sub-sections briefly summarize these challenges. While the issues due to these challenges are not the main focus of this research, they have been encountered during the course of the studies and overcome using existing solutions in the literature. Thus, the following sub-sections also provide theoretical foundations for some of the method chosen for the research.

1.6.1. SPC challenges in continuous processes

This sub-section summarizes the additional challenges that may emerge when applying SPC methods to continuous processes.

Multivariate nature of process data

Researchers in different areas are increasingly focusing on issues related to managing big data. The accelerated advancement of sensing technology, such as IoT and high-throughput instruments, and the increasing availability of storage capacity allow for taking process measurements at multiple locations and with high sampling frequency (Woodall and Montgomery, 2014; Ferrer, 2014; Peterson et al., 2019). The uninterrupted flow of continuous processes can produce massive datasets of both variables and observations exhibiting varying degrees of autocorrelation and cross-correlation (Saunders and Eccleston, 1992; Hild et al., 2001; Vanhatalo, 2010; He, Q. P. and Wang, 2018). Vining et al. (2016) claim that any process and product improvement attempt should consider the complexity of the problem due to the new data-rich environment. SPC (and DoE) methods require more application-oriented and methodological studies to handle this modern challenge and meet the growing industry demand (Vining et al., 2016; Steinberg, 2016; Peterson et al., 2019).

The earliest SPC research and industrial applications focused mainly on univariate control charts, with the product quality characteristics monitored individually. In data-rich environments, such as those of continuous processes, the univariate monitoring of each process variable in separate control charts is often inefficient and misleading (Kourti and MacGregor, 1995; Bersimis et al., 2007; He, Q. P. and Wang, 2018). In 1997, MacGregor (cited in Ferrer, 2014) argued that monitoring a multivariate process using univariate charts is analogous to using one-factor-at-a-time experimentation: while the correlation of variables makes it difficult to interpret univariate SPC charts, factor interactions make it difficult to interpret the results obtained from one-factor-at-a-time experimentation. To overcome this problem, researchers have adopted multivariate SPC allowing for the simultaneous monitoring of multiple process variables.

Multivariate monitoring charts based on latent variable techniques, such as principal component analysis (PCA) and partial least squares (PLS), have been used in industrial applications successfully (see, for example, Kourti et al., 1996; Qin, 2012; Ferrer, 2014; Zhang et al., 2014; Silva et al., 2017; Silva et al., 2019). The strength of latent variable techniques relies on their dimensionality reduction properties. Through the cross-correlation of process variables, these techniques can reduce an original dataset to a few linear process variable combinations (or principal components), which can be considered the main drivers of the process events (MacGregor and Kourti, 1995; Yoon and MacGregor, 2001; Kourti, 2005; De Ketelaere et al., 2015; Rato et al., 2016). Typically, two control charts are commonly used for process monitoring, a Hotelling T^2 control chart on the first retained principal components of the PCA/PLS model, and the squared prediction error (*SPE* or *Q*) chart on the model residuals.

Autocorrelated data

Control charts based on PCA are well equipped to handle cross-correlation, but not autocorrelation (Vanhatalo and Kulahci, 2015). Autocorrelation is an inherent characteristic of continuous processes due to process inertia, continuous flow of material, EPC, and high sampling frequencies (Atienza et al., 1998; Noorossana et al., 2003; Prajapati and Singh, 2012). Autocorrelation in data violates the basic assumption of time-independent observations that the SPC methods rely on, affecting both univariate and multivariate SPC techniques (Mastrangelo and Forrest, 2002; Woodall and Montgomery, 2014). According to Prapajati and Singh (2012), in practice, positive autocorrelation is more often encountered than negative autocorrelation, leading to deflated control limits in control charts and increased false alarm rates (Mastrangelo and Montgomery, 1995; Runger, 1996; Woodall, 2000; Bisgaard and Kulahci, 2005; Vanhatalo et al., 2017).

The literature describes two main solutions to dealing with autocorrelated data (Prajapati and Singh, 2012). The first is to use a standard control chart and adjust the control limits to achieve the desired false alarm rate (Russell et al., 2000; Vermaat et al., 2008; Rato and Reis, 2013b; Vanhatalo and Kulahci, 2015; Vanhatalo et al., 2017). This approach requires an ad-hoc adjustment to each case, which is cumbersome and time-consuming. The second solution requires "filtering out the autocorrelation" using a time series model and then applying a control chart to the model residuals (Harris and Ross, 1991; Kruger et al., 2004; Pacella and Semeraro, 2007; Rato and Reis, 2013a; Reis and Gins, 2017). Most of the studies using this approach are based on the assumption of a known time series model (Woodall and Montgomery, 2014). Furthermore, fitting a time series model for many variables is challenging because a large number of parameters must be estimated (Rato and Reis, 2013a).

To monitor autocorrelated large-scale processes, Ku et al. (1995) proposed a modified version of the PCA framework, known as dynamic PCA (DPCA). The DPCA approach suggests applying the usual PCA method to an augmented data matrix obtained by appending its time-shifted duplicates to the original dataset. The Hotelling T^2 and Q charts based on dynamic principal components can then be used to monitor the process.

1.6.2. DoE challenges in continuous processes

This sub-section summarizes the additional challenges that may emerge when applying DoE methods to continuous processes.

Large-scale and costly experimentation

Continuous process plants are usually spread out over a large area and operate around the clock. Experimentation in full-scale continuous processes may involve the majority of production staff, making coordination and information flows essential (Vanhatalo and Bergquist, 2007). Experimental campaigns can continue for a long time, jeopardizing the production plans and leading to off-grade products. Time and cost are often significant constraints (Kvist and Thyregod, 2005; Bergquist, 2015b).

Continuous production process characteristics unavoidably affect the experimentation strategy. Planning, conducting, and analyzing experiments require proper adjustments in continuous process settings (Vanhatalo and Vännman, 2008). An experimental campaign should always begin with careful planning because planning is critical to successfully solving the experimenters' problem (Coleman and Montgomery, 1993; Box et al., 2005; Freeman et al., 2013). Vanhatalo and Bergquist (2007) provide a checklist for planning experiments in continuous process settings, where limited number of experimental runs, easy-/hard-to-change factors, randomization restrictions, and design preferences are particularly relevant. Time restrictions and budget constraints force the analyst to consider experiments with few factors and runs. Thus, two-level (fractional) factorial designs are important, but replicates of the experiments may not always be possible (Bergquist, 2015a). Analyzing unreplicated designs might not always be easy because of the impossibility of estimating experimental random variations and lack of degrees of freedom when calculating the model unknowns (i.e., the factors' effects). When split-plot designs are needed, for example, to reduce the transition times between runs, the analysis might become further complicated (see, for example, Vanhatalo and Vännman, 2008; Vanhatalo et al., 2010)

Time series nature of process data and process dynamics

Random process disturbances and unforeseen control action seldom let the experimental factors remain constant during experimentation in a continuous process (Vining et al., 2016). Moreover, high sampling frequencies produce a chronological sequence of observations. Thus, both experimental factors and response variables should be viewed as time series (Storm et al., 2013; He, Z. et al., 2015). Production steps such as mixing, melting, reflux flows, or product state changes make the process dynamic (Lundkvist and Vanhatalo, 2014). In a dynamic process, changed process inputs affect the response variables gradually, and the process stabilizes to a new steady state (Nembhard and Valverde-Ventura, 2003; Vanhatalo et al., 2010; Bisgaard and Khachatryan, 2011; Lundkvist and Vanhatalo, 2014). Vanhatalo et al. (2010) defined the time taken for a response to reach a new steady state as transition time, arguing that its characterization is crucial when experimenting in continuous processes.

To correctly estimate the factors' effects on the response variables, the process needs to reach a steady-state condition. That is, the transition times affect the run length of the experiments (Vanhatalo and Vännman, 2008; Vanhatalo et al., 2010). By knowing the transition times, the experimenter can avoid unnecessary long and costly or too short run lengths that yield misleading estimates of the effects. However, to determine the transition times in continuous processes is not easy for several reasons. Factors' levels change often affects the response variables in several ways, and the transition times may vary for different responses in terms of both length and behavior. For example, Vanhatalo et al. (2010) developed a method to estimate the transition times in dynamic processes by combining PCA and transfer-function noise modeling. However, the method is an offline method that has to determine the transition times a priori during the planning phase of the experiment. Methodological research on online estimation of transition times in continuous processes can help solve the aforementioned experimentation challenges in such production environments.

Autocorrelated and cross-correlated responses

In continuous processes, high sampling frequency induces a positive correlation in the response variables (Hild et al., 2001; Prajapati and Singh, 2012). Ignoring the autocorrelation in responses might lead to ineffective or erroneous analysis of the experimental results. For example, using the run averages of responses might be a poor alternative and can lead to incorrect estimation of the effects. Time series analysis could be a useful tool to analyze the experimental results because both the time series nature and autocorrelation of data can be taken into account. However, few attempts have been made to combine the benefits of DoE and time series analysis. As shown in Vanhatalo et al. (2010), the dynamic relationships between process inputs and response variables can be modeled using transfer-function noise modeling and intervention analysis to improve the efficiency of the results (Bisgaard and Kulahci, 2011; Vanhatalo et al., 2013; Lundkvist and Vanhatalo, 2014).

In continuous processes, the response variables are often related to each other, making it difficult to identify the process inputs that can be changed independently from one another and used as experimental factors (Hild et al., 2001). A change in one experimental factor often affects several response variables because they are simply reflections of the same underlying event (Kourti and MacGregor, 1995; Kourti and MacGregor, 1996; Kourti, 2005). Moreover, small changes in a factor might lead to unacceptable changes in process operating conditions and exorbitant production costs of a large volume of off-spec products (Kvist and Thyregod, 2005). A multivariate analysis approach using latent variable techniques, such as PCA and PLS, should be preferred to a univariate approach. Moreover, in many experimental situations, the main interest might be to characterize how a function (a surface or profile) changes over time within an experimental design region (see, for example, Storm et al., 2013; He, Z. et al., 2015). However, existing methods do not allow for designing and analyzing these experimental scenarios, and further research is needed to address these challenges (Vining et al., 2016).

1.7. Introduction and authors' contributions to appended papers

This section introduces the appended papers and highlights the relationship between them and their connection with the research aims. The authors' contributions to the appended papers are also presented.

Paper A: "Managerial Implications for Improving Continuous Production Processes." Capaci, F., Vanhatalo, E., Bergquist, B., and Kulahci, M. (2017).

Paper A outlines the SPC and DoE implementation challenges described in the literature for managers, researchers, and practitioners interested in continuous production process improvement. Besides the research gaps and state-of-the-art solutions, the paper illustrates the current challenges. This is the first appended paper since it introduces the research topic and relates to aim I of the research.

This paper was conceived by Francesca Capaci when an opportunity arose to submit a contribution to the 24th International Annual EurOMA Conference. Francesca Capaci carried out the four phases and eight stages of the literature review process including searches for data collection, screening steps, and analysis of data. The co-authors provided support throughout the emerging analysis steps. Francesca Capaci wrote the paper, with contributions from all co-authors.

Paper B: "Exploring the Use of Design of Experiments in Industrial Processes Operating Under Closed-Loop Control." Capaci, F., Bergquist, B., Kulahci, M., and Vanhatalo, E. (2017).

Paper B conceptually explores issues of the experimental design and analysis in processes operating under closed-loop control, and illustrates how DoE can help in improving and optimizing such processes. The Tennessee Eastman (TE) process simulator is used to illustrate two experimental scenarios. Paper B relates to aim II of the research.

All the authors jointly developed the idea of exploring the use of DoE in processes operating under closed-loop control. Francesca Capaci tried to understand the TE process simulator in order to find viable scenarios for conducting the experiments. Francesca Capaci planned, simulated, and analyzed the experimental scenarios, while all authors were involved in the discussions leading up to the results. Francesca Capaci wrote the paper, with contributions from all co-authors.

Paper C: "The Revised Tennessee Eastman Process Simulator as Testbed for SPC and DoE Methods." Capaci, F., Vanhatalo, E., Kulahci, M., and Bergquist, B. (2019).

Paper C provides guidelines on how to use the revised TE process simulator, run with a decentralized control strategy, as testbed for SPC and DoE methods in continuous processes. Flowcharts detail the necessary steps to initiate the Matlab/Simulink® framework. The paper also explains how to create random variation in the simulator, with two examples illustrating two potential applications in the SPC and DoE contexts. Paper C mainly relates to aim III of the research.

The proposal to use the revised TE process as testbed for SPC and DoE methods development for continuous processes was jointly developed by all the authors. Francesca Capaci located the revised simulator, performed all work required to understand the details of the simulator, and developed the idea on how to create random variation in the simulator. Francesca Capaci also designed the illustrated examples, and was responsible for all simulations and analyses. All the authors were involved in the discussions leading up to the results. Francesca Capaci wrote the paper, with contributions from all co-authors.

Paper D: "On Monitoring Industrial Processes under Feedback Control." Capaci, F., Vanhatalo, E., Palazoglu A., Bergquist, B., and Kulahci, M., (2019).

Paper D explores the use of SPC in single-input single-output[6] processes controlled by variations in the proportional-integral-derivative (PID) control scheme, illustrating whether and how common disturbances (i.e., mean shifts or trends) manifest themselves on the controlled and manipulated variables. The implications of process monitoring for these scenarios are discussed. Two simulated examples in Matlab/Simulink® illustrate two industrial applications. Paper D relates to aim II of the research.

The proposal to study the signatures of step and ramp disturbances in single-input single-output processes came from Francesca Capaci while taking a course in "Basics of Control Theory." Francesca Capaci had to understand how step and ramp disturbances are handled by variations in the PID control scheme and how they manifest themselves on the controlled and manipulated variables. Francesca Capaci also developed the simulators used in the two examples, performed the simulations, and analyzed the results. Ahmet Palazoglu provided support to properly set up the control scheme in the simulated examples. Francesca Capaci wrote the paper, with contributions from all co-authors.

Paper E: "A Two-Step Monitoring Procedure for Knowledge Discovery in Industrial Processes under Feedback Control." Capaci, F. (2019).

Paper E explores the use of SPC in multiple-inputs multiple-outputs[7] processes under feedback control, illustrating a two-step monitoring procedure in which the process variables are classified prior to the analysis and then monitored separately by means of a multivariate monitoring scheme. The revised TE process simulator under a decentralized feedback control strategy is used to apply the two-step monitoring procedure. The results of the two simulated scenarios are compared with the approach of monitoring the variables simultaneously in the same multivariate chart(s). Paper E relates to aim II of the research.

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[6] In this thesis, the term "single-input single-output process" refers to a process with one process input and one response variable.

[7] In this thesis, the term "multiple-inputs multiple-outputs process" refers to a process with several process inputs and several response variables.

As the sole author, Francesca Capaci designed the study, carried out the simulations, analyzed the data, and wrote the paper. Erik Vanhatalo, Bjarne Bergquist, and Murat Kulahci contributed with valuable feedback.

PART II: EMPIRICAL WORK AND FINDINGS

"If we knew what it was we were doing,
it would not be called research, would it?"
Albert Einstein

2. RESEARCH METHOD

This chapter outlines the research design and describes the tools and methods used for data collection and analysis in the research. The chapter provides the relationships between the studies and frames them in the research aims. The studies are presented in relation to the research aims and do not follow their chronological development (i.e., the order of the appended papers).

2.1. Research design

To fulfill the overall research objective, the research was organized around three topics, one for each research aim. To reach the research aims, five studies were totally conducted, as illustrated in Figure 2.1.

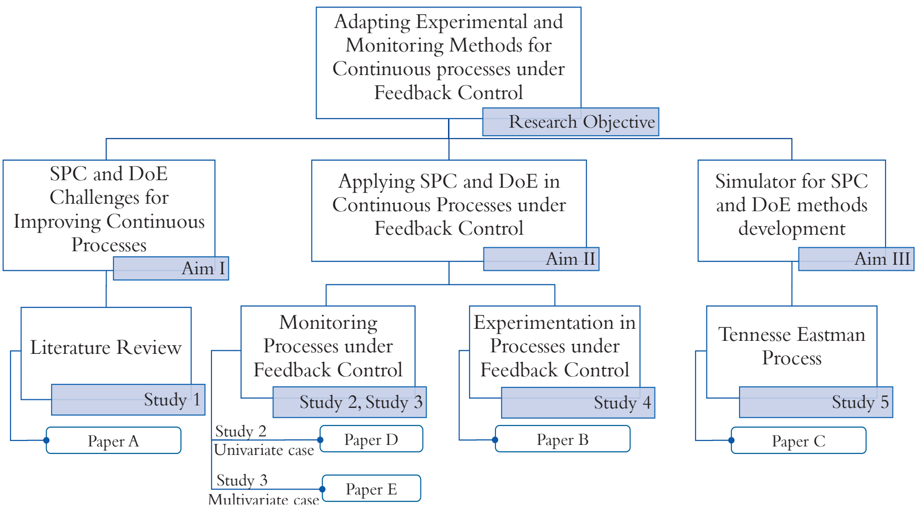

Figure 2.1. Design of research and studies conducted.

A literature review is summarized in Paper A. This was required to achieve aim I of the research objective. The review was motivated by the need for a theoretical foundation for the research and to summarize the results of the searches and readings in a systematic manner. This is an essential step in the research. A knowledge of the existing literature would help, for example, to determine what researchers already know about the research topic, summarize the research evidence from high-quality studies, identify the research gaps, and generate new ideas to fill those gaps (Tranfield et al., 2003; Briner and Denyer, 2012).

Aim II of the research objective was defined on the basis of the literature review. The review highlighted several challenges faced when applying SPC and DoE to continuous processes. Among them, the need for more research to adapt experimental and monitoring methods for processes under feedback control emerged. This became the focus of aim II of the research objective. Three studies were conducted to achieve aim II of the research objective. The first and second studies (studies 2 and 3 in Figure 2.1) investigated the use of SPC methods in processes under feedback control; this led to the development of Papers D and E. Study 2 focused on the application of SPC methods to single-input single-output processes under feedback control, while study 3 investigated the use of SPC methods in multiple-inputs multiple-outputs processes under feedback control. The third study (study 4 in Figure 2.1) delved into the problem of adapting DoE methods for processes under feedback control, leading to the development of Paper B.

The research strategy relating to aim II of the research objective was based on simulations. The main reason for choosing this approach was that the project did not involve industrial collaborators where SPC and DoE methods could be studied. Even with access to industrial processes, it would have been difficult to obtain processes allowing for full-scale methods developments. To develop and test SPC methods, datasets with specific characteristics such as sample size, sampling time, and the occurrence of known faults are required. Furthermore, DoE applications in full-scale industrial processes may unavoidably jeopardize the production plants and thus affect the production goals. This could make it difficult to convince top management to adopt large and costly experimental campaigns.

Finding a realistic simulator for SPC and DoE methods development was a priority, and led to the definition of aim III of the research objective. This simulator needed to offer a good balance between realistic simulation of a continuous process and flexibility necessary for testing new SPC and DoE methods. To achieve aim III, the research strategy was to search the literature for available simulators that can mimic the features of continuous processes. A literature search highlighted that many published studies in chemometrics, an important field of research connected to continuous processes, used the TE process as testbed for new methods developed (see, for example, Lee et al., 2004; Liu et al., 2015; Rato et al., 2016). Downs and Vogel (1993) originally proposed the TE process as a test problem, providing a list of potential applications in a wide variety of topics such as plant control, optimization, education, and non-linear control. In addition, Reis and Kenett (2017) classified the TE simulator as one of the more complex simulators (medium-/large-scale nonlinear dynamic simulator), suggesting its use for advanced applications in high-level statistical courses. The TE process simulator can emulate many of the challenges frequently found in continuous processes, such as multivariate nature of the data, process dynamics, and autocorrelated and cross-correlated responses. The process operating conditions can be disturbed activating 21 pre-programmed process disturbances of different types, such as step and random variation. Most importantly, the TE process simulator has to be run with an implemented control strategy to overcome its open-loop instability.

The above-mentioned features and the need to run the TE process simulator under a designed control strategy supported an in-depth study of the simulator, since it could allow for the development of studies 3, 4, and 5. Numerous control strategies were available to control for and stabilize the TE process. Among them, the decentralized control strategy proposed by Ricker (1996; 2005) was the most suitable for this research, with the following advantages:

- the set-points of the controlled variables and process inputs (not involved in control loops) can be modified as long as they are maintained within the process operations constraints,
- the analyst can specify the characteristics of the simulated data (e.g., length of experiment, sampling frequency, types of process disturbances), and
- the simulator is free to access.

Building on this knowledge, study 5 of the research aimed to make an in-depth study of the TE process simulator and investigate its suitability for SPC and DoE methods development in continuous process settings.

The decentralized TE simulator devised by Ricker (2005) was first used to run the experiments for study 4. The analyses made during this study highlighted an important limitation of the decentralized TE process simulator, that is, it is almost deterministic in nature. Measurements of the decentralized TE process variables were affected only by white Gaussian noise, with standard deviation typical of the measurement type and thus mimicking a measurement error. Repeated simulations with the same starting conditions and setup produced the same results, except for measurements errors. The impossibility to simulate replicated experiments did not allow for estimating the experimental error and determining whether the observed differences in data were really statistically different. Moreover, the value of a model containing only measurement noise is limited when running repeated simulations to assess the performance of an SPC method.

The knowledge gained during study 4 called for revision of the research design. Additional research was needed to understand whether the limitations of the decentralized TE process simulator of Ricker (2005) could be overcome to make it suitable for studies 3 and 5. A literature search led to the release of the decentralized TE process simulator, known as the revised TE process model, implemented in Matlab/Simulink® (Bathelt et al., 2015a; 2015b). Among other possibilities, the revised simulator allowed for scaling the disturbances introduced to the process and changing the seed of each simulation. Scaling the random variation disturbances allowed for adding variability to the simulation results without overly distorting them. Moreover, the seed change of random numbers could force the simulator to generate different results for repeated simulations with the same starting conditions. Combining these two features, the deterministic nature and limitations of the simulator could be overcome, making the revised TE model suitable for testing the SPC and DoE methods in continuous process settings. The revised TE process was then used for studies 3 and 5.

2.2. Aim I: SPC and DoE challenges for improving continuous processes

This section highlights the tools and methods used for data collection and analysis in study 1 related to aim I of the research objective.

2.2.1. Study 1: Literature review

The literature review highlighted the SPC and DoE implementation challenges for managers, researchers, and practitioners interested in improving continuous production processes. It was conducted in four phases based on the eight review stages suggested by Briner and Denyer (2012), as shown in Table 2.1.

The review stages of the "to plan" phase were outlined using Cooper's literature review taxonomy (Randolph, 2009) as follows:

- Review stage 1:
  - *Focus:* to identify methods for SPC and DoE in continuous processes;
  - *Goal:* to identify and classify central issues related to the identified methods;
  - *Perspective:* to present the review findings assuming a neutral position (i.e., reporting the results).
- Review stage 2
  - *Coverage:* a representative sample of publications central or pivotal to achieving the goal.

- Review stage 3
  - *Organization:* to be structured around concepts (i.e., around the central issues identified by the literature review);
  - *Audience:* researchers and practitioners in the field, as well as top management.

Table 2.1. Four phases and eight review stages of the literature review process [adapted from Briner and Denyer (2012)].

Phase	Review stage
To plan	1. Identify and clarify the question(s) to be addressed 2. Determine the types of studies that will answer the question(s) 3. Establish the audience
To conduct	4. Search the literature to locate relevant studies 5. Sift through the studies and include or exclude following predefined criteria
To analyze	6. Extract the relevant information from the studies 7. Classify the findings from the studies
To remember	8. Synthesize and disseminate the findings from the studies

The other phases shown in Table 2.1 were conducted twice in five review stages, first for the SPC field, and then for the DoE field. Review stage 4 of the "to conduct" phase was realized in April 2017 using the Scopus database, limiting the search to publications in English during the past 30 years. Sequential searches were conducted using keywords and combined queries such as "statistical process control" *AND* "continuous process" *OR* "continuous production" for the SPC literature searches, and "design of experiments" AND "continuous process" OR "continuous production" for the DoE literature searches. Starting from the search results, the items were sequentially screened (review stage 5), excluding all items not related to SPC and DoE applications to continuous processes, and those that did not highlight the potential challenges in applying SPC and DoE methods to continuous processes. Conference articles were excluded if a later journal article by the same authors and with the same title was found. In review stages 6 and 7 (the "to analyze" phase in Table 2.1), the relevant information from the remaining publications was extracted and classified to identify the challenges or development needs of SPC and DoE methods in continuous processes. The classification stage was conducted using a Microsoft Excel® worksheet. Then, relevant publications not found by searches were added to the classified publications. The reference lists of the classified publications were also examined to minimize the risk of missing out other important publications. This final step provided the pivotal or central publications making up the representative sample which the results of Paper A were based on (review stage 8 of the "to remember" phase in Table 2.1).

2.3. Aim II: applying SPC and DoE to continuous processes under feedback control

The following sections explain the tools and methods used for data collection and analysis used in studies 2, 3, and 4 related to aim II of the research objective.

2.3.1. Study 2: monitoring univariate processes under closed-loop control

Study 2 focused on the use of statistical process control charts in univariate processes (single-input single-output processes) controlled by variations in the proportional-integral-derivative (PID) control scheme. The study explored how commonly occurring disturbances (step and ramp) manifest themselves in univariate processes by studying their signatures on the controlled and manipulated variables. Moreover, monitoring the controlled and manipulated variables separately helps in better understanding the process and controller performance in cases of out-of-control conditions. Formulas to quantify the steady-state values of controlled and manipulated variables were also derived. These formulas were based on mathematical derivations applying the principles and theorems used in control theory, such as the superposition principle and final value theorem (for further details, see Ogata, 2010; Romagnoli and Palazoglu, 2012). Two common textbook industrial applications were used to exemplify the theoretical results and illustrate the implications for process monitoring. For further information, the reader can refer to Paper D, which also provides all the details of the simulators employed for the study. These simulators can be used as testbeds for SPC methods in univariate processes under closed-loop control. Hence, study 2 relates to aim II and, to a lesser extent, aim III of the research objective.

The two simulated examples were implemented in Matlab/Simulink®. The first example simulates a heat-exchanger controlled by a proportional (P) controller. The proportional gain of the controller was tuned using the Ziegler-Nichols technique (see, Ogata, 2010; Romagnoli and Palazoglu, 2012). The second example simulates a steel rolling mill with a proportional-integral (PI) controller. In this case, the proportional and integral gains of the controller were tuned using the internal model control rule (see, for example, Romagnoli and Palazoglu, 2012). In both examples, the controlled and manipulated variable values were collected twice during the continuous process operations. The processes were upset the first time by a step disturbance and the second time by a ramp disturbance. Prior to data analysis, the observations collected during the process startup were discarded to allow for a more stable estimation of the process parameters in Phase I.

The simulated data were analyzed using Matlab® scripts and the free R statistics software. In the heat-exchanger example, time series plots of the controlled and manipulated variables were used to analyze the results. In the steel rolling mill example, standardized CUSUM charts applied separately to the controlled and manipulated variables were used to analyze the results. Step and ramp disturbances do not typically result in large shifts of the process variables in the presence of the PI controller. Thus, CUSUM charts were considered a good alternative to detect potential out-of-control signals. Of course, other control charts with comparable detection abilities, such as the exponentially weighted moving average (EWMA) chart, could have been used. However, a different choice of control chart would not have changed the final conclusions of the study.

2.3.2. Study 3: monitoring multivariate processes under closed-loop control

Study 3 explored the use of control charts in multivariate processes (multiple-inputs multiple-outputs processes) under feedback control. The study focused on a two-step monitoring procedure for multivariate processes, first [1] classifying the process variables into groups as controlled, manipulated, and measured variables, and then [2] monitoring each group of variables separately using a multivariate monitoring scheme. The two-step monitoring procedure was adopted to better understand the process and the controllers' performance in multivariate processes in case of out-of-control signals. From this perspective, study 3 can be considered an extension of study 2. The results of study 3 are reported in Paper E.

The revised TE process under a decentralized feedback control strategy (Bathelt et al., 2015b) was used as a testbed for the two step-monitoring procedure, as advised in Paper C. Two simulated scenarios were illustrated and discussed. The results were also compared with the commonly used approach of monitoring the process variables together in the same multivariate control charts.

In the first step of the two-step monitoring procedure, the TE process variables were classified as controlled, manipulated, and measured variables using a qualitative approach. The information for classification was mainly extracted from the work by Ricker (1996), who explained the design phases of the TE process decentralized control strategy. The knowledge gained during the development of study 5 (conducted prior to study 3) also supported the TE process variables classification. The support tool for the classification was a Microsoft Excel® sheet.

In the second step of the two-step monitoring procedure, the controlled, manipulated, and measured variables were monitored separately using a multivariate monitoring scheme. The revised TE simulator (Matlab/Simulink®) was run twice to collect two datasets, one for each illustrated example. Throughout the simulations, a step-change disturbance was introduced into the process to collect the faulty datasets (for details, see Paper E). Using a Matlab® script, the phase I samples of the controlled, manipulated, and measured variables were produced by removing the observations during the transition time on process startup. Steady-state values of the variables provide a more stable estimation of the covariance matrices and hence of the in-control models. The TE process variables exhibit moderate to high autocorrelation coefficients. Thus, a multivariate monitoring scheme based on DPCA was applied to each group of variables.

Hotelling T^2 and Q charts built on the basis of DPCA models in phase I were used to monitor separately the controlled, manipulated, and measured variables in phase II. For comparative purposes, the phase I and phase II samples consisting of controlled, manipulated, and measured variables were used for monitoring all the variables simultaneously. The data analysis was conducted using the free R statistics software.

2.3.3. Study 4: experimentation in processes under closed-loop control

Study 4 relates to aim II of the research objective. The study explored the experimental design and analysis issues to explain to researchers and practitioners how DoE can add value to the processes under closed-loop. Two experimental scenarios were designed to exemplify the study's conceptual ideas.

Design Expert® (version 9) was used to generate the experimental designs and analyze the experimental results, and the experiments were simulated using the decentralized TE process simulator implemented in Matlab/Simulink® as a testbed (Ricker, 1996; 2005).

The first scenario illustrated an experiment in which the control strategy is disturbed by level change of process inputs not involved in control loops. Process inputs not involved in control loops can be considered as disturbances in closed-loop systems and thus viewed as experimental factors. The TE process has three inputs not involved in any control loop that can be used as experimental factors. However, even a small factor-levels change can be exaggerated to unacceptable effects that lead to a process shutdown. A 2^2 randomized factorial design with three replicates was generated to estimate the location effects (main effects and interactions) of two inputs not involved in control loops on the controlled and associated manipulated variables. The second scenario exemplified a screening design using the set-points of controlled variables as experimental factors. In this case, a factor-level change will move the process from one operating region to another. A two-step sequential experiment estimated the set-points' impact on the process operating cost. A 2_{III}^{9-5} fully randomized fractional factorial design with four additional central points was followed by a full fold-over in a new block to explain some aliased effects. The final design was of resolution IV.

In both experimental scenarios, the analysis of experimental results for analysis of variance (ANOVA) was based on the averages of each experimental run. Matlab scripts and Microsoft Excel® sheets were used for extracting averages and saving results. Vanhatalo et al. (2013) recommend removing apparent dynamic behavior at the beginning of each run to avoid the biased estimation of effects. Nevertheless, in the first experimental scenario, the initial observations were included in calculating the run averages since an effective control action should be able to remove the impact of the factors' level change on the controlled variables. In the second experimental scenario, a transition time of 24 hours was removed prior to the calculation of the run averages. In this case, the response variables were not involved in control loops and the factors' level changes can take time before reaching its full effect.

2.4. Aim III: a simulator for SPC and DoE methods development

The following section highlights the tools and methods used for data collection and analyses in study 5 related to aim III of the research objective.

2.4.1. Study 5: the Tennessee Eastman (TE) process simulator

Study 5 examines how to use the revised TE process simulator (Bathelt et al., 2015b) run under a decentralized control strategy as testbed for SPC and DoE methods. During the study, the guidelines on the required steps to initialize the revised TE process simulator and simulate data for SPC and DoE applications were formulated and illustrated by means of flow charts. The flow charts were created using Bizagi modeler® based on the business process modeling notation (BPMN) (see, for example, Chinosi and Trombetta, 2012; the BPMN archive, 2011). Furthermore, two simulated examples were conducted to demonstrate the strategy for creating random variability in the simulator and potential SPC and DoE applications. For further details, see Paper C, which mainly relates to aim III and, to a lesser extent, aim I of the research objective. The revised TE simulator can in fact simulate most of the challenges described in Paper A.

The first example demonstrates how closed-loop operations affect the shift-detection ability of control charts. The revised TE process simulator was used to simulate Phase I and Phase II data. The free R statistics software was used to analyze the collected data, that is, to build a Hotelling T^2 control chart on the controlled and manipulated variables. The second example employs a response surface methodology approach. The levels change of five controlled variables' set-points were analyzed through sequential experimentation to improve the process operating cost of the TE process. While the revised TE simulator, Microsoft Excel®, and Matlab Scripts were used to simulate the experiments, Design Expert® (version 10) was used to generate the experimental designs and analyze the experimental results.

The sequential experimentation started with a 2_V^{5-1} fully randomized fractional factorial design, with four additional center points to screen the set-points of five controllers. Then, a central composite design was created by augmenting the resolution V fractional factorial design with ten additional axial points run in a new block, allowing for estimation of a second-order model. The numerical optimization tool in Design Expert® (version 10) was used to search for design space and find the settings for the set-points that would produce the lowest predicted cost. Three additional runs were simulated for confirmation. During the sequential stages, the experimental results were analyzed using ANOVA tests based on the averages of each run after removing 24 hours of transition time, as suggested by Vanhatalo et al. (2013).

2.5. Summary of methods used in appended papers

Table 2.2 provides an overview of the methods chosen for the studies connected to the five appended papers and the papers' relationship with the aims of the research objective.

Table 2.2. Overview of the methods choices made in the studies reported in the appended papers.

	Paper A	Paper B	Paper C	Paper D	Paper E
Aim of the research objective	I	II	I, III	II, III	II
Type of paper	Literature review	Research	Research	Research	Research
Target audience	Quality managers, researchers, and practitioners	Researchers and practitioners	Researchers and practitioners	Researchers and practitioners	Researchers and practitioners
Data collection (tools)	Scopus	TE process	Revised TE process	➢ Heat exchanger ➢ Steel rolling mill	Revised TE process
Data collection (methods)	Searches using keywords and queries	➢ DoE ➢ Simulations	➢ DoE ➢ SPC ➢ Simulations	➢ Mathematical derivations ➢ SPC ➢ Simulations	➢ Article by Ricker (1996) ➢ SPC ➢ Simulations
Data analysis (tools/methods)	Sequential screening and classification of publications identified during the searches	ANOVA	➢ ANOVA ➢ Time series plots ➢ Hotelling T^2 chart	➢ Time series plots ➢ CUSUM chart	➢ Qualitative classification of the TE process variables ➢ DPCA ➢ Hotelling T^2 and Q charts
Illustration of the results	Conceptual classification of SPC and DoE challenges in continuous processes	Two simulated examples	➢ BPMN flow charts ➢ Two simulated examples	➢ Mathematical formulas; ➢ Two simulated examples;	Two simulated examples
Software	Microsoft Excel®	➢ Design Expert 9 ➢ Matlab/Simulink ➢ Matlab ➢ Microsoft Excel	➢ Bizagi Modeler ➢ Design Expert 10 ➢ Matlab/Simulink ➢ Matlab ➢ Microsoft Excel ➢ R	➢ Matlab/Simulink ➢ Matlab ➢ Microsoft Excel ➢ R	➢ Matlab/Simulink ➢ Matlab ➢ Microsoft Excel ➢ R

3. RESULTS AND DISCUSSION

This chapter summarizes the results of the studies presented in the five appended papers and discusses the main contributions, implications, and limitations of the research. The results are conceptually organized in relation to the research aims (i.e., around related topics) and therefore do not necessarily follow the order of the appended papers.

3.1. Aim I: SPC and DoE challenges for improving continuous processes

The literature review highlighted several challenges that may arise when applying SPC and DoE methods to continuous processes. As explained in section 2.2.1, these challenges were classified in categories. Figure 3.1 illustrates the categories of SPC and DoE challenges identified during the classification procedure of the literature review and the following sections summarize the main findings. Further details are provided in Paper A.

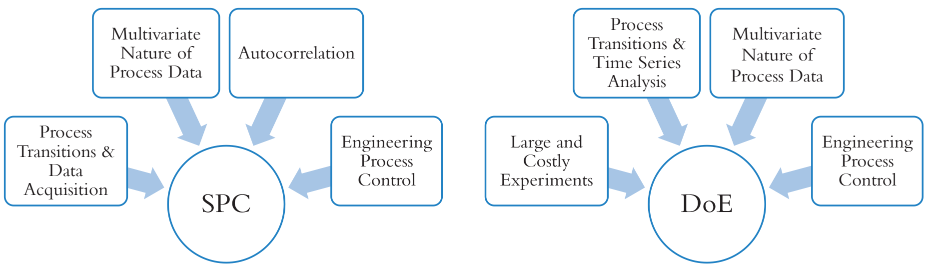

Figure 3.1. SPC and DoE challenges for improving continuous processes identified during the literature review.

SPC in continuous processes

In continuous processes, operating conditions frequently change owing to grade changes, restarts, or process adjustments and process inertia leads to transition phases. Data storage should be designed to preserve the history of transition phases and the interrelation of variables during transitions (Kourti, 2003). The monitoring phase in SPC should begin after the transition is complete (Duchesne et al., 2002). The existing SPC literature recognizes the need for multivariate control charts to monitor multiple quality characteristics or process variables simultaneously as in continuous processes (Ferrer, 2014). Several options need to be considered here. The Hotelling T^2 control chart is commonly used for monitoring up to ten variables exhibiting moderate cross-correlation. When the number of variables is larger, other multivariate SPC methods are available (Shi and MacGregor, 2000; Qin, 2012; Ge et al., 2013). Ge et al. (2013) classify the available process monitoring methods into five categories:

1. Gaussian process monitoring methods (e.g., latent structure variable techniques such as PCA/PLS),
2. Non-Gaussian process monitoring methods (e.g., independent component analysis),
3. Non-linear process monitoring methods (e.g., neural networks),
4. Time-varying and multimode process monitoring (e.g., adaptive/recursive methods), and
5. Dynamic process monitoring (e.g., dynamic multivariate SPC methods).

In these cases, the choice of multivariate SPC methods should depend on the process characteristics (for example, Gaussian/non-Gaussian, stationary/non-stationary, and linear/non-linear) and level of data autocorrelation.

Among the above-mentioned methods, process monitoring based on PCA/PLS is an important quality improvement tool for data-rich environments already used successfully in the process industry (see, for example, Ferrer, 2014; Zhang et al., 2014; Silva et al., 2019). Using PCA/PLS reduces the high-dimensional monitoring problems to a few orthogonal principal components, which can be monitored either individually or simultaneously. Control charts based on PCA/PLS are well equipped to deal with cross-correlated, independent, and stationary data, but autocorrelation and non-stationarity affect their performance (De Ketelaere et al., 2015). To cope with autocorrelation or non-stationarity, certain extensions of the PCA/PLS monitoring methods are also available in the literature. For autocorrelated data and stationary processes, Ku et al. (1995) suggest expanding the original data matrix by adding time-lagged versions of the original variables and transforming the autocorrelation into cross-correlation. The performance of PCA on this extended data matrix is referred to as DPCA. For independent data and non-stationary processes, recursive and adaptive methods are available (see, for example, Li et al., 2000; De Ketelaere et al., 2015). Figure 3.2 illustrates the PCA/PLS methods available for process and data challenges.

The literature review presented in Paper A also highlight some technical issues and development needs to improve the applicability of these methods. While knowledge of the above-mentioned solutions support the adoption of these methods, researchers and practitioners should be aware of the following issues that need to be overcome. Among others, the relevant problems include the following:

- How to simultaneously handle autocorrelation and non-stationarity? (De Ketelaere et al., 2015),
- How to select the number of latent variables to retain and lags to add in DPCA? (Himes et al., 1994; Ku et al., 1995; De Ketelaere et al., 2015; Vanhatalo et al., 2017),
- Fault detection and isolation (Kourti and MacGregor, 1996; Dunia et al., 1996; Yoon and MacGregor, 2001), and
- Handling of outliers in the data (Stanimirova et al., 2007; Serneels and Verdonck, 2008).

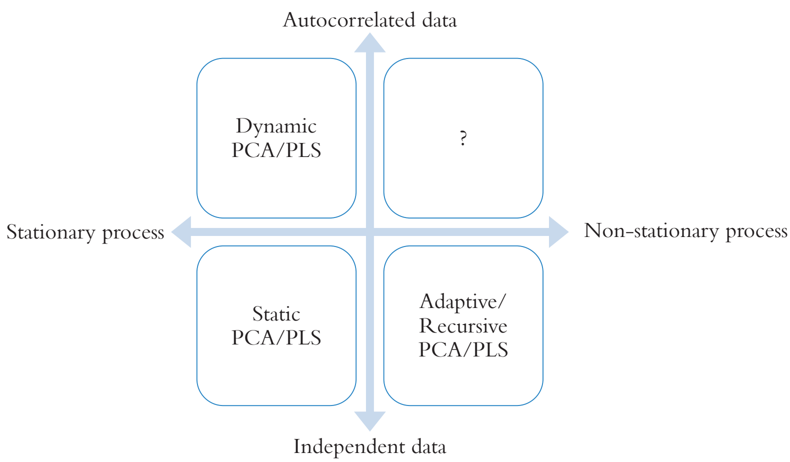

Figure 3.2. Process and data challenges, and available PCA/PLS methods.

Another important SPC challenge that emerged during the literature review is the need to run continuous processes under EPC, such as for feedback controllers. Feedback controllers mitigate unwanted deviations of controlled variables through continuous adjustment of related manipulated variables (see, for example, Ogata, 2010; Romagnoli and Palazoglu, 2012). The propagation of a disturbance through the process might not always be visible in the controlled response variable, but may be displaced to the related manipulated variable (Akram et al., 2012; Siddiqui et al., 2015). The SPC examples simulated in the revised TE process presented in Papers C and E and in the heat exchanger and steel rolling mill simulators presented in Paper D illustrate this behavior.

To detect out-of-control process conditions, the traditional approach of applying a control chart to controlled variable(s) is often replaced with a control chart applied to manipulated variable(s) or a multivariate control chart monitoring the controlled and manipulated variables together (Montgomery et al., 1994; Tsung, 1999). However, the study results presented in Papers D and E show that these approaches might hinder deeper process insight and understanding of out-of-control process conditions. Further details on the implications of monitoring either the manipulated or controlled and manipulated variables in the same multivariate chart(s) will be discussed in section 3.2.1.

DoE in continuous processes

The literature review highlighted both the challenges and existing solutions when conducting experiments in continuous processes. While the challenges affect all the experimental phases (i.e., planning, conducting, and analysis of experiments), the literature review shows that related solutions are not always available, and if available, need to be developed further.

Following the recommendations of Coleman and Montgomery (1993), who highlight the critical importance of the planning phase, Vanhatalo and Bergquist (2007) provide a systematic approach to planning an industrial experiment in continuous processes. The authors present twelve steps for the planning phase, which need to have both technical and organizational choices due to the complexity of large-scale experimentation. The choice of design preferences and factor levels and need for restricted randomization are as critical as the requirement for assigning responsibilities in coordinating the experiment or collecting relevant background information. Vanhatalo and Bergquist (2007) also recommend identifying the presence of controlled variables in the planning phase, suggesting that closed-loop operations affect the entire experimental strategy. Paper A classifies the experimentation in processes under closed-loop control as one of the important issues in continuous process experiments, as conventional DoE methods implicitly assume open-loop operations (Montgomery, 2012a). For further details, see section 3.2.2 and Paper B summarizing the results of study 4, which focuses on the use of DoE in processes under closed-loop.

Planning and conducting experiments in continuous processes also imply unavoidable cost and time constraints (Vanhatalo, 2010). The often lengthy experimental campaigns jeopardize the production plan since the production plant could be unavailable during an experimental campaign or produce off-spec products (Bergquist, 2015b). Nevertheless, the need for improvement often calls for experimentation. The use of simulators to test methodological ideas prior to implementation might be helpful to improve continuous processes. The results of study 5 are presented assuming this perspective (see section 3.3 and Paper C). Moreover, two best practices need to be promoted: [1] support and allocate resources to the planning phase, and [2] create awareness of experimental strategies suitable for large-scale experimentation (Vanhatalo and Bergquist, 2007).

Paper A presents the potential issues that emerge when analyzing experiments conducted in continuous processes. The experimental factors and responses from continuous processes can typically be represented as time series (Vining et al., 2016). In these cases, the existing methods are inadequate to design the experiments and properly analyze them. The literature review highlights that analytical methods such as functional data analysis, shape analysis, and time series analysis receive increasing attention from both academia and industry owing to their considerable importance (He, Z. et al., 2015; Vining et al., 2016). Moreover, continuous processes are dynamic systems with inertia, meaning that the impact of factors' level changes on responses can take time to reach its full impact (Nembhard and Valverde-Ventura, 2003; Vanhatalo et al., 2010; Lundkvist and Vanhatalo, 2014). These transition times need to be considered in the planning and analysis phases because they might affect, for example, the length of experimental runs or estimation of effects.

Other challenges in the analysis phase relate to the use of multivariate methods to analyze the experimental results. In continuous processes, the presence of several cross-correlated responses suggests that a univariate approach to analyses might be ineffective (Ferrer, 2014; Vanhatalo and Vännman, 2008). Latent variable techniques can be used to summarize the information in experimental response variables. The latent variables can then be used as new responses to test the statistical significance of the experimental factors effects. El-Hagrasy et al. (2006), Vanhatalo and Vännman (2008), Baldinger (2012), Souihi et al. (2013), and Storm et al. (2013), among others, provide examples of multivariate analysis combined with DoE.

3.2. Aim II: applying SPC and DoE to continuous processes under feedback control

The following sub-sections summarize the results of studies 2, 3, and 4 in terms of aim II of the research objective, that is, to propose new or adapted SPC and DoE methods to overcome some of the issues due to the presence of feedback controllers. For more details, see Papers B, D, and E.

3.2.1. Monitoring processes under closed-loop control

In a closed-loop system, quality characteristics or process variables that might be interesting to monitor are usually controlled for and kept around desired target values (i.e., set-points). Monitoring only the controlled variables in a control chart will often be unsuccessful because of the controllers' potential masking effect of external disturbances. The literature recommends two basic approaches to monitor a process under feedback control: [1] monitoring the control error, that is, the difference between the controlled variable and set-point value (see, for example, Faltin et al., 1993; Montgomery et al., 1994) and [2] monitoring the manipulated variable (MacGregor, 1991; Faltin et al., 1993). To maximize the chances of detecting out-of-control process conditions, a combined approach of monitoring the controlled variable (or control error) and the manipulated variable in the same bivariate control chart has also been proposed (Tsung, 1999). The same approaches can also be extended to monitor multivariate processes. For further details, see section 1.4.1.

The results of studies 2 and 3, summarized in Paper D and E, indicate that the above-mentioned approaches are valuable for detecting out-of-control process conditions, but might hinder deeper process insight. Instead, as will be explained later, monitoring both controlled and manipulated variables in separate charts might increase the knowledge of the process and controller performance when out-of-control situations occur.

Study 2 deals with single-input single-output processes and illustrates whether and how step and ramp disturbances manifesting themselves on the controlled and manipulated variables depend on the control mode used [proportional (P), proportional-integral (PI), or proportional-integral-derivative (PID)]. The study shows that the ongoing disturbance (step or ramp) and control mode used (P, PI, or PID) determine the pattern (mean shift or trend) of the disturbance signatures on the controlled and manipulated variables. The upper part of Table 3.1 shows on which variables (manipulated and/or controlled) the signature of a step or ramp disturbance manifest itself depending on the control mode used (P, PI, or PID) and the pattern (mean shift or trend) of the signatures. Assuming a set-point equal to zero, the lower part of Table 3.1 provides the formulas for calculating the steady-state values of the controlled and manipulated variables, knowing the step magnitude ($\bar{d}$) or slope of the ramp ($\hat{d}$) and the process (k_p) and controller parameters (k_c, and τ_I). Generally, knowing the magnitude or slope of a disturbance is not a realistic situation. However, using the true steady-state values of the controlled and manipulated variables calculated from the process data, the inverse formulas can be useful to calculate, for example, the magnitude or slope of a disturbance.

Table 3.1. (Upper part) Signatures of step and ramp disturbances on the controlled and manipulated variables depending on the control mode (P, PI, or PID). (Lower part) Steady-state values of the controlled and manipulated variables as functions of the step magnitude ($\bar{d}$) or slope of the ramp ($\hat{d}$) and the process (k_p) and controller parameters (k_c, and τ_I).

Control Mode	Step Disturbance		Ramp Disturbance	
	Controlled variable	Manipulated variable	Controlled variable	Manipulated variable
P	Mean shift	Mean shift	Trend	Trend
PI, PID	No signature	Mean shift	Mean shift	Trend
Control Mode	**Steady-state values**		**Steady-state values**	
P	$\frac{\bar{d}}{1+k_c k_p}$	$-\frac{k_c \bar{d}}{1+k_c k_p}$	$+\infty$	$-\infty$
PI, PID	0 (= set-point)	$-\frac{\bar{d}}{k_p}$	$\frac{\tau_I}{k_c k_p}\hat{d}$	$-\infty$

As an illustration of the results in Table 3.1, Figure 3.3 displays the time series plot and CUSUM chart of the controlled (a-b) and manipulated (c-d) variables of a steel rolling mill under a PI controller. Paper D provides full details on this example. A disturbance occurs around the 500th observation. An analysis of the CUSUM charts on the controlled and manipulated variables indicates that the controller is active (manipulated variable out-of-control), but unable to fully remove the disturbance effect on the controlled variable (i.e., the controlled variable is out-of-control and the process is not performing satisfactorily). Moreover, the (slight) mean shift of the controlled variable and trend pattern of the manipulated variable shown in the time series plots might be a hint of an ongoing ramp disturbance (see Table 3.1).

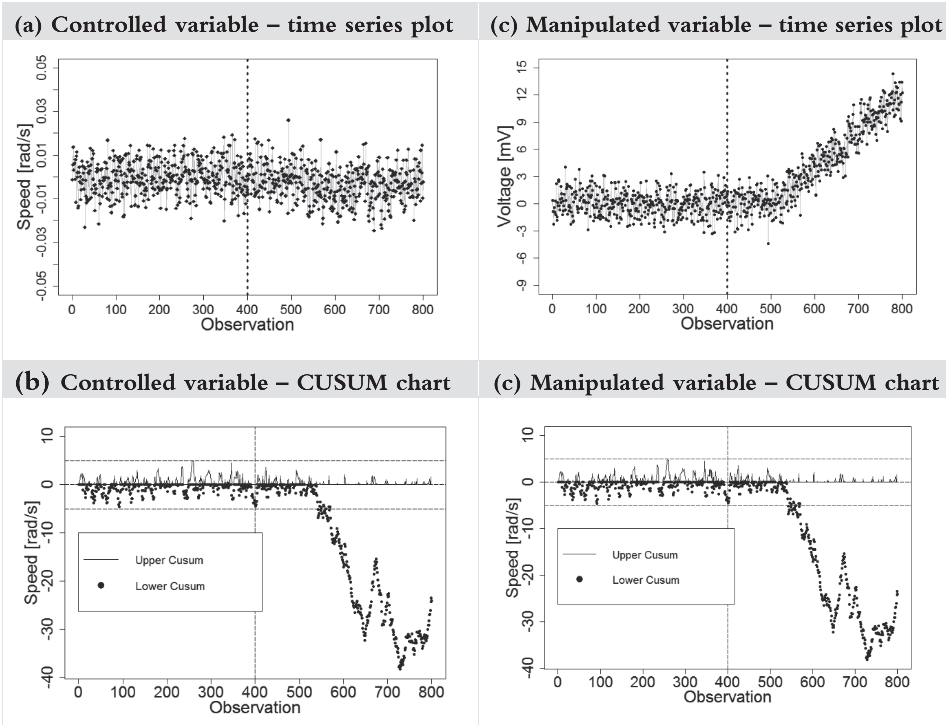

Figure 3.3. Time series plot and CUSUM chart of the controlled (a-b) and manipulated (c-d) variables of a steel rolling mill under a PI controller. The vertical dotted lines divide Phase I and Phase II data. A disturbance occurs around the 500th observation.

The general implication of the results in Table 3.1 is that the P, PI, and PID control modes have limitations on the type of disturbances they can handle. Moreover, the results in Table 3.1 imply that monitoring the steady-state error, manipulated variable, and controlled and manipulated variables together in the same control chart (in this case, a bivariate chart) should enable detection of an out-of-control situation when a step or ramp disturbance occurs. However, none of the approaches illustrated in the literature can provide information on the process and controller performance simultaneously. This process insight can be gained when controlled and manipulated variables are monitored using separate charts.

Study 3 summarized in Paper E can be considered, to some extent, as an extension of study 2 to multivariate processes. In multivariate processes (with multiple inputs and several response variables), feedback controllers need to keep several controlled variables at their set-point values and several manipulated variables are likely to be adjusted. Typically, control loops involve crucial quality characteristics or process variables that need to be kept around target values, for example, to ensure product quality specifications or stable process conditions within equipment constraints. Other response variables related to process performance indicators, such as energy consumption or product waste, might be more difficult or too expensive to control for and are not usually involved in any control loop. These additional response variables (called measured variables here) are generally affected by the process operating conditions and hence assess the overall process performance.

The author of this thesis argues that in a multivariate process (with multiple inputs and several response variables), the response variables can be classified into at least three categories: controlled, manipulated, and measured variables. Akin to study 2 in Paper D, grouping these response variables (the controlled, manipulated, and measured variables) and monitoring them in separate multivariate charts, rather than jointly, might improve the process knowledge as well as controllers' performance when out-of-control conditions occur.

In general, a combined study of the control charts applied to controlled and measured variables provides information on process performance. As mentioned earlier, controlled variables usually relate to the quality characteristics of a product or the process producing it. Out-of-control signals in control chart(s) on the controlled variables might indicate that the process performance and hence product quality are most likely critically affected. However, out-of-control signals in control chart(s) on the measured variables might indicate that the process performance is compromised, even though the product quality might most likely be unaffected.

As in the univariate case, the combined study of the control charts on the controlled and manipulated variables would show the controllers' performance. An analyst can check whether the control action is active or inactive (manipulated variables out-of-control or in control) and its ability or inability to partially or fully compensate for the disturbance (controlled variables out-of-control or in-control). More details on the potential scenarios that an analyst might encounter are provided in Paper E.

The approach often used to monitor all the variables together in the same multivariate chart(s) is valuable to detect out-of-control process conditions. However, this approach does not directly provide the process insight gained by monitoring the variables in groups as illustrated above. Moreover, in case of an out-of-control signal, the suggested approach might support the search of disturbance. When an out-of-control situation occurs, the controllers' action propagates the effect of a disturbance to several process variables, making the contribution plots difficult to interpret (Yoon and MacGregor, 2001; Qin, 2003). Classifying the process variables in "blocks" (or groups) can reduce the "smearing effect" of the contribution plots on non-faulty variables (see, for example, MacGregor and Kourti, 1995; Qin et al., 2001), as the analyst will have to analyze the contribution plots for groups of variables rather than all the variables together.

3.2.2. Experimentation in processes under closed-loop control

Designed experiments imply deliberately changing a set of experimental factors in order to study how important process variables or quality characteristics react. In an open-loop process, the experimenter can discover the potential impact of factor-level changes in the process response(s). In this case, the purpose of DoE is essentially to reveal the potential causal relationships between the experimental factors and process response(s). Typically, in a closed-loop system, the causal relationships between the process inputs (or manipulated variables) and controlled response variables are already established and known, and are normally not the focus of the designed experiment. Generally, the existing relationships between process inputs and response variables are discovered using system identification methods dealing with building dynamic models (usually a set of differential equations) based on observed data from the system (Ljung, 2007). In system identification, experimental data are used to find the optimal input signals and model the system to ensure stability. However, as Paper B shows, designed experiments can improve industrial processes under feedback control supporting in factor screening, factor characterization, or process improvement and optimization.

Closed-loop operations affect all the experimental phases; that is, planning, conducting, and analyzing. Continuous interference by controllers makes the experimentation challenging, as the control action might neutralize the factors' level change impact on the response variables. Moreover, if the experimental factors are not properly chosen in the planning phase, all attempts to change the experimental factors' levels may prove futile because the feedback controllers might counteract their deliberate changes. That is, the input variables involved in control loops (or manipulated variables) cannot be considered as potential experimental factors since they are not free to vary independently.

Study 4, summarized in Paper B, illustrates two potential scenarios for experiments in processes under closed-loops (see Table 3.2). In the first scenario, the experimenter can consider any set of inputs not involved in control loops as potential experimental factors. In a closed-loop system, input variables not involved in control loops behave as disturbances and thus can be viewed as experimental factors. In this case, both the controlled and manipulated variables are interesting response variables. An analysis of the controlled variables will provide information on the presence of controllers if in doubt, and their performance. An analysis of the manipulated variables will reveal whether experimental factors affect the important process phenomena controlled in the loops. To better clarify this concept, consider Figure 3.4.

Table 3.2. Potential experimental scenarios to conduct designed experiments in processes under closed-loop control.

Experimental scenario	Experimental factors	Response variable(s)
1	Process inputs not involved in control loops	Controlled and manipulated variables
2	Controlled variables' set-points	Process performance indicators (e.g., operating cost, energy consumption and, product waste)

Figure 3.4 shows the behavior of the manipulated and controlled variables of the TE process control loop 16 when two inputs not involved in control loops are used as experimental factors. The charts show (a) the controlled variable XMEAS(9), and (b) the manipulated variable XMV(10). The coded levels of the experimental factors XMV(9) and XMV(12) are superimposed in both charts. A simple visual inspection of the charts reveals that the controlled variable is insensitive to the factors' level changes, suggesting the presence of a full-operational controller. Moreover, an analysis of the manipulated variable's chart suggests that the factors' level changes affect the process phenomena controlled in the loop.

In the second scenario, the experimenter can change the controlled variables' set-points to study their effect on process performance indicators, such as cost, product waste, and energy consumption (experimental scenario 2 in Table 3.2). In this case, the change in the set-points' levels is equivalent to moving the process from an operating condition to another. The process performance indicators can be improved by finding "better" set-points-level settings.

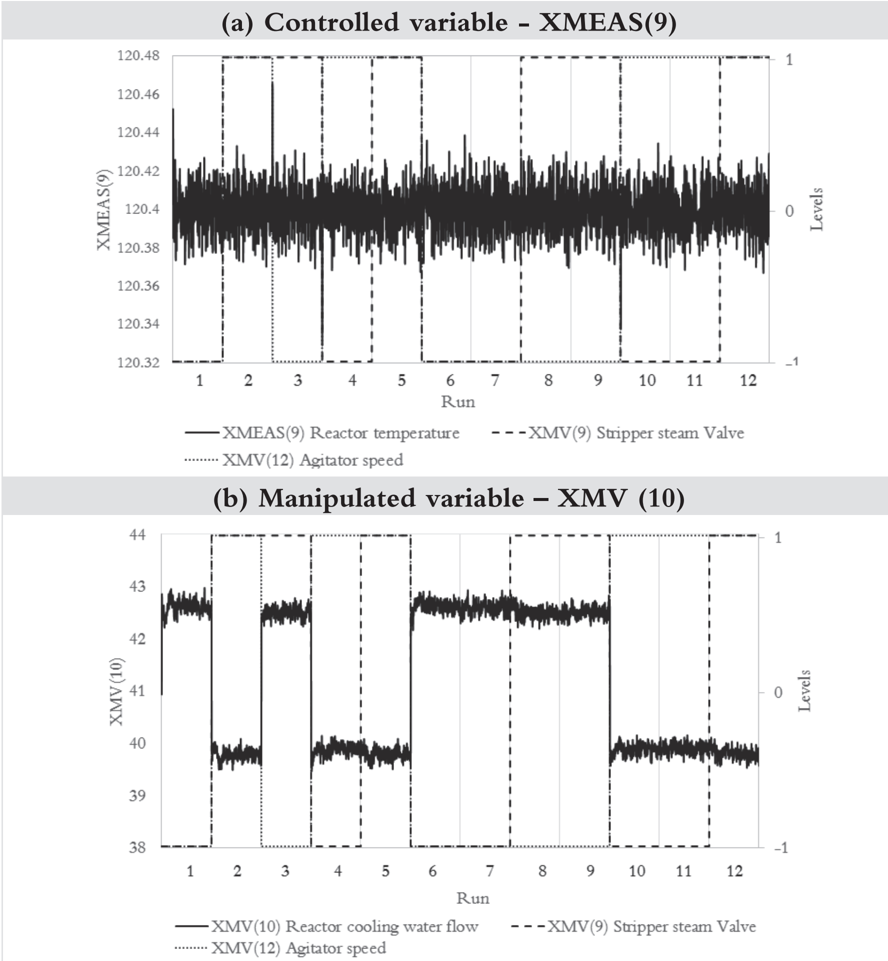

Figure 3.4. Impact of inputs not involved in control loops on the (a) controlled and (b) manipulated variables of the TE process loop 16.

The suggested experimental scenarios for experiments in closed-loop systems can generate knowledge and contribute to process improvement, making it possible to study

- the presence of controllers if in doubt,
- the performance of controllers, that is, whether they are functioning well,

- the impact of experimental factors on process phenomena, and
- how the controlled variables' set-points affect the process performance indicators.

3.3. Aim III: the TE simulator for SPC and DoE methods development

New SPC or DoE methods development is generally difficult to test in real continuous process plants. SPC method development does not usually affect the production plant, but the need for datasets with specific characteristics, such as sample size, sampling time, and occurrence of a known fault, could limit or slow down the testing process. Conversely, DoE method development may jeopardize the production plant and affect the production goals. Production engineers and managers may find it inconvenient to invest time and money on lengthy experimental campaigns. Simulation tools can thus be instrumental in SPC and DoE method development.

Reis and Kennet (2017) map a wide variety of resources and simulators that can be used to teach statistical methods, such as Rice Virtual Lab in Statistics, StatLab, and PenSim[8]. The authors classify the simulators based on three characteristics: [1] linear/non-linear elements in the simulation model, [2] time-independent/time-dependent behavior, and [3] size of simulator. In this classification, the TE process is considered one of the most complex and realistic simulators since it mimics a large-scale, non-linear, and dynamic process. Moreover, the TE process simulator has to be run with an implemented control strategy to overcome its open-loop instability (Downs and Vogel, 1993).

The decentralized control strategy of the TE process (Ricker, 1996) is attractive from an SPC and DoE methods development perspective because it can mimic the challenges frequently found in continuous processes (see sections 1.4 and 1.6). Ricker (1996) devised the decentralized control strategy of the TE process and implemented a simulator in Matlab/Simulink® (Ricker, 2005). Recently, Bathelt et al. (2015a; 2015b) implemented an upgraded version of Ricker's simulator, the revised TE process simulator, in Matlab/Simulink®. Table 3.3 compares the main characteristics

[8] Rice Virtual Lab in Statistics offer an online statistics open textbook and additional resources to assist students in understanding statistical concepts (http://onlinestatbook.com/rvls.html). StatLab is a free web-based application for supporting teaching the basics of DoE (https://www.win.tue.nl/statlab/). PenSim is a web-based simulator designed for students' education that simulates a fed-batch penicillin production (http://simulator.iit.edu/web/pensim/).

of the decentralized TE process simulator strategy of Ricker (2005) and the revised TE process simulator strategy of Bathelt et al. (2015b).

From Table 3.3., the revised TE process simulator offers more flexibility than the simulator originally developed by Ricker (2005). These new possibilities discovered while developing study 5 and summarized in Paper C widen the usability of the revised TE process simulator, making it more suitable for testing the SPC and DoE methods. The illustrated examples in Papers B and C simulated using Ricker's simulator and the revised TE process, respectively, highlight this concept as well. Among the most relevant features, the possibility of changing the seed of each simulation and scaling random disturbances allows for introducing random variation in the simulation results, which is essential for testing SPC and DoE methods. Moreover, from an SPC perspective, the possibility of scaling process disturbances allows for testing the sensitivity of SPC methods. However, the revised TE process lacks a graphical user interface (GUI). New users might find it challenging to understand the details of the revised TE process and to run it. Thus, the results of Paper C are illustrated in order to support the interaction between a new user and the simulator. Flowcharts using the Business Process Modelling Notation (BPMN) provide a step-by-step description of how to use the simulator, and simulate data for SPC and DoE applications.

Table 3.3. Comparison of the main characteristics of the decentralized TE process of Ricker (2005) and the revised TE process of Bathelt et al. (2015b).

Characteristic	Decentralized TE process (Ricker, 2005)	Revised TE process (Bathelt et al., 2015b)
Set simulation seed	No	Yes
Set simulation length and sampling frequency	Yes	Yes
Introduce process disturbances	Yes	Yes
Scale process disturbances	No	Yes
Monitor output of the disturbances	No	Yes
The random generator uses different state variables for process disturbances and measurements noise	No	Yes
Possibility to pause and resume the simulation using final process conditions	Yes	Yes
Repeatability of simulation results	No	Yes
Graphical user interface (GUI)	No	No

3.4. Research limitations

The conclusions and recommendations drawn from the studies related to aim II of this thesis are based on data collected through simulations. Papers B and E used the TE process as testbed for the adapted SPC and DoE methods. The data for Paper D were collected using simulators of two common industrial applications, that is, a heat exchanger and a steel rolling mill.

The method chosen for data collection via simulations has both advantages and disadvantages. From an SPC perspective, the use of simulators implies the immediate availability of datasets with the desired characteristics (sampling time, number of observations, type of process disturbance, and so on). From a DoE perspective, the use of TE simulators implies the availability of a realistic process to test new experimental methods. Finding industrial partners willing to share their production data for SPC methods development is potentially easier than finding those willing to share their production plants for conducting lengthy and costly experimental campaigns. Testing new DoE methods would be feasible if the company is proposing to run experiments with the sole aim of improving the production process. Thus, DoE methods development might be limited due to the lack of available industrial partners willing to support the research ideas.

The main drawback of working with simulators is that the SPC analyst or experimenter cannot consider the challenges that would emerge when working in real environments. Among them, in SPC applications, the collection of data from multiple and interconnected sources and massive datasets is common for continuous processes. Thus, what data and how to handle them properly will become crucial in addressing questions of interest. In DoE applications, planning, conducting, and analyzing experiments would need a transversal organization in real processes. Moreover, replicates of experiments will most likely not be possible. Unforeseen events, unexpected complications during experimental runs, or lack of coordination and information might also affect the experimental results, thus further challenging the testing process of the methods.

The suggested SPC and DoE methods in the research tested on simulated data can be applied to real continuous processes. However, one can fairly expect these methods to be implemented considering the needs of the production environments.

3.5. Main contributions

This research explored the challenges usually encountered when applying SPC and DoE methods to continuous processes, with focus on the adapted strategies to overcome some of the issues due to one of the identified challenges, the presence of feedback controllers. This research also proposed simulation tools that can be used in SPC and DoE methods development.

Creating awareness of potential challenges when applying SPC and DoE methods to continuous processes is an essential step supporting the development of these methods. This research reinforces the knowledge of SPC and DoE methods development needs and suggests the current remedies found in the literature to overcome these challenges. A first contribution of this research is to show the researchers the SPC and DoE challenges that need to be overcome and to encourage practitioners and quality engineers to adopt these methods and benefit from them.

Other contributions of this research come from the SPC and DoE methods suggested for application to continuous processes under feedback control. Feedback controllers challenge the implicit SPC and DoE assumption of open-loop operations. From an SPC perspective, feedback controllers imply that the quality characteristics or process variables potentially interesting to be monitored are controlled for and kept around desired target values. Generally, the impact of external process disturbances are displaced from the controlled to manipulated variables. Monitoring only the controlled variables might be futile. The approaches suggested in the literature for monitoring processes under feedback control mainly focus on detecting out-of-control process conditions (see section 1.4.1). Certainly, the detection of out-of-control conditions is a key aspect of an effective process monitoring procedure. However, this research assumes a broader perspective. The suggested SPC methods for monitoring under feedback control emphasize how the process knowledge and understanding can improve when an out-of-control situation occurs. Another contribution of this research is to suggest a monitoring procedure for processes under feedback control that jointly uses the information from the control charts and controllers to improve the process knowledge and the controllers' performance when out-of-control situations occur. This enhanced knowledge can be achieved monitoring the controlled, manipulated, and measured variables (if they exist) simultaneously, but in separate charts. The following questions can be answered simultaneously using the suggested approach: Is the compensatory control action active? Is the controller able to fully remove the impact of a disturbance on the controlled variables? Is the disturbance affecting the process phenomena controlled for in a closed-loop? Is the controller in place able to handle the ongoing disturbance?

A direct implication of this enhanced knowledge is to provide support to search and identify the disturbance. In single-input single-output processes controlled for by varying the PID controllers, step and ramp disturbances leave distinctive signatures on the controlled and manipulated variables. Thus, monitoring the controlled and manipulated variables simultaneously and in separate charts provides information on process and controller performance and indicates the potential disturbances affecting the process.

As in single-input single-output processes, an SPC analyst can monitor the controlled, manipulated, and measured variables of a multivariate process under feedback control in separate control charts. This will show the SPC analyst whether the control action is active, its ability or inability to deal with the ongoing disturbance, and whether an out-of-control condition is affecting the process phenomena controlled for in a loop. Although it is more challenging to understand the disturbance signature in a multivariate process than in a univariate process, the suggested approach can support the search and identification of an ongoing disturbance. As for an out-of-control condition, identification of the disturbance might be easier because the analyst will have to analyze the contribution plots for groups of variables rather than for all the variables at once. The suggested approach can thus mitigate the so-called smearing effect (Yoon and MacGregor, 2001; Qin, 2003), that is, the spreading of disturbance on the non-faulty variables.

From a DoE perspective, the main contribution of this research pertains to the benefits of using experimental methods in process under closed-loop, a different framework compared to the one usually found in textbooks or traditional DoE applications. The research provides an adapted framework to widen the applicability of DoE methods to industrial processes under feedback control. The traditional open-loop experimental framework is adjusted to the closed-loop framework and the implications are discussed. In this adjustment, the two suggested experimental scenarios classify the potential experimental factors as either a set of inputs not involved in the control loops, or the set-points of the controlled variables (see Table 3.2). In the former case, the manipulated and controlled variables become the responses. In the latter case, the typical responses include process performance indicators such as cost, product waste, or energy consumption.

The adapted SPC and DoE methods for application to processes under feedback control constitute a contribution to the quality engineering field, and also provide useful suggestions to industrial practitioners and engineers interested in quality control and improvement of continuous processes.

The last main contribution of this study is to provide detailed guidelines on how to use the TE process, a flexible simulation tool, to further develop SPC and DoE methods and overcome the challenges presented by continuous processes. The TE process has been used for methodological work especially in the SPC field for a long time. However, the previous simulator's deterministic nature has most likely hampered the researchers in choosing development work and making fair comparison of methods. This study promotes the use of the TE process simulator widely used in the control theory field for SPC and DoE methods development. Following the ideas and recommendations presented in this study, the deterministic nature of the TE process can be overcome and the simulator can become a valuable tool for SPC and DoE methods development. Moreover, the TE simulator can play a key role in teaching SPC and DoE concepts in statistical and quality engineering courses in academia. Thus, this last contribution of the study is undoubtedly the most valuable one for researchers interested in SPC and DoE methods development and academics interested in teaching SPC and DoE concepts.

PART III: FUTURE RESEARCH

"Somewhere, something incredible is
waiting to be known."
Carl Sagan

4. FUTURE RESEARCH DIRECTIONS

This chapter presents ideas and new questions for future research that emerged during the Ph.D. research education and that I would like to pursue in the future.

SPC and DoE methods can be valuable to support product and process quality improvement, but companies will not gain full advantage without adjusting these statistical methods to the new production environments. In later years, the research community can reasonably be assumed to focus increasingly on the challenges offered by data-rich manufacturing environments. Moreover, SPC and DoE methods and their implementation can be affected by the new industrial revolution, Industry 4.0. SPC and DoE methods will most likely be increasingly used along with machine learning and artificial intelligent to gain full advantage from simultaneous application. Nevertheless, both methodological and application-oriented SPC and DoE research will still be needed to solve problems arising from the process industry.

Considering the background and development of this research, future studies can explore both methodological and applied directions. The availability of the revised TE process as flexible simulator and testbed for method development allows for undertaking more theory-oriented studies of the challenges described in the thesis, such as the multivariate nature of process data, process dynamics, and closed-loop operations. Moreover, thus far, most of the multivariate SPC methods suggested in the literature have been tested using pre-simulated training and testing datasets from the TE process. The characteristics of the revised TE simulator make it possible to revisit the suggested multivariate SPC methods and perform improved and more realistic comparative studies between existing methods or between existing and new methods.

The research related to the challenge of applying SPC and DoE methods in continuous processes under EPC is a very recent topic, and could offer a rich research path to explore in the future. A natural continuation of the research undertaken in Paper D could be, for example, to run extensive simulations and study the sensitivity of commonly used control charts in processes governed by variations of PID controllers in relation to the controllers' parameters. This type of studies could benefit both univariate and multivariate processes. Further development of the research in Paper E could investigate how different types of disturbances manifest themselves on the controlled, manipulated, and measured variables of a multivariate process. The results could be valuable to support the search and identification of process disturbances. More research related to fault identification and isolation tasks in processes under EPC is also needed. In the future, an integrated framework that helps in understanding controller and process performances simultaneously can provide more powerful tools for improved disturbance diagnosis.

More research to develop the adapted or new DoE methods for processes operating under EPC can provide useful contributions to the DoE field. For example, analysis methods to model the dynamic relations between several experimental factors and the time series response(s) would be interesting to explore. From this perspective, the first experimental scenario described in Paper B is of special interest (see Table 3.2). A more in-depth study of the process control theory could lead to more advanced analysis methods of experimental results, where a closed-loop system could be transformed into its relative open-loop system. If the effect of control action could be filtered back from the controlled variable, the experimental factors change effects on the "back-filtered" variables could be analyzed and compared with those on the manipulated and controlled variables.

Further interesting research relates to how to adapt and apply sequential experimentation methods such as response surface methodology (RSM) and evolutionary operations (EVOP), to processes under feedback control. Adjustments of the experimentation strategies may be needed in this framework because, for example, the response variable(s) to be optimized may not be immediately clear.

A more in-depth study of the process control and system identification theory is therefore crucial and highly necessary to develop the above-mentioned ideas and nurture further research in developing SPC and DoE methods.

APPENDIX – Research Process

Figure A.1 illustrates a Gantt chart showing the main research activities of this doctoral study that led to the five appended papers. The authors' contributions to the appended papers are also highlighted (for more information refer back to section 1.5). In the chart, upside down triangles mark the beginning of a research study, circles indicate conference presentations for the appended papers, and triangles and diamonds indicate the papers that have been submitted or accepted for publication, respectively.

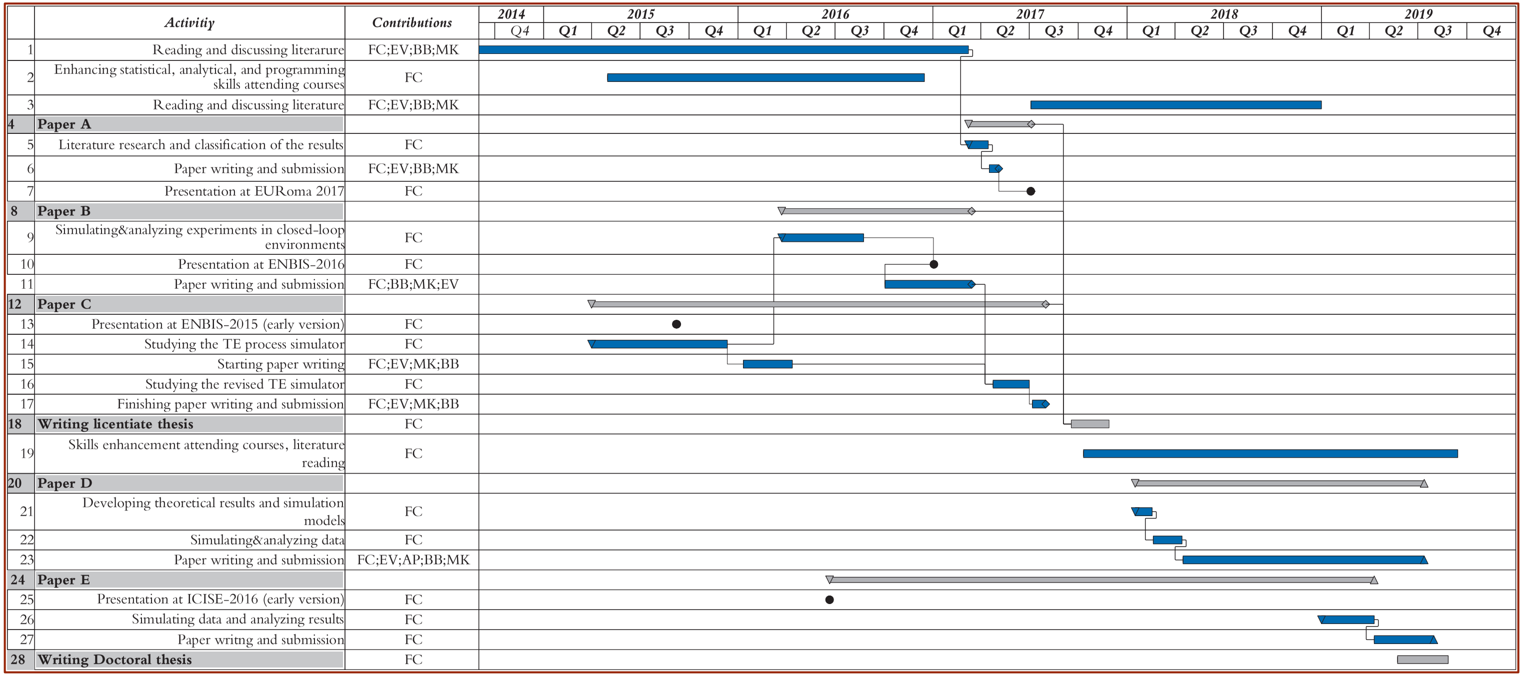

Figure A.1. Gantt chart showing the main research activities from the beginning of my research education until the doctoral defense seminar. The authors' contributions to the appended papers are also highlighted (FC = Francesca Capaci; EV = Erik Vanhatalo; BB = Bjarne Bergquist; MK = Murat Kulahci; AP = Ahmet Palazoglu)

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PART IV: APPENDED PAPERS

"It always seems impossible
until it's done."
Nelson Mandela

PAPER A

Managerial Implications for Improving Continuous Production Processes

Capaci, F., Vanhatalo, E., Bergquist, B., and Kulahci, M. (2017)

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Managerial implications for improving continuous production processes

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Abstract

Data analytics remains essential for process improvement and optimization. Statistical process control and design of experiments are among the most powerful process and product improvement methods available. However, continuous process environments challenge the application of these methods. In this article, we highlight SPC and DoE implementation challenges described in the literature for managers, researchers and practitioners interested in continuous production process improvement. The results may help managers support the implementation of these methods and make researchers and practitioners aware of methodological challenges in continuous process environments.

Keywords: Productivity, Statistical tools, Continuous processes

Introduction

Continuous production processes (CPPs), often found in, e.g., pulp and paper, chemical, steel, or other process industries, constitute a significant part of goods production. In a CPP, the product is gradually and often with minimal interruption refined through different process steps (Dennis and Meredith, 2000). Raw materials in these processes often stem directly from natural resources and characteristics of inputs such as ores or wood will therefore vary substantially. CPPs are often large-scale and tend to include interconnected process steps and complex flows. Continuous production environments are typically inflexible producing only one or a few products, require large investments, and occupy a large area. Wear and varying raw material characteristics are examples of frequent disturbances, making engineering process control (EPC) necessary to stabilize product quality and process characteristics (Montgomery et al., 1994; Box and Luceño, 1997). Although EPC keeps quality characteristics on target, CPPs require continuous improvements to remain competitive (Hild et al., 2001).

The main possibilities to learn and improve any process come from the analysis of observational and experimental process data. While first principles support correlations among observational data, process analyst usually needs experiments to discover causal relationships in industrial processes (Montgomery, 2012).

In this article, we focus on statistical process control (SPC) and design of experiments (DoE) since they constitute two fundamental process improvement methodologies. The purpose of SPC is to monitor the process and reduce process variation through identification and elimination of assignable causes of variation. In the SPC field univariate and multivariate control charts constitute the most important improvement tools. Alarms issued by control charts indicate the presence of potential assignable causes (i.e., unusual events). Root-cause analysis is the next step to uncover reasons for these events and if possible, to eliminate their causes. SPC is a long-term improvement methodology, while EPC is a short-term control strategy that transfers variability from the controlled variable to manipulated variables (MacGregor and Harris, 1990). The purpose of DoE is to plan, conduct and analyse experiments to improve products and processes in a systematic and statistically sound manner.

Since their introduction in the early twentieth century, management controlled improvement programs such as Robust Design, Total Quality Management, and Six Sigma have been promoting these methodologies. Their apparent omission from the currently popular lean program descriptions, as well as methods within popular data analytics and machine learning, indicate that textbook implementation of these methods may be ill-suited for today's production environment. It is becoming increasingly apparent that standard SPC and DoE methods need to be adapted to challenges such as rapid data collection from multiple and interconnected sources and massive datasets (Vining et al., 2015), which are common for CPPs. We argue that DoE and SPC are far from obsolete and that companies will not take full advantage of the big data transition without such proper statistically based methodologies for learning and improvements. However, practitioners must be aware of the challenges that this data rich environment brings to SPC and DoE.

McAfee et al. (2012) highlight leadership and decision-making as important management challenges in the big data era. If managers of CPPs understand SPC and DOE challenges, they can support pairing their data with effective improvement methods. Hild et al. (1999) suggest using thought maps to promote improvement methods and critical thinking. While managers need to be aware of techniques such as DoE and SPC to reduce resources, to meet customer requirements and, perhaps most important, they should also promote their use (Lendrem et al., 2001; Bergquist and Albing, 2006; Tanco et al., 2010).

The purpose of this article is to highlight challenges and development needs described in the literature for SPC and DoE in CPPs. We also provide some examples of state-of-the-art solutions to current challenges.

Method

Literature searches were conducted in April 2017 using the Scopus database, limited to publications in English in the last 30 years (1987->). Table 2 and 3 show sequential search steps and keywords used. We examined reference lists of selected publications in Search 4 to minimize the risk of missing relevant publications, following recommendation by Randolph (2009).

Table 2 – Search terms and number of publications in each step in the SPC search.

Search #	*Search terms and queries*	*Step 1*	*Step 2*	*Step 3*	*Step 4*	*Step 5*
Search 1	(“statistical process control”) *AND* (“continuous process” *OR* “continuous production”)	136	32	14	Classification	23 (7)
Search 2	(“statistical process monitoring”) *AND* (“continuous process” *OR* “continuous production”)	16	2	0		
Search 3	(“statistical process monitoring”) *AND* (“process industry”)	9	4	3		
Search 4	References of selected publications in Search 1, 2 and 3	436	64	35		

The initial sample from Step 1 is the number of publications found using the keywords in Scopus. Duplicates were deleted in each search. In Step 2, the initial sample was reduced by screening titles, author keywords, and sources. Conference articles were excluded if a later journal article of the same authors and with the same title was found. Many publications were rejected after abstracts were read in Step 3. We then classified challenges or development needs for DoE and SPC in CPPs in Step 4. Publications were further analysed in Step 5 to identify the central or pivotal publications on which our results are mainly based. Additional relevant publications known by the authors (indicated in brackets at Step 5 in Tables 2 and 3) were also added and analysed.

Table 3 – Search terms and number of publications in each step in the DoE search.

Search #	*Search terms and queries*	*Step 1*	*Step 2*	*Step 3*	*Step 4*	*Step 5*
Search 1	(“design of experiments”) *AND* (“continuous process” *OR* “continuous production”)	49	27	8	Classification	20 (11)
Search 2	(“experimental design”) *AND* (“continuous process” *OR* “continuous production”)	50	25	15		
Search 3	(“experimental design”) AND (“process industry”)	12	7	2		
Search 4	References of selected publications in Search 1, 2 and 3	877	66	40		

SPC challenges in continuous production processes

The literature review revealed many technical solutions to challenges arising when using SPC in continuous processes. The aim of this section is to provide an overview of challenges and potential strategies that managers can promote. Technical details are therefore not be completely covered in this article.

Process transitions and data acquisition

Operating conditions frequently change due to grade changes, restarts or process adjustments and process inertia leads to transition phases. Data storage should be designed as to preserve the history of transitions phases and interrelation of process variables during transitions (Kourti, 2003). Process transitions may involve loss of production time and increased costs due to produced sub-grade products. The monitoring phase in SPC should begin after the transition is complete (Duchesne et al., 2002). Moreover, properly stored historical data is crucial to gain process knowledge.

Multivariate nature of process data

Important reactions such as phase changes from ore to metal are difficult to measure accurately. Instead, engineers try to measure a multitude of secondary variables such as temperatures and pressures as proxies to the real, hidden process events. Technological development continuously reduces sensor costs and increases data storage capacity.

Today measuring, e.g., a reactor temperature at multiple locations is easily achieved. With many underlying phenomena, the analyst soon has hundreds of cross-correlated variables that need simultaneous monitoring. A univariate approach with each variable in separate control charts is inefficient and often misleading.

Fortunately, there are many multivariate SPC tools available (see, e.g., Shi and MacGregor, 2000; Qin, 2012, and Ge et al., 2013). These methods can be classified in five categories: *Gaussian process monitoring methods* (e.g. latent structure variable methods), *non-Gaussian process monitoring methods* (e.g. independent component analysis), *non-linear process monitoring methods* (e.g. neural networks), *time varying and multimode process monitoring* (e.g. adaptive/recursive methods), and *dynamic process monitoring* (e.g. dynamic multivariate SPC methods). The choice of multivariate SPC method depends on assumed process characteristics: Gaussian/non-Gaussian, static/dynamic, and linear/non-linear. Data characteristics such as if data are two or multidimensional or if data can be assumed to be time independent also affect the choice. An important multivariate process monitoring technique is to use a few linear combinations of the process variables (the so-called latent variables). Multivariate monitoring based on latent variables such as Principal Component Analysis (PCA) and Partial Least Square (PLS) are popular and important especially due to their dimensionality reduction properties (Frank and Friedman, 1993; MacGregor and Kourti, 1995). Kourti et al. (1996) provide a review of examples with industrial applications of latent variable monitoring techniques in process plants such as a chemical smelter, a polymerization process, a pulp digester, and others. Ferrer (2014) illustrates how latent variable methods for process understanding, monitoring and improvement can be used effectively in a petrochemical CPP. Latent variable techniques use the process variables' cross-correlation. Process monitoring uses a few linear combinations of the process variables (the so-called latent variables). Commonly, a Hotelling T^2 control chart simultaneously monitors the retained latent variables from the PCA/PLS model whereas the squared prediction error (Q) chart monitors the model's residuals. When the charts signal an out-of-control observation, these composite statistics are often decomposed into the original variables for fault identification (Himes et al., 1994; Ku et al., 1995; Kourti and MacGregor, 1996; Yoon and MacGregor, 2001; De Ketelaere et al., 2015)

Serial correlation (autocorrelation)

Process variables in CPPs are often highly (and positively) autocorrelated due to high sampling rates and process dynamics. This challenge is increasing due to sensor development and availability of almost unlimited data storages. Serial correlation usually means that the current observation is similar to the previous one. Since autocorrelation affects the estimation of the process' variability, autocorrelation can lead to increased false alarm rates in both univariate and multivariate control charts or incorrectly estimated process capability indices (Tracy et al., 1992; Runger, 1996; Mastrangelo et al., 1996; Bisgaard and Kulahci, 2005; Jarrett and Pan, 2007).

Two ways to handle SPC of multivariate, autocorrelated data have been suggested. The first employs a standard univariate or multivariate control chart but with adjusted control limits to achieve the desired in-control alarm rate. The second requires 'filtering out the autocorrelation' through a univariate or multivariate time series model and applying a control chart to the residuals from this model. However, fitting a multivariate time series model with many variables is difficult.

Latent variables based SPC is recommended for cases with multiple and highly cross-correlated process variables. Vanhatalo and Kulahci (2015) show that autocorrelated process variables still affect the monitoring performance of PCA based control charts since the principal components also are autocorrelated. Control charts based on PCA/PLS are well equipped to deal with cross-correlated, independent, and stationary data but will be affected by autocorrelation. De Ketelaere et al. (2015) review extensions of PCA/PLS based monitoring methods available for more complex process and data characteristics, see Figure 1. Specifically, dynamic PCA/PLS have been promoted for handling the autocorrelation by adding time-lagged variables (Ku et al., 1995) to transform autocorrelation into the cross-correlation that is suitable for PCA/PLS.

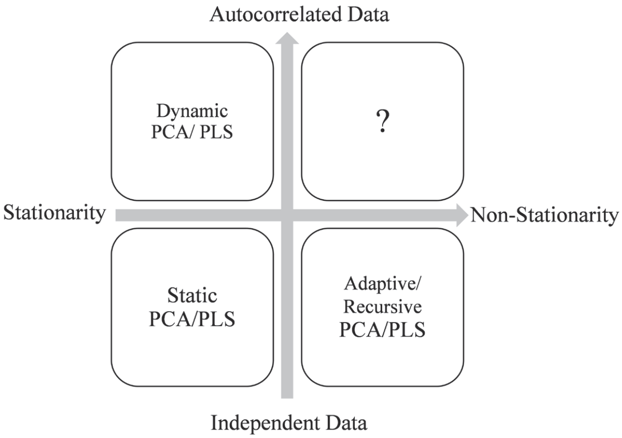

Figure 1 – Process and data challenges and available PCA/PLS methods.

Process capability analyses are important and popular for assessing process performance, frequently used in six sigma companies and promoted by various management and industrial systems standards. However, positive autocorrelation would lead to an overestimation of process capability indices (Shore, 1997; Zhang, 1998; Sun et al., 2010; Lundkvist et al., 2012).

The literature seems to lack a comprehensive solution to assessing process capability from processes with autocorrelated and multivariate data. Pan and Huang (2015) develop two multivariate process capability indices for autocorrelated data and compare their performance via a simulation study and, Mignoti and Oliveira (2011) propose an adjustment of multivariate capability indices to handle autocorrelation.

Presence of engineering process control

Fault detection using SPC control charts could fail when EPC is applied. Integrating SPC and EPC requires applying control charts to manipulated and not to controlled process variables. Box and Kramer (1992) provide a comprehensive discussion on the interface between EPC and SPC and Montgomery et al. (1994) demonstrate the effectiveness of integrating SPC and EPC in process surveillance. Contributions related to this challenge for most CPPs can also be found in Box and Luceño (1997), Janakiram and Keats (1998), Capilla et al. (1999), Tsung (2000) and in Huang and Lin (2002).

DoE challenges in continuous production processes

The literature seems unanimous on the benefits of using DoE but also on the need of managerial support for increased use of DoE in industry (Tanco et al., 2009; Bergquist, 2015b). In this section, we describe specific challenges when applying DoE in CPPs but also suggest remedies.

Large scale and costly experimentation

Operations in CPP plants typically occur around the clock with few operators in charge. Full-scale experiments may thus involve the majority of the production staff, making managerial support, coordination, and information flow essential. Moreover, the often lengthy experimental campaigns can jeopardize the production plan. Previously unexplored factor settings may lead to production of low-grade products. Time and costs are therefore unavoidable constraints. Nevertheless, the need for improvements often make experimentation necessary. Relevant examples include Wormbs et al (2004) who describe experimentation to evaluate production methods of milk using a three factors, two-levels full factorial design in a dairy company and, Gonnissen et al. (2008) who show how a continuously produced powder mixture can be optimized using DoE.

We have found two best practices that managers can promote: (i) support and allocate resources to the planning phase of the experiment and (ii) create awareness of experimental strategies suitable for large scale experimentation.

Montgomery (2012) and Box et al. (2005) highlight the planning activities preceding the actual experiments. However, recognizing that the planning phase is seldom a taught skill, Coleman and Montgomery (1993) provide a systematic approach to plan an industrial experiment. Later, Vanhatalo and Bergquist (2007) adapt this approach to CPPs. Beside a well-chosen design, the planning phase should include, e.g., a clear problem statement, background such as expert knowledge or previous experiments, and someone responsible for coordination and information flow. Of special importance for CPPs is a list of experimental restrictions such as the number of possible experimental runs, easy/hard-to-change factors, randomization restrictions and design preferences.

Due to restrictions, cost, and time constraints, experiments in CPPs typically involve few factors, runs and replicates (Vanhatalo and Bergquist, 2007). Two-level (fractional) factorial designs are especially important to reduce the number of runs and factor level changes (Bergquist, 2015a). Box-Behnken designs also require few runs and are particularly suitable when extreme regions of the experimental space need to be avoided (Stazi et al., 2005; Kamath et al., 2011; Iyyaswami et al., 2013). Needs for restricted randomization, for instance to minimize transition times, may require split-plot designs (Sanders and Coleman, 1999; Bjerke et al., 2008; Vanhatalo and Vännman, 2008).

Response surface methodology (Box and Wilson, 1951; Myers et al., 2004) and evolutionary operation (Box, 1957) are two useful sequential experimental strategies when the goal is process optimization. Kvist and Thyregod (2005) demonstrate evolutionary operation for optimizing an industrial enzyme fermentation process.

Closed loop process operation

Applying EPC means running CPPs under closed-loop control, which complicates experimental design and analysis. Conventional DoE methods make the implicit assumption of open-loop operation in which effects of changes of experimental factors on responses may be studied directly. In closed-loop, many potentially interesting variables are kept around a certain values (set-points) to achieve desired product quality and/or for plant safety reasons. Potential effects of experimental factors on controlled variables are masked when manipulated variables are adjusted to counteract their deviations from set-points (Figure 2).

Capaci et al. (2017) suggest two closed-loop experimental strategies that classify the potential experimental factors as either a set of system inputs not involved in control loops or the actual control loop set-points, see Figure 2. In the former case, the manipulated variables become the responses. The experimenter can also use controlled variables as responses to study controller effectiveness. In the latter case, typical responses include overall process performance indicators such as cost and/or quality.

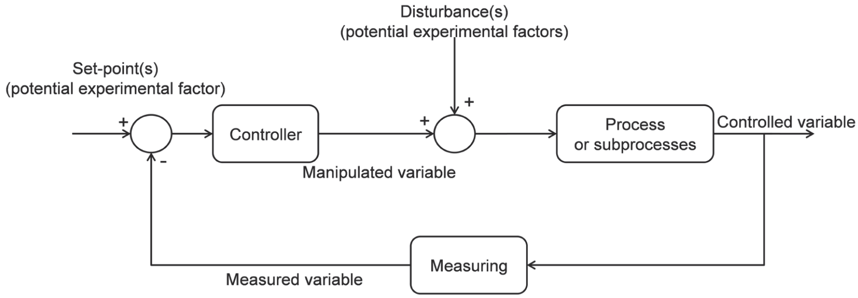

Figure 2. Schematic overview of process operating under closed-loop control

Process transitions and time series responses
High sampling frequencies in CPPs produce time series responses. Moreover, process dynamics often cause effects of experimental factors to develop gradually and then stabilize (Nembhard and Valverde-Ventura, 2003; Bisgaard and Khachatryan, 2011). These process transitions need consideration. Vanhatalo et al. (2013) develop possible analysis methods for experiments with time series responses. If the analyst can estimate the transition time (see for example Vanhatalo et al., 2010), the analyst can (i) use averages of the response in each run after eliminating transition time or (ii) use transfer function-noise modelling. However, transition times may prolong experimentation since it may be unclear when the process reaches steady state. Lundkvist and Vanhatalo (2014) apply a version of the second method to model time series of factors and responses of a full-scale blast furnace experiment. He et al. (2015) provide a recent review of additional available methods to analyse dynamic process responses in DoE.

Multivariate responses
Cross-correlations among responses often make multivariate analysis methods effective. Applications of multivariate projection methods such as PCA and PLS have been used to reduce the dimensionality and restrict the loss of information compared to univariate response analysis. A multivariate analysis approach also controls the Type I error rate. Vanhatalo and Vännman (2008) use principal components as new responses for a blast furnace experiment. El-Hagrasy et al. (2006), Baldinger (2012) and Souihi et al., (2013) provide additional multivariate analysis examples in DoE.

Conclusions and discussions
In this article, we focus our attention on discussing challenges of employing SPC and DoE for improving CPPs. Existing challenges do not mean that these methods cannot be used or should be discouraged. Similar or other challenges will be encountered also in other data analytics methods as in machine learning or neural networks. Managers of CPPs environments need to be aware that data-rich environments produce challenges for most employed methods. This is true also in applying SPC and DoE. We are aware that many of the mentioned challenges are not unique for CPPs and lie outside of the general managerial knowledge domain. A managerial implication is thus to guide analysts to a proper choice of tools by posing questions of how to address these challenges. We recommend that managers should solicit the competence of a statistically trained data

analyst until process engineers gain such competence. This is especially true during SPC method selection, or when designing and analysing experiments.

Our literature review has revealed challenges in using SPC and DoE in CPPs, but also many remedies to overcome those challenges. Applications of SPC in CPPs are often multivariate, need to deal with autocorrelation and process transitions, as well as to work alongside EPC procedures. DoE may need to deal with the large-scale, closed-loop operation and multivariate time series responses. An important message is also that SPC and DoE methods can be applied readily using proper adjustments presented in the literature. We also recommend managers to make sufficient resources available to engineers and analysts to adapt methods and to acquire software that can support application. Software are continuously developing to meet some of the challenges we highlight in this article. Examples of commercial software that can aid the application of SPC in CPPs are Prosensus® (www.prosensus.com), Simca® (www.umetrics.com), and Unscrambler X® (www.camo.com). Available DoE software include JMP® (www.jmp.com), Design Expert® (www.statease.com), and Modde® (www.umetrics.com). For the more experienced analyst free software such as the R statistics software are interesting alternatives.

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PAPER B

Exploring the Use of Design of Experiments in Industrial Processes Operating Under Closed-Loop Control

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Exploring the Use of Design of Experiments in Industrial Processes Operating Under Closed-Loop Control

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Industrial manufacturing processes often operate under closed-loop control, where automation aims to keep important process variables at their set-points. In process industries such as pulp, paper, chemical and steel plants, it is often hard to find production processes operating in open loop. Instead, closed-loop control systems will actively attempt to minimize the impact of process disturbances. However, we argue that an implicit assumption in most experimental investigations is that the studied system is open loop, allowing the experimental factors to freely affect the important system responses. This scenario is typically not found in process industries. The purpose of this article is therefore to explore issues of experimental design and analysis in processes operating under closed-loop control and to illustrate how Design of Experiments can help in improving and optimizing such processes. The Tennessee Eastman challenge process simulator is used as a test-bed to highlight two experimental scenarios. The first scenario explores the impact of experimental factors that may be considered as disturbances in the closed-loop system. The second scenario exemplifies a screening design using the set-points of controllers as experimental factors. We provide examples of how to analyze the two scenarios. © 2017 The Authors Quality and Reliability Engineering International Published by John Wiley & Sons Ltd

Keywords: Design of Experiments; engineering control; feedback adjustment; simulation; Tennessee Eastman process

1. Introduction

Industrial processes often involve automated control systems to reduce variation of quality characteristics or variables affecting plant safety. Sometimes, the control relies on human intervention, such as subjective evaluation of the process state followed by an operator's control action. Processes operating under such control regimes are operating under some form of closed-loop control. Experimenting in these processes will be challenging due to controllers' continuous interference, see Box and MacGregor.[1,2] Because the control action will potentially eliminate the impact of experimental factor changes, experimentation in closed-loop systems may be seen as futile. However, we argue that well designed and properly analyzed experiments run under such conditions can yield valuable information.

This article relates to system identification, which aims at building mathematical models of dynamic systems based on observed data from the system, see Ljung.[3] Experimental design in that sense typically concerns the selection of a proper input signal disturbance to discover the causal relationships between the disturbance and the responses or manipulated variables. This way, system identification allows for the estimation of model parameters to optimize a feedback controller, see, e.g. Jansson.[4] Typically, experimental design research in the system identification field studies 'optimal' input signals to model the system.

In this article, we are primarily concerned with factor screening, factor characterization or process improvement and optimization rather than modeling process dynamics through factors that are already known to affect the response. Similar to system identification experiments, allowable factor ranges are usually restricted, the experiments could be run in full-scale production and the number of experimental runs are limited. However, compared to system identification, the experiments we consider are run for longer periods of time and, most importantly, they have a more overarching purpose of improving or optimizing a process rather than to guarantee stability of a control loop.

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Closed-loop environments add complexity to experimental design and analysis because the control strategy affects the choice of experimental factors. For example, some input variables are manipulated within control loops and therefore may not be suitable as experimental factors. Moreover, even though closed-loop operation is common, we argue that Design of Experiments (DoE) literature typically rests on the implicit assumption that the studied system is operating in open loop, hence allowing the experimental factors to freely affect the response(s). However, as pointed out by, e.g. Vanhatalo and Bergquist[5] and Hild *et al.*,[6] process control systems are designed to maintain the important process variables at their set-points with low variability. Hence, control loops may counteract deliberate changes of experimental factors and thereby displace the effect from typical responses to manipulated variables. An analysis implication is that these manipulated variables instead may have to be used as responses to understand the experimental factors' impact on the system.

The purpose of this article is therefore to explore experimental design and analysis issues in processes operating under closed-loop control and to illustrate how DoE can add value in improving or optimizing such processes. We will pursue this through the help of a process simulator. Process simulators in general have limitations in mimicking the behavior of a real process, but they also offer the flexibility required for methodological developments without jeopardizing plant safety or product quality.

A well-known simulator in the engineering control community is the Tennessee Eastman (TE) challenge chemical process simulator first described by Downs and Vogel.[7] The TE simulator has been primarily used in the development of different process control strategies and for the development of statistical process monitoring methods mainly in chemometrics literature, see for example Kruger *et al.*[8] In this article, we run the TE process with a decentralized control strategy to simulate and illustrate experiments in a closed-loop system.

The remainder of this article is organized as follows: Section 2 establishes important concepts and provides a general comparison of open loop and closed-loop systems from a DoE perspective. Section 3 provides a general description of the TE process simulator and the chosen control strategy. Section 3 also outlines the two experimental scenarios we illustrate in closed-loop operation of the process. The experimental scenarios are elaborated and analyzed in Sections 4 and 5, respectively. Finally, conclusions and discussion are provided in Section 6.

2. Experiments run in open vs. closed-loop systems

Experiments imply that one or many input variables (experimental factors) are allowed to vary to affect the output (response(s)) with the aim of revealing potential causal relationships (effects) between factors and responses, and providing estimates of these effects. The response could be also affected by random disturbances, see Figure 1.

In a process operating under closed-loop control, unwanted variable deviations are mitigated by adjusting a manipulated variable, see Figure 2.

From an experimental perspective, the manipulated variables involved in control loops are not potential experimental factors. In fact, because manipulated variables are involved in control loops, the control engineers have an idea, e.g., from a past experiment, how the manipulated variables affect the response. In relation to Figure 2, the experimental factors in a closed-loop setting should be viewed as disturbances to the system operating under closed-loop control. The potential effects of a disturbance on the controlled variable(s) are therefore typically masked and displaced to one or several manipulated variables if the control system is working

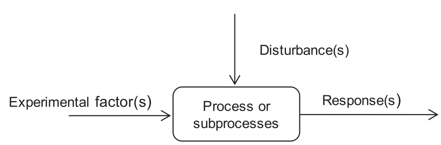

Figure 1. Experimental paradigm for open-loop operation. Figure inspired by Montgomery.[9]

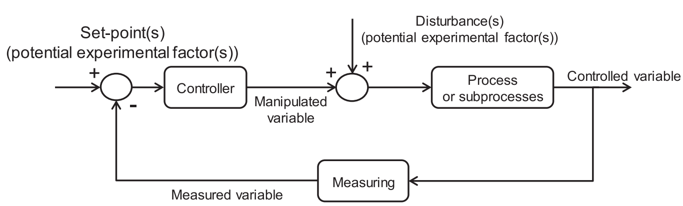

Figure 2. Schematic overview of a process under closed-loop control.

properly. This constitutes the first message we would like to convey in this article. That is, if the control action is ignored, the experimental factor changes will likely not affect the response (the controlled variable) significantly. An erroneous conclusion from the lack of detectable reaction would then be, depending on the effectiveness of the control action, that the factor is unimportant. However, if the presence of the controller is suspected or known, controlled variables may be used as responses primarily to test the presence and the effectiveness of the controllers. Manipulated variables may thus be considered as responses to study the impact of the experimental factors on the system and its dynamics due to the displacement of the potential effects from controlled to manipulated variables.

We classify experimental factors for processes operating under closed-loop control as (i) either a set of system inputs not involved in any control loop (should be viewed as disturbances in Figure 2) or (ii) the actual set-point values in the control loops. In the former scenario, both the manipulated and controlled variables can be used as experimental responses, while in the latter case more natural responses may be overall process performance indicators such as cost and/or product quality.

3. The Tennessee Eastman process simulator

Downs and Vogel[7] introduced the TE chemical process simulator for studying and developing engineering control design. The process is open loop unstable meaning that it will deviate and stop after a certain time period without any active control. With an appropriate control strategy, however, the process will remain stable. Several different control strategies for the TE process have been proposed; see for example McAvoy,[10] Lyman and Georgakis,[11] and Ricker.[12] The TE process has also been used as a test-bed for methodological development of multivariate statistical process monitoring.[8,13–16]

In the remainder of this section, we will describe some of the details of the TE process to facilitate the understanding of the experimental scenarios we use.

3.1. Process description

The TE process is a chemical process for which the components, kinetics, processing and operating conditions have been modified for proprietary reasons, see Downs and Vogel.[7] Following four irreversible and exothermic reactions, the process produces two liquid products from four gaseous reactants. With an additional byproduct and an inert product, eight components are present in the process. The process has five major unit operations: a *reactor*, a *product condenser*, a *vapor–liquid separator*, a *recycle compressor* and a *product stripper* as shown in a simplified process overview in Figure 3. A more detailed process map is given in the original reference.[7]

The physical inputs to the process consist of four gaseous streams, out of which three are fed to a reactor. After the reaction, the product mixture flows into a condenser, in which most of the gas is condensed. Some non-condensable components remain as vapors and the two phases are separated in the vapor–liquid separator. Vapor is partially recycled and purged together with the inert product and the byproduct. The product stripper separates remaining reactants from the products. The reactants are recycled, and the products exit the process from the stripper.

The TE process simulator has 12 manipulated variables (XMVs) and 41 measured variables (XMEASs). Out of 41 measured variables, 22 are measured directly while the remaining 19 variables can be calculated by the composition of the directly measured streams. In addition to XMVs and XMEASs, operating costs, production and product quality data are also recorded.

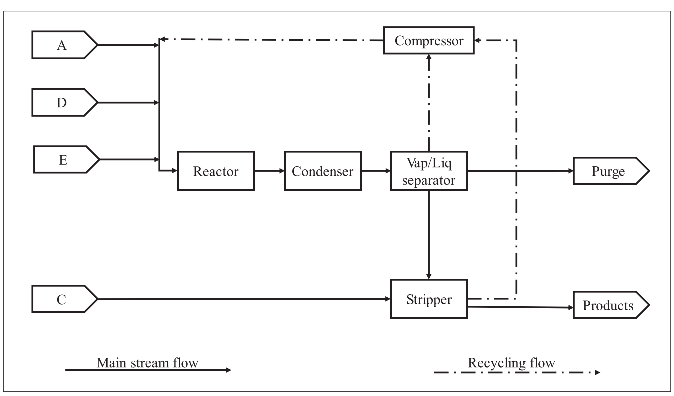

Figure 3. A schematic overview of the TE process.

The TE process has six different operating modes based on the production ratio of the two products and the production rate. Mode 1 is the most commonly used base case in research articles, which we also employ in this article. Five operating constraints need to be fulfilled to avoid process shutdown. There is also a possibility to activate 20 pre-set process disturbances (IDVs) during process operation. Downs and Vogel[7] provide more information on manipulated and measured variables, operating constraints, disturbances and the different operating modes.

3.2. *Implemented process control strategy*

A control strategy is a prerequisite for experimentation in the TE process because it is open loop unstable. Ricker[12] developed a decentralized control strategy for the TE process for improved performance, especially for the maximization of the production rate. The decentralized approach partitions the TE plant into 19 sub-units to each of which a controller is added. Tables I and II list the control loops, controlled variables, their set-points and manipulated variables. Note that we also provide XMV(i) and XMEAS(j); the i^{th} manipulated variable and the j^{th} measured variable given in Tables III and IV of the original article by Downs and Vogel[7] for ease of comparison. The manipulated variables listed with different codes, such as F_p, r_7 etc. come from the decentralized control strategy settings given in Ricker.[12]

We use a Matlab/Simulink decentralized control simulator (available at: http://depts.washington.edu/control/LARRY/TE/download.html#MATLAB_5x). In this configuration, all constraints are satisfied and the process can operate without undesired shutdowns. Moreover, the set-point values for some controlled variables and the values of inputs (XMVs) not involved in control loops may be varied, thereby allowing for experimentation.

The override loops 18 and 19 are exceptions to the control procedure described in Section 2. These control loops are only active when abnormal conditions occur that require an operating strategy change. Severe disturbances such as an introduction of the feed loss of A (IDV 6) activate the override loops. The production index F_p and the compressor recycle valve XMV(5) are not manipulated when the process operates without disturbances. All variables that can be manipulated except for the stripper steam valve XMV(9) and the agitator speed XMV(12) are involved in control loops in the decentralized control strategy. Consequently, XMV(9) and XMV(12) may be varied during experimentation and should then be viewed as disturbances in Figure 2.

3.3. *Chosen experimental scenarios in the TE process*

Two experimental scenarios in the TE process will illustrate experimentation in a process under closed-loop control. The first scenario will demonstrate an experiment when the system is disturbed by experimental factors. Input variables not involved in control loops can act as such disturbances and therefore be defined as experimental factors. The second scenario will demonstrate the use of the set-points of the control loops as experimental factors.

3.3.1. Scenario 1. The aim of this scenario is to demonstrate and visualize how experimental factor variation effects are distributed among the controlled and manipulated variables and how these effects can be analyzed. Recall that the stripper steam valve XMV(9)

Table I. Control loops for the decentralized control strategy (Ricker[12])

Loop	Controlled variable: Name	Controlled variable: Code	Manipulated variable: Name	Manipulated variable: Code
1	A feed rate (stream 1)	XMEAS(1)	A feed flow	XMV(3)
2	D feed rate (stream 2)	XMEAS(2)	D feed flow	XMV(1)
3	E feed rate (stream 3)	XMEAS(3)	E feed flow	XMV(2)
4	C feed rate (stream 4)	XMEAS(4)	A and C feed flow	XMV(4)
5	Purge rate (stream 9)	XMEAS(10)	Purge valve	XMV(6)
6	Separator liquid rate (stream 10)	XMEAS(14)	Separator pot liquid flow	XMV(7)
7	Stripper liquid rate (stream 11)	XMEAS(17)	Stripper liquid product flow	XMV(8)
8	Production rate (stream 11)	XMEAS(41)	Production index	F_p
9	Stripper liquid level	XMEAS(15)	Ratio in loop 7	r_7
10	Separator liquid level	XMEAS(12)	Ratio in loop 6	r_6
11	Reactor liquid level	XMEAS(8)	Set-point of loop 17	s.p. 17
12	Reactor pressure	XMEAS(7)	Ratio in loop 5	r_5
13	Mol % G (stream 11)	XMEAS(40)	Adjustment to the molar feed rate of E	E_{adj}
14	Amount of A in reactor feed, y_A(stream 6)	XMEAS(6)	Ratio in loop 1	r_1
15	Amount of A + C in reactor feed, y_{AC} (stream 6)	XMEAS(6)	Sum of ratio in loop 1 and 4	$r_1 + r_4$
16	Reactor temperature	XMEAS(9)	Reactor cooling water flow	XMV(10)
17	Separator temperature	XMEAS(11)	Condenser cooling water flow	XMV(11)
18	Maximum reactor pressure	XMEAS(7)	Production index	F_p
19	Reactor level override	XMEAS(8)	Compressor recycle valve	XMV(5)

Table II. Set-point values in the control loops for the decentralized control strategy (Ricker[12])

Loop	Controlled variable	Set-point	
		Base case values	Units
1	A feed rate (stream 1)	0.2505	kscmh
2	D feed rate (stream 2)	3664.0	kg h^{-1}
3	E feed rate (stream 3)	4509.3	kg h^{-1}
4	C feed rate (stream 4)	9.3477	kscmh
5	Purge rate (stream 9)	0.3371	kscmh
6	Separator liquid rate (stream 10)	25.160	m^3 h^{-1}
7	Stripper liquid rate (stream 11)	22.949	m^3 h^{-1}
8	Production rate (stream 11)	100	%
9	Stripper liquid level	50	%
10	Separator liquid level	50	%
11	Reactor liquid level	75	%
12	Reactor pressure	2705	kPa
13	Mol % G (stream 11)	53.724	mol%
14	Amount of A in reactor feed, y_A (stream 6)	54.95	%
15	Amount of A + C in reactor feed, y_{AC} (stream 6)	58.57	%
16	Reactor temperature	120.40	°C
17	Separator temperature	80.109	°C
18	Maximum reactor pressure	2950	kPa
19	Reactor level override	95	%

Table III. Potential experimental factors in scenario 1. Input variables not involved in control loops

Variable name	Code	Base case value (%)	Low limit (%)	High limit (%)
Compressor recycle valve	XMV(5)	22.210	0	100
Stripper steam valve	XMV(9)	47.446	0	100
Agitator speed	XMV(12)	50.000	0	100

Table IV. Potential experimental factors of the TE process: set-point values of the control loops

Loop	Controlled variable	Base set-point
7	Stripper liquid rate (production)	22.949 m^3 h^{-1}
9	Stripper liquid level	50%
10	Separator liquid level	50%
11	Reactor liquid level	75%
12	Reactor pressure	2705 kPa
13	Mole % G	53.724 mol%
14	Amount of A in reactor feed (y_A)	54.95%
15	Amount of A + C in reactor feed (y_{AC})	58.57%
16	Reactor temperature	120.40 °C

and the agitator speed XMV(12) are the only two manipulated variables not involved in control loops. Moreover, if the process is run without introducing any of the pre-set disturbances (IDVs), the compressor recycle valve XMV(5) is not manipulated and can be considered as another possible experimental factor. Because the TE simulator is designed the way it is, these factors not involved in control loops can be seen as potential experimental factors (disturbances), and an experiment can be designed to evaluate their impact on the system. We would like to note that in a real process the experimental factors need not only come from a list of numeric input variables not involved in control loops but can rather be drawn from a variety of potential disturbances to the system, such as different raw materials, methods of operation etc. Our choice here is convenient because XMV(5, 9, and 12) can be changed rather easily in the simulation model.

Three experimental factors are thus available in this scenario. Response variables will be the controlled variables as well as the manipulated variables in the control loops (see Section 2). Table III presents base case values of XMV(5, 9 and 12) and their allowed ranges in operating Mode 1 of the TE process.

3.3.2. Scenario 2. The aim of this scenario in the TE process is to explore the set-points of the controllers to reveal their potential impact on the process operating cost. That is, to see causal relationships between the process' operating conditions and an important process performance indicator. By changing the set-points, the second experimental scenario indirectly uses the levels of the controlled variables as experimental factors. However, some of the set-points are actually controlled in a cascaded procedure based on directives generated by other controllers. Thus, only a subset of the controlled variables may be considered potential experimental factors. Table IV lists the controlled variables that may be used as potential experimental factors and their set-point values for operating Mode 1.

4. Scenario 1: design and analysis

This section and Section 5 through examples illustrate the two experimental scenarios explained above. We would like to clarify that the aim of these examples is not to show the 'best' experimental designs or analysis procedures but rather to illustrate issues related to experimentation in closed-loop operation.

4.1. A two-level factorial design

Scenario 1 involves a 2^2 randomized factorial design with three replicates with the aim of estimating location effects (main effects and interaction) of the stripper steam valve XMV(9) and of the agitator speed XMV(12) on controlled variables and associated manipulated variables. Control loops 9, 10, 11, 12 and 16 (see Table I) include constraints implemented for securing plant safety and adequate control actions to avoid shutdown.

The run-order of the experiments and the averages of the controlled and manipulated variables are given in Table V. The TE process was run for 36 h under normal operating conditions, i.e., the base case values for operating Mode 1, before starting the first experimental run. This 'warm-up phase' allows for the process to reach a steady-state condition before the manipulated variables are changed. Thereafter, every run lasted 50 h, and all 12 runs were run in sequence during continuous operation of the process. We did not apply any of the possible pre-set disturbances (IDVs) during experimentation. Including the warm-up phase, the entire experiment contained 636 h of simulated operation (real simulation time is only 115 s on a computer using an Intel® Core™ i5-4310 U processor running at 2.0 GHz with 16 GB of RAM.) The controlled and manipulated variables were sampled every 12 min.

Due to the process' continuous nature, the experimental factors and responses need to be viewed as time series. For example, Figure 4 illustrates the impact of the experimental factors on the controlled and manipulated variables in Loop 16 which controls the reactor temperature, XMEAS(9), by adjusting the reactor cooling water flow, XMV(10).

As seen in Figure 4, the experiment has a substantial impact on the manipulated variable – reactor cooling water flow, XMV(10). However, even though the levels of the experimental factors are changing, the controlled reactor temperature XMEAS(9) exhibits a random variation around its set-point value, indicating that the impact on this controlled variable is small or non-existent. A similar behavior has been observed also for loops 9, 10 and 11.

4.2. Statistical analysis

In the first scenario, the manipulated variables of loops 9, 10, 11, 12 and 16 are considered as the main response variables. A simple but reasonable way to analyze the experiments with time series responses is to ignore the time series aspect of the responses and to calculate the average value for each run in Table V, see Vanhatalo *et al.*[17]. Vanhatalo *et al.*[18] recommend removing apparent dynamic behavior at the beginning of each run. However, the initial observations are here included to investigate if the control loops are effective because the control action may not succeed to remove the impact on the controlled variable instantly. The run averages can be used to perform analysis of variance (ANOVA). Table VI presents a summary of the ANOVA based on the averages in Table V. The analysis was performed using the software Design-Expert® version 9.

Based on the high p-values for the controlled variables in Loops 11, 12 and 16, the results do not indicate that the experimental factors affect their related controlled variables. However, as revealed by the low p-values for the manipulated variables in Loops 12 and 16 in Table VI, the experimental factors affect process phenomena controlled by these loops. Furthermore, Loops 9 and 10 fail to remove the full impact of the experimental factor variation on the controlled variables as indicated by the low p-values on the controlled variables. There is no evidence that the experimental factors are affecting process phenomena controlled by Loop 12. Furthermore, the low p-value of the main effect of the stripper steam valve XMV(9) on the stripper liquid level in Loop 9, XMEAS(15), is explained by the inclusion of the transition time. The run averages are affected because the control action of Loop 9 is delayed.

4.3. Concluding remarks for scenario 1

When experimenting in a closed-loop system, the analyst should expect that the impact of the experimental factors could be partly or completely displaced from the controlled variables to manipulated variables. This is true despite using inputs not involved in control loops as experimental factors, if the experimental factors affect the phenomena controlled in the loops. However, as illustrated, the analysis may reveal potential ineffectiveness of the controllers to completely or instantly remove disturbances acting on controlled variables. We therefore recommend viewing the responses as two important and closely related groups: [1] controlled variables and [2] manipulated variables when analyzing an experiment in a closed-loop system as illustrated above.

Table V. Run order and averages of the observations for the manipulated and controlled variables in the 2^2 factorial experiment

Run	Experimental factors		Manipulated variables (XMVs)					Controlled variables (XMEASs)				
	XMV(9) %	XMV(12) %	Loop 9 r_7	Loop 10 r_6	Loop 11 s.p. 17	Loop 12 r_5	Loop 16 XMV(10)	Loop 9 $j = 15$	Loop 10 $j = 12$	Loop 11 $j = 8$	Loop 12 $j = 7$	Loop 16 $j = 9$
1	40	40	0.2273	0.2489	80.3247	0.0034	42.5970	49.97	49.97	74.98	2705.03	120.40
2	60	60	0.2281	0.2500	80.2536	0.0034	39.7900	50.34	50.09	74.94	2705.04	120.40
3	60	40	0.2281	0.2500	80.2754	0.0034	42.4825	50.06	49.97	75.01	2705.03	120.40
4	40	60	0.2272	0.2489	80.3755	0.0034	39.8809	49.62	50.00	75.02	2704.99	120.40
5	60	60	0.2281	0.2501	80.2909	0.0033	39.7862	50.37	50.19	74.99	2704.95	120.40
6	40	40	0.2272	0.2488	80.3795	0.0033	42.6090	49.62	50.02	74.98	2705.02	120.40
7	40	40	0.2272	0.2489	80.3306	0.0033	42.5969	49.92	50.04	74.99	2705.00	120.40
8	60	40	0.2281	0.2501	80.2541	0.0033	42.4961	50.16	50.04	74.98	2704.99	120.40
9	60	40	0.2281	0.2501	80.2469	0.0033	42.5057	49.98	49.97	75.02	2705.01	120.40
10	40	60	0.2272	0.2487	80.3858	0.0033	39.8842	49.81	49.93	74.99	2705.05	120.40
11	40	60	0.2272	0.2489	80.3315	0.0033	39.8970	49.97	49.83	74.96	2704.95	120.40
12	60	60	0.2281	0.2500	80.2335	0.0033	39.8065	50.36	50.00	75.06	2705.01	120.40

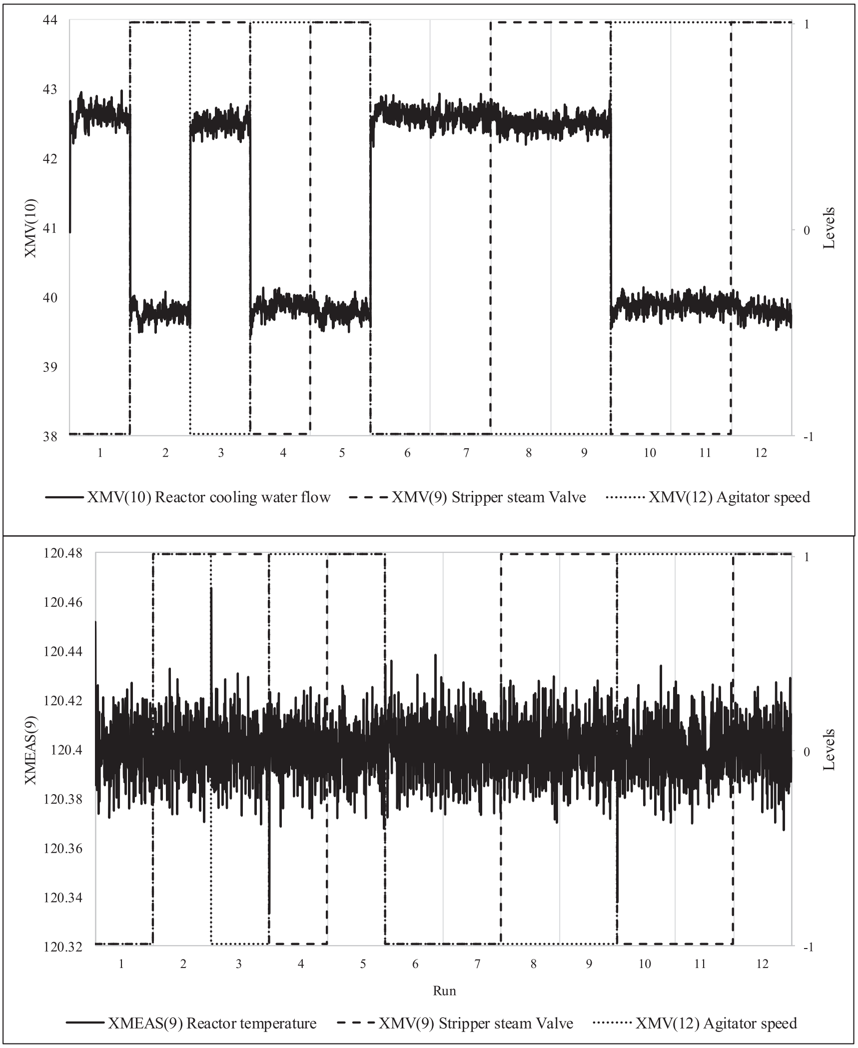

Figure 4. Overview of experimental factors' impact on variables related to control loop 16. The manipulated variable, XMV(10), is given in the top chart and controlled variable, XMEAS(9), in the bottom chart. The levels, in coded units, of the experimental factors XMV(9) and XMV(12) are superimposed on the plots. The duration of each experiment is 50 h.

5. Scenario 2: design and analysis

The second scenario illustrates a different way of running experiments in closed-loop controlled processes. Now, we consider the set-points of the control loops as experimental factors. Our major concern is no longer to reveal cause and effect relationships between inputs and important measured variables in the process. These should have been identified already in the engineering control design phase. Instead, we are exploring the set-points of the controllers to see causal relationships between the process operating conditions and process performance indicators with the aim of optimizing the process.

5.1. A screening experiment

In this case, we focus on the process operating cost as an important response. We have nine possible set-points to change (see Table IV), and we wish to test their impact on the process operating cost using a two-step sequential experiment. The starting point

Table VI. The *p*-values of the estimated effects based on ANOVA. Cells with bold text indicate the significant effects based on a significance level of 5%

Main effects and interaction	Manipulated variables					Controlled variables XMEAS(*j*)				
	Loop 9	Loop 10	Loop 11	Loop 12	Loop 16	Loop 9	Loop 10	Loop 11	Loop 12	Loop 16
	r_7	r_6	sp17	r_5	XMV(10)	$j = 15$	$j = 12$	$j = 8$	$j = 7$	$j = 9$
XMV(9)	$<$**0.0001**	$<$**0.0001**	$<$**0.0002**	0.7011	$<$**0.0001**	**0.001**	0.0937	0.4997	0.9031	0.9588
XMV(12)	0.9958	0.3744	0.5351	0.4029	$<$**0.0001**	0.1414	0.8736	0.8567	0.4668	0.1363
*XMV(9)*XMV(12)*	0.2754	0.9865	0.5564	0.9997	0.2759	0.0692	**0.0412**	0.7048	0.8390	0.6849

is a 2_{III}^{9-5} fully randomized fractional factorial design with four additional center points. This resolution III design is then followed by a full fold-over in a new block to entangle some aliased effects. The final design, i.e., the original plus the fold-over, is of resolution IV.

Some factor setting combinations will invoke a process shutdown and some shutdown limits are also given in the Downs and Vogel[7] paper. The base case value of each factor (rounded to the nearest integer) was chosen as either the low or high factor level in the design. The other level of each variable was defined by trial and error by either adding to or subtracting from the base case value while trying to keep the process from shutting down. Table VII provides the low and high levels of each experimental factor (set-point) used in the experiment.

Furthermore, we chose to keep XMVs (5, 9 and 12) fixed at their base case values given in Table III during the experiment because they are not involved in the loops but do affect the process behavior.

A 'warm-up phase' of 36 h was once again used before the start of the first run of the experiment. During this phase, the experimental factors (set-points) were fixed to their base case values for operating Mode 1. The 40 runs of the experiment are given in Table VIII. Each experimental run lasted 50 h. Including the warm-up phase, the entire experiment contained 2036 h of operation (simulation time was 147 s for all runs). From the TE simulator, the process operating cost ($/h) can be extracted, and we have the operating cost for every 12 min. Figure 5 illustrates the impact of the experimental factors on the process operating cost during the first three experiments in run order.

Table VII. Low and high level of the set-points used as experimental factors

Loop	Controlled variable	Base set-point	Low level	High level
7	Stripper liquid rate (production)	22.949 $m^3\ h^{-1}$	21 $m^3\ h^{-1}$	23 $m^3\ h^{-1}$
9	Stripper liquid level	50%	50%	60%
10	Separator liquid level	50%	35%	50%
11	Reactor liquid level	75%	70%	75%
12	Reactor pressure	2705 kPa	2600 kPa	2705 kPa
13	Mole % G	53.724 mol%	54 mol%	62 mol%
14	Amount of A in reactor feed (y_A)	54.95%	55%	65%
15	Amount of A + C in reactor feed (y_{AC})	58.57%	50%	59%
16	Reactor temperature	120.40 °C	120 °C	127 °C

Table VIII. Run order, standard order of the runs and average operating cost both before and after removal of transition time at the beginning of each run

Block 1: 2_{III}^{9-5} experimental design				Block 2: Full fold-over			
Run order	*Standard order*	*Operating cost ($/h)*	*Operating cost ($/h) (after removing transition time)*	*Run order*	*Standard order*	*Operating cost ($/h)*	*Operating cost ($/h) (after removing transition time)*
1	14	201.11	201.68	21	38	139.46	130.84
2	2	156.51	154.51	22	26	130.55	131.72
3	9	148.60	143.56	23	34	152.75	146.08
4	4	127.37	140.00	24	27	156.25	157.61
5	6	185.37	172.01	25	35	182.89	170.58
6	20	124.19	129.89	26	22	125.28	126.76
7	1	139.87	141.24	27	30	175.37	157.19
8	17	133.27	131.09	28	39	120.70	131.02
9	11	123.56	129.74	29	33	151.78	150.66
10	12	255.76	215.15	30	24	166.46	155.20
11	8	175.52	187.61	31	29	129.43	142.91
12	16	164.44	160.05	32	31	186.93	167.84
13	18	127.84	130.15	33	28	166.30	167.94
14	15	147.23	142.59	34	36	164.98	165.41
15	19	130.64	132.81	35	37	128.14	132.72
16	5	104.70	109.27	36	21	145.67	140.70
17	13	181.27	161.61	37	32	104.34	115.46
18	3	128.85	127.87	38	23	174.01	166.69
19	7	182.26	177.45	39	25	213.02	198.88
20	10	117.49	127.62	40	40	127.23	135.06

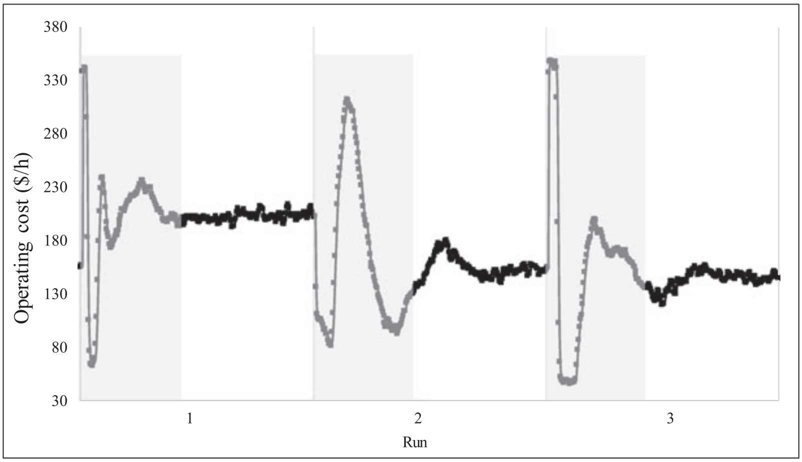

Figure 5. The operating cost during the first three runs of the experiment. Note the dynamic behavior of the response during the first part of each run. The shaded areas highlight the removed observations before calculating the run averages. The duration of each experiment is 50 h.

5.2. Statistical analysis

The aim of the experiment is to find set-points which reduce the long-term operating cost. In contrast to scenario 1, it makes sense to remove transition time from the runs and then use the remaining observations to calculate run averages. To keep the observations during the transition time in the calculation of run averages will lead to an underestimation of the location effect of the factors and interactions, see Vanhatalo et al.[17] The process operating cost exhibits some transition time before reaching the steady state as illustrated in Figure 5. A visual inspection of the operating cost reveals that 24 h can be considered as a reasonable transition time (grey shaded area in Figure 5), and thus the observations obtained during the first 24 h of all runs were removed before calculating the run averages, see Table VIII.

Table IX presents an ANOVA table of the 40-run experimental design in Table VIII based on a significance level of 5%. We have also repeated the analysis including the transition time. The results of that analysis are not reported in this article, but with the transition time included, the same main effects turn out to be active, but the significant interaction effects differ. As seen in Table IX, seven main effects and eight two-factor interaction alias strings are active (interactions of order three or higher are ignored). It is perhaps not surprising that most factors affect the operating cost because control loops aim to control important process phenomena which tend to affect the production cost. Moreover, the interconnectedness of the different control loops is demonstrated by the many significant interactions.

Note that the curvature test is significant and that the model exhibits significant lack of fit, suggesting that a higher order model is appropriate. The fitted model in Table IX is thus ill-suited for optimization and prediction but provides a starting point for future response surface experimentation. The many significant two-factor interaction alias strings would need further investigation to decide which among the aliases are actually active. However, as we mentioned earlier, the main purpose of this article is not necessarily to provide an optimization procedure on a simulated process but rather to draw attention to possibilities and pitfalls in experimentation under closed-loop operation. Hence, for demonstration purposes, we simply assume that the first interactions of the interaction strings in Table IX are the important ones, ignoring the interactions in brackets. We proceed to use the estimated model to provide suggested factor settings for the lowest operating cost within the experimental region. In this case, the lowest cost will be at a corner point on the multidimensional hyperplane. The settings of the factors and the predicted operating cost at this point (104.5 $/h) are provided in Table X. The significant curvature, the lack of fit tests and the R^2 for prediction indicate that the predictive ability of the model is poor. A confirmation run in the TE process simulator using the suggested factors settings gives the long-term average operating cost 109.1 $/h. The 4.6 $/h discrepancy between the predicted cost and the confirmation run is likely due to the models' poor predictive ability. Nevertheless, this rough analysis provides a significant improvement of the process operating cost. A simulation of the process keeping the factors settings at the base set-points values given in Table VII gives a long-term average operating cost of 170.2 $/h. Hence, running the process at the suggested factors settings leads to a substantial cost reduction of 61.1 $/h. Further reduction of the operating cost is likely possible but outside the scope of this article.

5.3. Concluding remarks for scenario 2

The second scenario illustrates how designed experiments can be used to improve process performance indicators using the set-points of variables controlled in closed-loop. This scenario also exemplifies the importance of considering, and here removing, the transition time during analysis. We want to point out that the set-points of the controllers in this example and in real life in general affect important process operating conditions. The experimenter should therefore expect that improper choices of factor levels of the

Table IX. ANOVA and estimated effects based on the averages of the response after removing the transition time. The model includes only terms significant at 5% level. Aliased two-factor interaction aliases that based on the heredity principle are less likely given in italic text within brackets. The control loop numbers are indicated by (#) in the factor names

Source	Sum of squares	*df*	Mean square	*F* value	Prob $> F$	Estimated standardized effects
Block	15.11	1	15.11			
Model	18 431.18	15	1228.75	83.97	$<$0.0001	
A: #7—Production	3946.30	1	3946.30	269.68	$<$0.0001	11.11
D: #11—Reactor level	321.10	1	321.10	21.94	0.0001	3.17
E: #12—Reactor pressure	3131.68	1	3131.68	214.01	$<$0.0001	−9.89
F: #13—Mole %G	4085.75	1	4085.75	279.21	$<$0.0001	−11.30
G: #14—y_A	443.48	1	443.48	30.31	$<$0.0001	−3.72
H: #15—y_{AC}	2444.72	1	2444.72	167.07	$<$0.0001	8.74
J: #16—Reactor temp	126.25	1	126.25	8.63	0.0076	−1.99
AD (*BH CG* FG)	124.36	1	124.36	8.50	0.0080	1.97
AF (*BG CH* DE)	207.73	1	207.73	14.20	0.0011	−2.55
AG (*BF CD* EH)	78.98	1	78.98	5.40	0.0298	−1.57
AH (*BD CF* EG)	151.98	1	151.98	10.39	0.0039	−2.18
AJ	532.42	1	532.42	36.38	$<$0.0001	−4.08
FJ	282.93	1	282.93	19.34	0.0002	2.97
GJ	619.92	1	619.92	42.36	$<$0.0001	4.40
HJ	1933.59	1	1933.59	132.14	$<$0.0001	7.77
Curvature	3415.43	1	3415.43	233.40	$<$0.0001	
Residual	321.93	22	14.63			
Lack of Fit	305.16	16	19.07	6.82	0.0129	
Pure Error	16.77	6	2.80			
Cor Total	22 183.66	39				
				R^2		83.1%
				Adjusted R^2		72.1%
				R^2 prediction		67.2%

Table X. Suggested settings of the set-points of the control loops to provide the lowest operating cost of the estimated model within the experimental region

Loop	Set-point	Suggested setting
7	Stripper liquid rate (production)	21 $m^3\ h^{-1}$
9	Stripper liquid level	Not in model, use base case
10	Separator liquid level	Not in model, use base case
11	Reactor liquid level	70%
12	Reactor pressure	2705 kPa
13	Mole % G	62 mol%
14	Amount of A in reactor feed (y_A)	65%
15	Amount of A + C in reactor feed (y_{AC})	50%
16	Reactor temperature	120 °C
Resulting predicted process operating cost:		104.5 $/h

set-points may lead to unexpected process behavior or even shutdown. Special care should be taken in choosing the levels because the window of operability may be irregular or unknown.

6. Conclusion and discussion

This article explores important issues in designing and analyzing experiments in the presence of engineering process control. The closed-loop operation increases process complexity and influences the strategy of experimentation. Two experimental scenarios based on the TE process simulator are used to answer the questions *why* and *how* to conduct and analyze experiments in closed-loop systems.

Even though we have prior experience with experiments lasting several weeks in continuous processes, the 2038 h of experimentation we use in our examples may admittedly be considered unrealistically long in practice. This is, however, beside the point because the examples we provide are for demonstration purposes, and we did not necessarily focus on shortening the duration of the experiments.

The first experimental scenario illustrates how the experimental factors not directly involved in control loops impact the closed-loop system and how the controllers affect the analysis. The controllers adjust manipulated variables to limit or eliminate the experimental factor effects on the controlled variable(s). We note that this will only occur if the experimental factors affect phenomena/variables governed by the closed-loop system. The effect on the controlled variables is partly or fully transferred to the manipulated variables depending on the effectiveness of the controllers. Hence, both the controlled and manipulated variables should be used as responses. Analyzing the effects of experimental factors on controlled variables may give important information about the effectiveness of the engineering process control. The effects on the manipulated variables instead reveal whether the experimental factors affect important process behavior.

In the second scenario, the experimental factors are the set-points of the controlled variables. The set-points are target values for the controlled variables and are typically closely tied to important process operating conditions. A level change of the set-points can therefore be considered equivalent to shifting the location of the process. Overall process performance indicators such as operating cost or product quality may then be suitable responses.

Using two scenarios we have illustrated that DoE can generate knowledge and aid process improvement in closed-loop systems. More specifically, DoE can be used to study:

- if the engineering process control is efficient and cost effective;
- if experimental factors affect important process phenomena; and
- how controlled variable set-points affect important process performance indicators.

We believe simulation software like the TE process offer great opportunities for methodology development in experimentation in closed-loop systems. In this article, we simply provide some basic ideas and approaches, but more research is needed for further development of experimentation and analysis methods for better process understanding and optimization in closed-loop systems.

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PAPER C

The Revised Tennessee Eastman Process Simulator as Testbed for SPC and DoE Methods

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The revised Tennessee Eastman process simulator as testbed for SPC and DoE methods

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ABSTRACT
Engineering process control and high-dimensional, time-dependent data present great methodological challenges when applying statistical process control (SPC) and design of experiments (DoE) in continuous industrial processes. Process simulators with an ability to mimic these challenges are instrumental in research and education. This article focuses on the revised Tennessee Eastman process simulator providing guidelines for its use as a testbed for SPC and DoE methods. We provide flowcharts that can support new users to get started in the Simulink/Matlab framework, and illustrate how to run stochastic simulations for SPC and DoE applications using the Tennessee Eastman process.

KEYWORDS
closed-loop; design of experiments; engineering process control; simulation; statistical process control; tutorial

Introduction

Continuous production during which the product is gradually refined through different process steps and with minimal interruptions (Dennis and Meredith 2000) is common across different industries. Today these processes manufacture both consumption goods such as food, drugs, and cosmetics, and industrial goods such as steel, chemicals, oil, and ore. Full-scale continuous production plants present analytical challenges since they are characterized by, for example, high-technological and complex production machinery, low flexibility, engineering process control (closed-loop operations) and high production volume. Automated data collection schemes producing multi-dimensional and high-frequency data generate additional analytical challenges. However, these processes still need to be improved continuously to remain competitive. Statistical process control (SPC) and design of experiments (DoE) techniques are essential in these improvement efforts.

The main challenge of applying SPC and DoE in continuous process settings comes from that these processes are run under engineering process control (EPC). EPC works by adjusting process outputs through manipulated variables. This autonomous control implies that when EPC is in place, the traditional SPC paradigm to monitor the process outputs needs to be adjusted to be effective since the process output(s) most likely follows the set-point(s) closely. However, the primary goals of EPC and SPC differ. SPC as a methodology is not aimed to produce feedback-controlled stability, but to help the analyst detect and eliminate unexpected sources of variation and disturbances that otherwise may go undetected. Also, while EPC can be used to compensate for a process disturbance, it has limits to what disturbance types and sizes it can handle. However, delving deep into the possibilities and obstacles of EPC in these settings goes beyond the scope of this article, as we wish to study the place for SPC and DoE in an environment containing EPC.

DoE involves deliberately disturbing the process to study how the process reacts, and traditionally, this involves studying an important response such as a product quality characteristics or a process output such as the yield. In the process industrial context where processes are run under EPC, such efforts may be futile as EPC may counteract any deliberate changes. However, better process conditions may be found by changing set-points or studying manipulated variables. Adding SPC and working with improvements using DoE to a process already operating under EPC may thus help improve processes, as we further demonstrate in this article.

The literature on the use of SPC and DoE in process industrial applications is extensive. However, a

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majority of these examples fail to capture essential challenges that analysts face when applying these methods in modern continuous processes. Recent SPC literature highlights the need to adapt SPC practices to the new manufacturing environments with massive datasets, multistep production processes, or greater computing capabilities (Ge et al. 2013, Ferrer 2014, Vining et al. 2015). Similarly, features of continuous processes unavoidably affect experiments and how experimental design strategies should be adapted, see, e.g., Vanhatalo and Bergquist (2007) and Capaci et al. (2017).

Methodological work to upgrade current SPC and DoE methods to address the continuous production challenges is needed, but it is often overly complicated to do methodological development using real processes. Tests of SPC or DoE methods in full-scale plants tend to require considerable resources and may jeopardize the production goals. Simulators may offer a reasonable trade-off between the required flexibility to perform tests and the limitations in mimicking the behavior of a real process.

Reis and Kenett (2017) map a wide range of simulators that can be used to aid the teaching of statistical methods to reduce the gap between theory and practice. They classify existing simulators based on various levels of complexity and guide educators to choose a proper simulator depending on the needed sophistication. Reis and Kenett (2017) classify the Tennessee Eastman (TE) process simulator (Downs and Vogel 1993) as one of the more complex simulators (medium-/large-scale nonlinear dynamic simulator) suggesting its use for advanced applications in graduate or high-level statistical courses. Downs and Vogel (1993) originally proposed the TE process as a test problem providing a list of potential applications in a wide variety of topics such as plant control, optimization, education, non-linear control and, many others. However, older implementations of the TE process that we have come across have a fundamental drawback in that the simulations are deterministic, apart from the added measurement error. An almost deterministic simulator is of limited value in statistical methodological development, since random replications as in Monte Carlo simulations are not possible.

The revised TE process by Bathelt et al. (2015a) does provide sufficient flexibility to create random errors in simulations. Especially after this latest revision, we believe that the TE process simulator can help bridge the gap between theory and practice as well as provide a valuable tool for teaching. However, as argued by Reis and Kenett (2017), the TE process simulator together with other advanced simulators lack an interactive graphical user interface (GUI), which means that the methodological developer still needs some programming skills.

In this article, we aim to provide guidelines for how to use the TE process simulator as a testbed for SPC and DoE methods. We use the revised TE process presented in Bathelt et al. (2015a) run with a decentralized control strategy (Ricker 1996). Flowcharts based on the Business Process Modelling Notation (BPMN) illustrate the required steps to implement the simulations (Chinosi and Trombetta 2012). Finally, we provide examples of SPC and DoE applications using the TE process.

The next section of this article provides a general description of the revised TE process simulator and the chosen control strategy. Sections 3 and 4 describe how to run simulations for SPC and DoE applications, respectively. We then present two simulated SPC and DOE examples in the TE process (Sections 5 and 6). Conclusions and discussion are provided in the last section.

The Tennessee Eastman process simulator

The TE process simulator emulates a continuous chemical process originally developed for studies and development of engineering control and control strategy design. See, for instance, plant-wide strategies (Lyman and Georgakis 1995), or model predictive control strategies (Ricker and Lee 1995). Independently of the chosen control strategy, the TE process mimics most of the challenges continuous processes present. The TE process has also been popular within the chemometrics community. Simulated TE process data have been used extensively for methodological development of multivariate statistical process control methods. For instance, the TE process simulator has been used for work on integrating dynamic principal component analysis (DPCA) into process monitoring, see Ku et al. (1995), Rato and Reis (2013), and Vanhatalo et al. (2017). Other TE process simulator examples for multivariate monitoring include Kruger et al. (2004), Lee et al., (2004), Hsu et al., (2010), and Liu et al., (2015). However, examples of DoE applications using the TE process are limited. Capaci et al. (2017) illustrate the use of two-level factorial designs using the TE process run under closed-loop control. Likely, methodological work has been hampered by the previous TE process simulator's deterministic nature.

From an SPC and DoE method development perspective, the decentralized control strategy proposed by Ricker (1996) and later revised by Bathelt et al. (2015a) is attractive because of the characteristics of the simulator under this strategy. Therefore, we intend to illustrate how the new revised simulation model of the decentralized TE process implemented by Bathelt et al. (2015b) can be adjusted to allow stochastic simulations and replications. The simulator has the following additional advantages:

- the simulator is implemented in the Simulink/Matlab® interface and can be obtained for free,
- the set-points of the controlled variables and the process inputs can be modified as long as they are maintained within the restrictions of the decentralized control strategy,
- the analyst can specify the characteristics of the simulated data as, for example, length of experimentation, sampling frequency, type and magnitude of process disturbances, and
- the simulation speed is fast. For example, to simulate the SPC example in this article with 252 hours of operation in the TE process takes less than a minute (56.26 seconds) on a computer using an Intel® Core™ i5-4310U processor running at 2.0 GHz with 16 GB of RAM.

Process description

The TE process plant involves five major units: a reactor, a condenser, a vapor-liquid separator, a product stripper and a recycle compressor (Downs and Vogel 1993). The plant produces two liquid products (G and H) from four gaseous reactants through a reaction system composed of four irreversible and exothermic reactions. It also produces an inert product and a byproduct purged as vapors from the system through the vapor-liquid separator (Figure 1).

Reactants A, D and E flow into a reactor where the reaction takes place. The output from the reactor is fed to a condenser. Some non-condensable vapors join the liquid products, but the following vapor-liquid separator again splits the substances into separate flows. Vapor is partially recycled and partially purged together with the inert product and the byproduct. The stripper separates the remaining A, D and E reactants from the liquid and another reactant, C, is added to the product. The final products then exit the process and the remaining reactants are recycled.

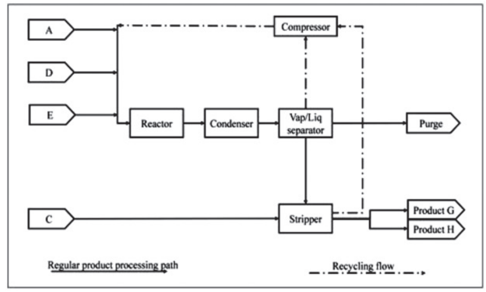

Figure 1. A simplified overview of the TE process flow.

The TE process has 12 manipulated variables (XMVs) and 41 measured variables (XMEAs). Tables in Downs and Vogel (1993) provide detailed information about all the process variables and the cost function that provides the process operating cost in $/h. The combination of three G/H mass ratios and four production rates of the final products define six different operating modes of the process. The user can also choose to activate 20 preset process disturbances (IDVs).

The TE process is open-loop unstable and it will rapidly leave the allowed process operations window and then shut down if it is run without engineering process control. Therefore, a control strategy is necessary for process stability. To avoid shutdowns and for securing plant safety, the control strategy should abide by five operating constraints related to the reactor pressure, level and temperature, the product separator level, and the stripper base level. Even with controllers working correctly, the TE process is sensitive and may shut down depending on the controller tuning and the set-points of the controlled variables.

Decentralized control strategy

The decentralized control strategy partitions the plant into sub-units and designs a controller for each one, with the intent of maximizing the production rate. Ricker (1996) identified nineteen feedback control loops to stabilize the process. Table 1 provides the control loops and the related controlled and manipulated variables. The original article by Ricker (1996) provides detailed information about the design phases of the decentralized control strategy.

The revised TE simulation model

Ricker (2005) devised the decentralized TE control strategy as a Simulink/Matlab® code. Bathelt et al. (2015b) recently developed a revised version of the

Table 1. Controlled and manipulated variables in the 19 loops of the decentralized control strategy. The manipulated variables with codes such as F_p and r_7 come from the decentralized control strategy settings (Ricker 1996). XMV(i) and XMEAS(j) are numbered according to the original article by Downs and Vogel (1993).

Loop	Controlled variable	Code	Manipulated variable	Code
1	A feed rate (stream 1)	XMEAS(1)	A feed flow	XMV(3)
2	D feed rate (stream 2)	XMEAS(2)	D feed flow	XMV(1)
3	E feed rate (stream 3)	XMEAS(3)	E feed flow	XMV(2)
4	C feed rate (stream 4)	XMEAS(4)	A and C feed flow	XMV(4)
5	Purge rate (stream 9)	XMEAS(10)	Purge valve	XMV(6)
6	Separator liquid rate (stream 10)	XMEAS(14)	Separator pot liquid flow	XMV(7)
7	Stripper liquid rate (stream 11)	XMEAS(17)	Stripper liquid product flow	XMV(8)
8	Production rate (stream 11)	XMEAS(41)	Production index	F_p
9	Stripper liquid level	XMEAS(15)	Ratio in loop 7	r_7
10	Separator liquid level	XMEAS(12)	Ratio in loop 6	r_6
11	Reactor liquid level	XMEAS(8)	Set-point of loop 17	s.p. 17
12	Reactor pressure	XMEAS(7)	Ratio in loop 5	r_5
13	Mol % G (stream 11)	XMEAS(40)	Adjustment of the molar feed rate of E	E_{adj}
14	Amount of A in reactor feed, y_A(stream 6)	XMEAS(6)	Ratio in loop 1	r_1
15	Amount of A+C in reactor feed, y_{AC}(stream 6)	XMEAS(6)	Sum of loops 1 and 4 ratio	$r_1 + r_4$
16	Reactor temperature	XMEAS(9)	Reactor cooling water flow	XMV(10)
17	Separator temperature	XMEAS(11)	Condenser cooling water flow	XMV(11)
18	Maximum reactor pressure	XMEAS(7)	Production index	F_p
19	Reactor level override	XMEAS(8)	Compressor recycle valve	XMV(5)

simulation model. The revision is an update of Ricker's (2005) code that widens its usability by allowing for customization of the simulation by modifying a list of parameters in the process model function. Below we describe how to initialize the revised TE simulator and how to use the model function parameters to achieve intended simulator characteristics.

Initialization of the revised TE model

The files of the revised model are available as a Simulink/Matlab® code at the Tennessee Eastman Archive (Updated TE code by Bathelt et al. (2015b)). Figure 2 illustrates the workflow to initialize the simulator through a simulation test, using the BPMN standard (Chinosi and Trombetta 2012). The simulator requires three phases to be initialized: installation, test, and use. The installation mainly consists of downloading the files and setting them in the same computer directory. Then a simulation test can be launched to check if the installation has been successful. During the simulation test, four online plots display the reactor pressure, process operating cost, production flow, and product quality trend. When the simulation ends, the simulator provides datasets of XMVs and XMEAs as well as the related plots. The correct completion of the installation and test phases ensures that the simulator works properly and it is ready to be used. Initialization is then completed.

The simulator can be run in both operating Mode 1 and 3. Operating Mode 1, which we use in this article, seems to be the most commonly used in the literature. The model "MultiLoop_mode1" runs the process at Mode 1 when the set-points of the input variables not involved in control loops and of the controlled variables are set up according to the base case values given in Tables 2 and 3.

In Figure 2, "DoE applications" and "SPC applications" consist of different compound activities, expanded later, that the user must follow depending on which method is being applied. The definition of the model function parameters is one of these activities and can be done following the instructions below.

Using the model function parameters to customize the simulation

The model function "temexd_mod" contains the "TE code" and it is located in the "TE Plant" block of the Simulink model. A double-click on "temexd_mod" opens a dialog window. In the field "S-function parameters," the user can define three model function parameters separated by commas. Square brackets are used for undefined parameters. The simulation can be customized to fit different needs by changing these parameters. Table 4 provides more details of the model function parameters.

Parameter 1 relates to the initial values of the model states. Since we wish to run the process in Mode 1, we hereafter assume that this parameter is set as empty unless otherwise specified. Therefore, the default "xInitial" array is used when we launch the simulator. Parameters 2 and 3 enable the customizations introduced in the revised TE code.

The possibility to change the seed of each simulation (parameter 2) creates the opportunity to avoid deterministic simulations, but only when the user activates process disturbances (IDVs) of the type random variation in the model, see Table 5. Parameter 3

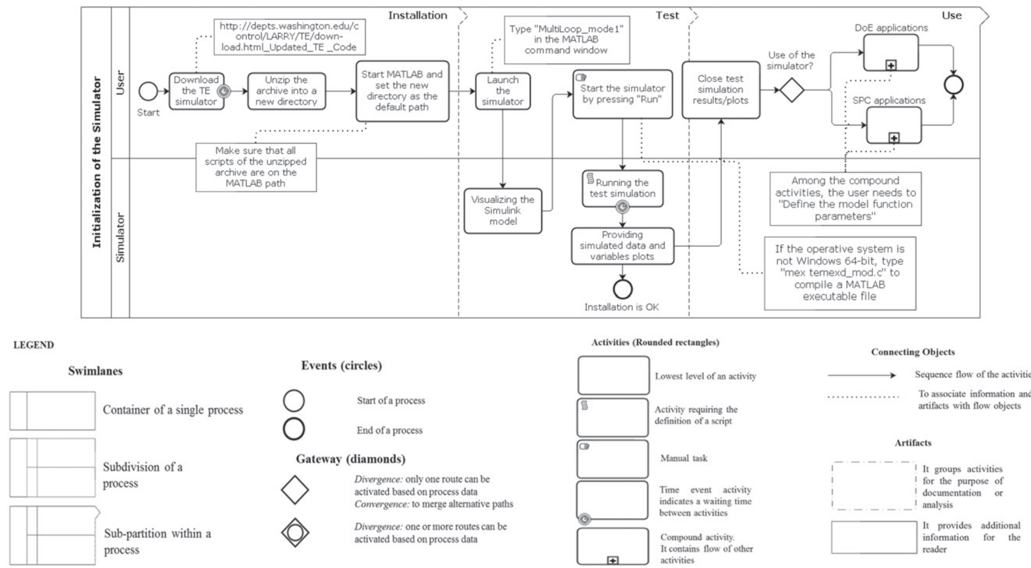

Figure 2. Main tasks required to initialize the simulator for operating Mode 1. Note that some symbols in the legend might be unused in this flowchart. Legend inspired by http://resources.bizagi.com/docs/BPMN_Quick_Reference_Guide_ENG.pdf

allows for activating/deactivating the model flags listed in Table 4. Each model flag corresponds to a bit that can be switched using the binary notation. The value of parameter 3 corresponds to the decimal integer of the binary number obtained after setting the value of each bit. For example, the binary number $(11100010)_2$ is equivalent to the parameter value of $(226)_{10}$, which produces the exemplified model structure given in Table 4. Note that for the right conversion from a binary to a decimal number, the binary number must be written starting from the highest to the lowest bit position (from 15 to 0).

As a rule of thumb, model flags 5 and 6 should be active during the simulation while the user can set the other model flags to adjust the model to the simulation needs. Further details of the model flag structure are given in Bathelt et al. (2015a).

Table 2. Base case set-points of the input variables not involved in control loops for operating Mode 1.

Variable name	Code	Base case value (%)	Low limit (%)	High limit (%)
Compressor Recycle Valve	XMV(5)	22.210	0	100
Stripper Steam Valve	XMV(9)	47.446	0	100
Agitator Speed	XMV(12)	50.000	0	100

Table 3. Base case set-points of the controlled variables (available experimental factors) in the TE process for operating Mode 1.

Loop	Controlled variable	Base set-point
7	Stripper liquid rate (production)	22.949 $m^3\ h^{-1}$
9	Stripper liquid level	50%
10	Separator liquid level	50%
11	Reactor liquid level	75%
12	Reactor pressure	2705 kPa
13	Mole % G	53.724 mol%
14	Amount of A in reactor feed (y_A)	54.95%
15	Amount of A+C in reactor feed (y_{AC})	58.57%
16	Reactor temperature	120.40 °C

Creating random simulations in the revised TE process simulator

The TE process is complex and in that sense mimics a real chemical process. While the high degree of complexity makes it useful as a testbed for methodological development, the same complexity imposes some limitations. As already stated, without customization, the TE simulator provides an output that does not differ much from a deterministic simulation where all measurement error is set to zero.

Figure 3 shows a schematic overview of the revised TE simulation model highlighting potential sources of random variation. Note that the TE process variables are only affected by white Gaussian noise mimicking typical measurement noise when random disturbances of type "random variation" are turned off. Thus, repeated simulations with the same setup will produce identical results, except for measurement error, which limit the model's value when running repeated simulations. Repeated simulations are for instance used when assessing the performance of an SPC method or when replicates of experimental runs are needed.

To overcome this limitation, we suggest running the simulator with added measurement noise and one or more of the random disturbances (IDVs) listed in Table 5 activated. Indeed, the possibility to scale random variation disturbances allows the user to add variability without overly distorting the results. The possibility to change the seed is also

Table 4. Description and settings of the parameter list for the process model function "temexd_mod" (Bathelt et al. 2015a). An example of settings for parameter 3 is given.

Parameter list of "temexd_mod"	Description		Setting	
1	An array of the initial values of the 50 states of the model. The user can specify a vector of 50 states of the model to run the simulator in a specific operating mode		Empty: default values of process operating Mode 1 are used (Downs and Vogel 1993).	
2	Initial value (seed) of the random generator		Every integer number greater than 0 is valid.	
	Model structure flag			
3	Bit	Description	Example	$(11100010)_2 = (226)_{10}$
	0	Additional measurements points	0	Integer value equivalent to the binary number activating/deactivating the bit of the model structure flag
	1	Monitoring outputs of the disturbances	1	
	2	Monitoring outputs of the reaction and process	0	
	3	Monitoring outputs of the component's concentration	0	
	4	Deactivation of measurement noise	0	
	5	Random generator uses different state variables for process disturbances and measurements noise	1	
	6	Solver-independent calculations of the process disturbances	1	
	7	Disturbances are scaled by the value of the activation flags	1	
	15	Reset model structure to original structure of Ricker (2005)	0	

Table 5. The 28 process disturbances available (Downs and Vogel 1993, Bathelt et al. 2015a).

Variable Number	Process Variable	Type
IDV(1)	A/C feed ratio, B composition constant (stream 4)	Step
IDV(2)	B composition, A/C ratio constant (stream 4)	Step
IDV(3)	D feed temperature (stream 2)	Step
IDV(4)	Water inlet temperature for reactor cooling	Step
IDV(5)	Water inlet temperature for condenser cooling	Step
IDV(6)	A feed loss (stream 1)	Step
IDV(7)	C header pressure loss- reduced availability (stream 4)	Step
IDV(8)	A,B,C proportion in stream 4	Random variation
IDV(9)	D feed temperature (stream 2)	Random variation
IDV(10)	A and C feed temperature(stream 4)	Random variation
IDV(11)	Water inlet temperature for reactor cooling	Random variation
IDV(12)	Ater inlet temperatur for condenser cooling	Random variation
IDV(13)	Variation coefficients of reaction kinetics	Random variation
IDV(14)	Reactor cooling water valve	Sticking
IDV(15)	Condenser cooling water valve	Sticking
IDV(16)	Variation coefficient of the steam supply of the heat exchanger of the stripper	Random variation
IDV(17)	Variation coefficient of heat transfer in reactor	Random variation
IDV(18)	Variation coefficient of heat transfer in condenser	Random variation
IDV(19)	Unknown	Unknown
IDV(20)	Unknown	Random variation
IDV(21)	A feed temperature (stream 1)	Random variation
IDV(22)	E feed temperature (stream 3)	Random variation
IDV(23)	A feed flow (stream 1)	Random variation
IDV(24)	D feed flow (stream 2)	Random variation
IDV(25)	E feed flow (stream 3)	Random variation
IDV(26)	A and C feed flow (stream 4)	Random variation
IDV(27)	Reactor cooling water flow	Random variation
IDV(28)	Condenser cooling water flow	Random variation

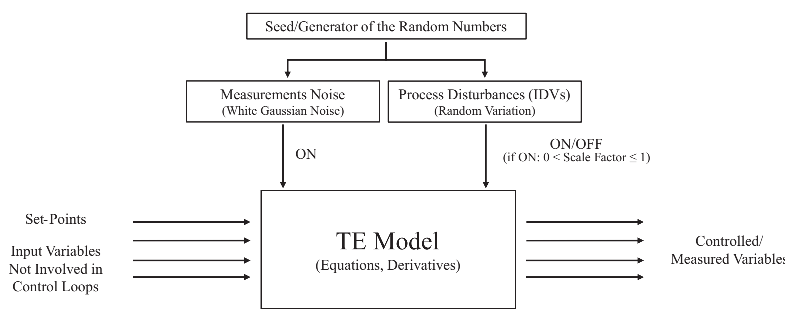

Figure 3. Schematic overview of the revised TE simulation model with a focus on potential sources of random variation.

important for our conclusion that the revised TE model is suitable for methodological tests of SPC and DoE methods.

It should be noted that the choice of the scale factor(s) to adjust the random variation depends on the random disturbance(s) introduced in the simulation model and the aim of the simulation study. The random disturbances vary in both magnitude and dynamics and hence impact the process differently. Therefore, we leave the choice of disturbances and the scale factor(s) to the user but explain the ideas behind our choices in our examples.

The TE process simulator in the SPC context

SPC applications require historical in-control data (Phase I dataset) and an online collection of data to perform Phase II analysis. Samples from Phase I and Phase II are typically collected in one shot in the TE process simulator. Using the BPMN standard, the upper half of Figure 4 presents the tasks required to simulate Phase I and Phase II data. Table 5 lists possible process disturbances (IDVs) that can be used as faults in Phase II. Note that the revised TE model adds eight "random variation" disturbances to the simulator, IDV(21)-IDV(28). A valuable characteristic of the revised simulator for SPC applications is the possibility to scale all process disturbances by setting their disturbance activation parameter values between 0 and 1.

Before we highlight three important SPC challenges that frequently occur in continuous processes and that the TE process simulator can emulate.

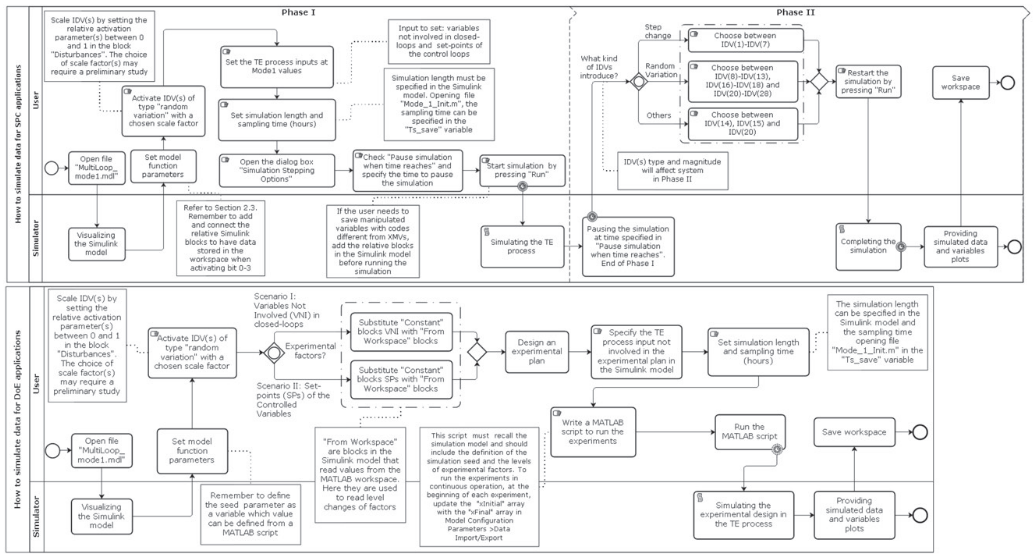

Figure 4. Overview of tasks required to simulate data for SPC (upper) and DoE (bottom) applications. Symbols are explained in Figure 2.

Multivariate data

The 53 variables available in the TE process (12 XMVs and 41 XMEAs), some of which are highly cross-correlated, allow for studies of multivariate monitoring methods. The TE process has been used extensively within the chemometrics literature to test monitoring applications and fault detection/isolation methods based on latent structures techniques such as principal component analysis (PCA) and partial least squares (PLS). The simulator does not produce missing data, but the analyst may remove data manually if needed.

Autocorrelated data

The user can choose the variables' sampling rate in the TE process, but for most choices, the resulting data will be serially correlated (autocorrelated). Autocorrelation will require adjustment of the control limits of control charts since the theoretical limits will not be valid. This faulty estimation will affect in-control and out-of-control alarm rates (Bisgaard and Kulahci 2005, Kulahci and Bisgaard 2006), and this also extends to process capability analysis affecting both univariate and multivariate techniques.

Closed-Loop Operation

Closed-loop engineering process control is constantly working to adjust process outputs through manipulated variables, which represents an interesting SPC challenge. Control charts applied to controlled outputs could fail to detect a fault and might erroneously indicate an in-control situation. The traditional SPC paradigm to monitor the process output when engineering process control is in place requires proper adjustments and the TE process simulator provides a good testbed for this.

The TE process simulator in DoE context

The lower part of Figure 4 provides a guide on how to simulate data in using the TE process for testing DoE methods for continuous processes operating under closed-loop control. Note that one of the early tasks is to activate one or more process disturbances of type "random variation," see Table 5, to overcome the deterministic nature of the simulator. Two experimental scenarios can, for example, be simulated using the TE process simulator (Capaci et al. 2017). In the first scenario, the experimental factors can include the three manipulated variables not involved in control loops, XMV(5), XMV(9), and XMV(12), see also Table 2, while the responses can include both manipulated and controlled variables. In the second scenario, the experimenter can use the set-point values of the control variables as experimental factors and the operating cost function as a response. However, a cascaded procedure based on directives generated by the decentralized control strategy will make some set-points dependent. Therefore, the experimenter only has the subset of the nine set-points given in Table 3 available as experimental factors in the second scenario.

The TE process simulator allows the user to pause, analyze the experiment, and make new choices based on the results. Thus, sequential experimentation, a cornerstone in experimental studies, is possible to simulate. The experimenter can repeat the experimental runs and expand the experiment with an augmented design since the seeds for the random disturbances can be changed. Hence, TE process simulator can emulate potential experimentation strategies such as response surface methodology (Box and Wilson 1951) and evolutionary operation (Box 1957). Even though cost and time concerns are irrelevant when experiments are run in a simulator and the number of experimental factor levels and replicates are practically limitless compared to a real-life experiment, there are only a few potential experimental factors available. The simulator may aid studies on the robustness and the analysis of an experiment where the number of experimental runs is limited, such as unreplicated designs with a minimum number of runs.

Below we highlight three challenges for the analyst when applying DoE in the TE process. These challenges are also commonly found in full-scale experimentation in continuous processes:

The closed-loop environment

The TE process experimenter must select experimental factors and analyze process responses while taking into account the presence of feedback control systems (Capaci et al. 2017). The decentralized control of the TE process will mask relationships between process input and output (see also McGregor and Harris 1990), and feedback control loops will limit the possibility to vary all the process inputs freely. Furthermore, the experimenter must restrict potential experimental factor changes within constrained operating regions to avoid any process shutdowns. As in open-loop systems, the choice of the experimental factor levels becomes crucial to assure the closed-loop process stability. However, one cannot expect the experimenter, new to the TE process, to predict the process behavior due to experimental factor changes. Instead, we have found that a trial-and-error approach of sufficiently stable operating regions has given sufficient a-priori knowledge of potentially feasible operating regions (such an approach is, of course, unfeasible in the real process case as it potentially involves multiple process shutdowns.) Later, results of the experimentation can provide an improved posteriori knowledge of actual feasible operating regions. Therefore, DoE methods can be used for factor screening, factor characterization, or process improvement and optimization in these processes. Moreover, it is fair to assume that a subsequent re-tuning of the control parameters at different sub-regions within the whole tolerable experimental region might lead to a further improvement of the process and an expansion of the region of tolerable operating conditions.

Transition times between runs

The time required for different responses to reach a new steady state in the TE process will differ depending on the factors and the magnitude of the change. The characterization of transition times is crucial to minimize their effect on the experimental results as well as to allocate the time needed for the treatments to take full effect (Vanhatalo et al. 2010). Long transition times between steady-state conditions add to the costs of randomizing the runs in a real experiment. The literature suggests using split-plot designs to restrict factor changes in this situation. Moreover, it is common to avoid resetting the levels of factors between consecutive runs where the factors are to be held at the same level for time and cost concerns. However, maintaining the factor level settings between adjacent runs and disregarding resetting lead to a correlation between neighboring runs and to designs called randomized-not-reset (RNR) designs (Webb et al. 2004). These can also be studied in the TE process.

Time series data for factors and responses

The continuous nature, the dynamic behavior, and the transition times of the TE process make it necessary to view experimental factors and responses as time series. The analysis of the experiments from the TE process allows for considering the time series nature of factors and responses. The response time series need to be summarized in averages or standard deviations to fit in a standard analysis such as the analysis of variance (ANOVA). Transfer function-noise modeling may be used to model the dynamic relations between experimental factors and the response(s) (Lundkvist and Vanhatalo 2014).

Example 1: The TE process simulator and SPC

Note that the aim of the example provided here (and in Section 6) is not to describe the most complex scenario available nor is it to suggest the “best solution” to the illustrated challenges. The examples are provided to show how the TE process can act as a testbed for developing and testing methodological ideas. In the first example, we illustrate how closed-loop operation can affect the shift detection ability of control charts. In particular, this example demonstrates how control charts applied to the (controlled) output could fail to detect a fault and, therefore, might erroneously indicate an in-control situation. It should be noted that this issue has been already handled in other research articles, see, for example, Rato and Reis 2014, 2015, and here we make use of it for illustration purposes.

The example focuses on control loops 9–12 and 16 (Table 1). These loops regulate the process operating constraints needed to secure plant safety and to avoid unwanted shutdowns. Five process inputs (r_5, s.p.$_{17}$, XMV(10), $r_{6,}$ and r_7), i.e., the manipulated variables, control the related TE process outputs (XMEAS 7–9, 12 and 15). We here refer to control loops 9–12 and 16, and their related variables as critical control loops, critical controlled variables (C-XMEAS) and critical manipulated variables (C-XMVs) respectively.

Selecting and scaling disturbances

After a preliminary study of the process disturbances of type random variation (Table 5) available in the TE process, we further analyzed the behavior of IDV(8) and IDV(13). IDV(8) varies the proportion of the chemical agents (A, B, C) in stream 4 of the process, mimicking a reasonably realistic situation, whereas IDV(13) adds random variation to the coefficients of reaction kinetics, propagating its impact through the whole process. We performed 4 sets of 20 simulations each with a scale factor of the disturbances equal to 0.25, 0.5, 0.75 and 1 to understand the impact of IDV(8) and IDV(13) on process behavior. Each simulation, run with a randomly selected seed, lasted 200 hours in the TE process and the outputs of the random disturbances were collected with a sampling interval of 12 minutes. We kept constant the set-points of the inputs not involved in control loops and of the controlled variables at the base case values of operating Mode 1 (Tables 2 and 3).

Based on the averages and standard deviations presented in Table 6, to achieve random variation in the TE process, we ran Phase I and Phase II data collection with both IDV(8) and IDV(13) active, with randomly selected scale factors between 0 and 0.25 and, 0 and 0.5 respectively.

We then performed a preliminary simulation with the same simulator settings for the random disturbances to select the magnitude of the step size (fault) for Phase II. Table 6 shows the magnitude of the step size for the scale factor equal to 0.25, 0.5, 0.75 and, 1. We, therefore, introduced a step change in the cooling water inlet temperature of the reactor in Phase II, i.e., IDV(4), with a randomly selected scale factor between 0.25 and 0.5.

Data collection

The TE process was first run for 144 hours at normal operating conditions (Phase I), i.e., base case values for operating Mode 1. A step change in the cooling water inlet temperature of the reactor (IDV4) was then introduced in the process for 108 hours (Phase II). The randomly selected scale factors of disturbances IDV(4), IDV(8) and IDV(13) in this simulation were 0.32, 0.1 and 0.25 respectively. Values on C-XMEAS and C-XMVs were collected in sequence during continuous operation of the process with a sampling time of 12 minutes.

Multivariate process monitoring

For illustration purposes, consider a standard Hotelling T^2 multivariate control chart for individual observations for the five critical controlled variables of the TE process (C-XMEAS). The Phase I sample was produced by excluding the start-up phase of the process. The critical controlled variables exhibit a dynamic behavior for about 36 hours or 180 samples at the start of the simulation. After this "warm-up phase," the TE process was deemed to have reached steady-state.

Samples of C-XMEAS collected during steady-state operation provide a more stable estimation of the sample covariance matrix, **S,** and thus of the T^2 values. We discarded the first 180 observations and used datasets of 540 samples both in Phase I and Phase II to build the Hotelling T^2 chart, see Figure 5. The standard sample covariance matrix was used to form the T^2 chart. The theoretical Phase I and Phase II upper control limits were based on the β and F distributions and on the assumption that observations are time-independent (Montgomery 2012). This assumption is unrealistic because of the observed positive autocorrelation in the critical controlled variables (and as a result also in the T^2 values), and consequently, the upper control limits should be adjusted, see Vanhatalo and Kulahci (2015). However, the point we want to make here will still be evident from the appearance of Figure 5 using the theoretical control limits and we here intentionally avoid a detailed discussion on adjusted control limits.

There are a few T^2 observations above the control limit in the Phase II sample based on C-XMEAS (top panel in Figure 5), but an analyst might as well conclude that there is little evidence to deem the process out-of-control. Moreover, a visual inspection of the C-XMEAS univariate plots in Figure 6 seems to support this conclusion, as the critical controlled variables appear to be insensitive to the step change in the cooling water inlet temperature of the reactor (IDV4). However, this conclusion is incorrect. Since the TE process is run in closed-loop operations, the analyst should know that the engineering process control seeks to displace most of the variability induced by the step change (fault) to some manipulated variable(s). In fact, the correct conclusion in this scenario is that the process is still working at the desired

Table 6. Averages and standard deviations of IDV(8) and IDV(13) based on 20 simulations. Step size of IDV(4) for different scale factor values.

Variable number	Process variable	Scale factor	Average	Step size	Standard deviation			
IDV(4)	Cooling water inlet temperature of reactor	$0.25n$ $n=0,1,\ldots,4$	35	$+1.25n$	-			
					$n=1$	$n=2$	$n=3$	$n=4$
IDV(8)	Proportion of A in stream 4	$0.25n$	48.51		0.372	0.748	1.126	1.50
	Proportion of B in stream 4	$0.25n$	0.50		0.038	0.074	0.110	0.15
	Proportion of C in stream 4	$0.25n$	50.99		0.374	0.751	1.130	1.51
IDV(13)	Variation coefficient of reaction kinetics $A+C+D \rightarrow G$	$0.25n$	1		$0.03n$			
	Variation coefficient of reaction kinetics $A+C+D \rightarrow G$		1					

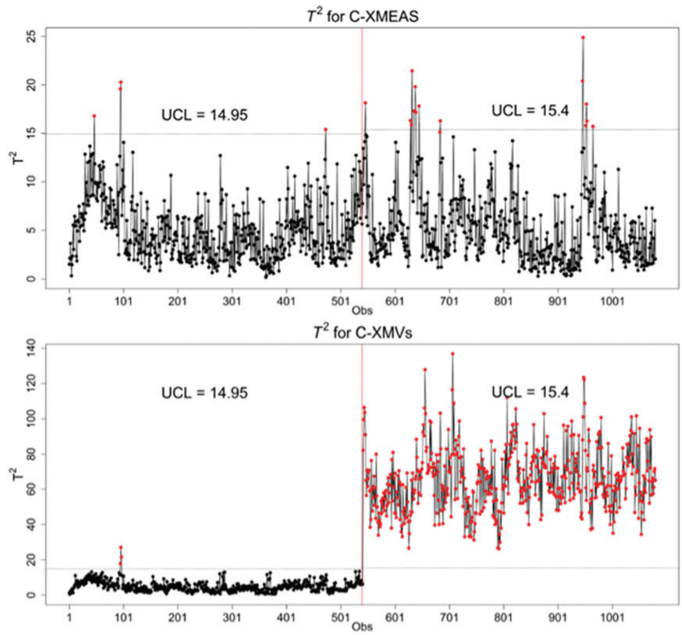

Figure 5. Hotelling T^2 chart based on individual observations for the C-XMEAS (top) C-XMVs (bottom). The vertical line divides Phase I and Phase II data.

targets thanks to the feedback control loops. If the C-XMVs are studied, the analyst would probably deem the process to be out-of-control. That the process is disturbed becomes evident by studying the Hotelling T^2 chart based only on the five C-XMVs (bottom panel in Figure 5). While one may consider the process in control during Phase I, it is out-of-control in Phase II. Moreover, a visual inspection of the univariate C-XMVs plots in Figure 6 suggests that an increase in the flow of the reactor cooling water, XMV(10) compensates for the effect of the introduced fault in the inlet temperature. Such a control action could, of course, increase waste of water and/or energy while trying to maintain product properties on target.

Closing remarks

The example above shows a possible application of how to use the TE process as a testbed for SPC methods. As the TE process is run in closed-loop operation, control actions may partly or entirely displace the impact of a disturbance from the controlled variables to manipulated variables. The traditional approach of applying a control chart on the (controlled) process output then needs to be supplemented with a control chart on the manipulated variables. The concurrent use of both of these control charts allows for [1] confirming the presence and effectiveness of the controller by analyzing the control chart for the controlled variables and [2] identifying potential assignable causes by analyzing the control chart for the manipulated variables.

Example 2: DoE in TE process simulator

This example illustrates a response surface methodology approach based on sequential experimentation using a subset of the set-points of the control loops in the TE process. The example starts with a two-level fractional factorial design, which is augmented to a central composite design, followed by confirmation runs in the simulator. The example describes how to use the TE process for experimentation. Hence, we conduct a simplified analysis of the experimental results applying ANOVA on the average values of the time series of the factors and the response of each experimental run, as suggested by Vanhatalo et al. (2013).

Closed-loop process performance may improve by exploring the relationships between the set-points of the controlled variables and an overall performance

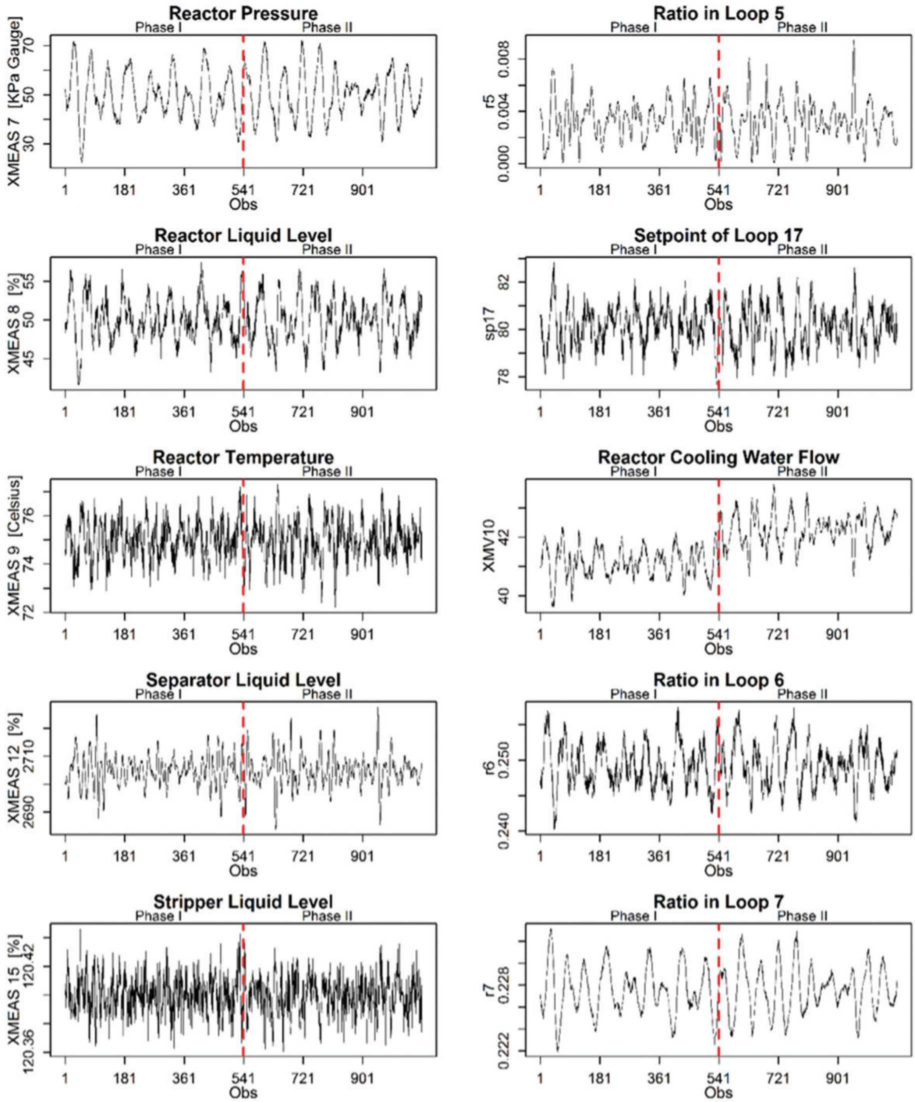

Figure 6. Univariate time series plots for C-XMEAS (left column) and C-XMVs (right column) during both Phase I and II.

indicator such as production cost. Consider an experiment where we first want to identify reactor set-points that affect the operating cost and then aim to minimize this cost. Our experimental factors are in this case the five set-points of the controlled variables in loops 11, 12, 14, 15 and 16. The response is the process operating cost ($/h). Table 7 presents the set-points of the starting condition, the average operating cost (long-term value) given these set-points, and the chosen levels of the set-points in the two-level experimental design. Note that the choices of experimental factor levels were found using trial-and-error by changing the base case values, testing that these values yield a stable process. The input variables that were not involved in control loops were set at operating Mode 1 values (Table 2) in all simulations.

Selecting and scaling disturbances

Real processes are often disturbed by unknown sources. The random process variation in the simulator needs to be comparable to disturbances affecting a

Table 7. Long-term average operating cost at the set-points of the starting condition. Low and high level of the set-points used as experimental factors.

Loop	Controlled variable	Set-points of the starting condition	Low level	High level
7	Stripper liquid rate (production)	22.949 $m^3\ h^{-1}$	-	-
9	Stripper liquid level	50%	-	-
10	Separator liquid level	50%	-	-
11	Reactor liquid level	75%	70%	75%
12	Reactor pressure	2705 kPa	2600 kPa	2705 Kpa
13	Mole % G (product quality)	62 mol%	-	-
14	Amount of A in reactor feed (y_A)	54.95%	55%	65%
15	Amount of A+C in reactor feed (y_{AC})	58.57%	50%	59%
16	Reactor temperature	120.40 °C	120 °C	127 °C
Long-term average operating cost		147.60 $/h		

real process. We used the random disturbances IDV(8) and IDV(13) to add random disturbances to the process. The impact of IDV(8) on the operating costs of the process was studied using ten simulations with the starting set-points given in Table 7. The scale factor of IDV(8) was then increased in increments of 0.1 in each run. Each simulation, run with a random seed, lasted 200 hours (simulation time, not real time) and the operating cost was sampled every 12 minutes (simulation time). We repeated the procedure for IDV(13), increasing the scale factor in increments of 0.1 in each run. Visual inspection of the resulting cost time series led us to the conclusion that the scale factors for both IDV(8) and IDV(13) should be set between 0.1 and 0.4 to produce reasonable random variability.

The scale factors of IDV(8) and IDV(13) were set to 0.31 and 0.1 respectively throughout the simulations after drawing random numbers from a uniform distribution between 0.1 and 0.4. From another set of 20 simulations with these selected scale factors, the average (long-term) operating costs were 147.60 $/h with a standard deviation of 36.75 $/h. Visual inspection shows that the process operating cost exhibits a transition time of approximately 24 hours before reaching the steady state. Therefore, we removed observations of the cost function during the first 24 hours before calculating the average and standard deviation of the time series of the process operating cost.

Experimental design and analysis

Analyses reported in this section were all made using Design Expert® version 10.

Phase I: Screening

We chose a 2^{5-1}_{V} fully randomized fractional factorial design with four additional center runs to screen the five factors (reactor set-points) in Table 7. The experiment started by a "warm-up phase" where the TE process was run for 36 hours (180 samples) using the starting set-point settings in Table 7. After these 36 hours, the TE process was deemed to have reached steady-state. At steady-state, all runs were conducted in sequence according to their run order during continuous process operation. The simulation runs lasted 50 hours each (250 samples) and the simulation seed was randomly changed before each run. The operating cost was sampled every 12 minutes.

We calculated response averages for each run to analyze the response time series of the cost. We removed the observations of the transition time before calculating the run averages to avoid a biased estimation of the main effects and their interactions (Vanhatalo et al. 2013). The transition time during some runs was determined to be approximately 24 hours through visual inspection. Some settings thus affected process stability, which meant that the run averages were based on the run's last 26 hours (130 samples). Table 8 shows the run order during the experiment and the averages of the process operating cost for each run.

Table 9 presents an ANOVA table of active effects (at 5% significance level) based on the first 20 experimental runs of Table 8. Four main effects and two two-factor interactions have statistically significant effects on the operating cost. We also included the main effect of factor E in the model due to effect heredity. However, the significant curvature suggests that a higher order model may be needed.

Phase 2: Second-order model

Augmenting the resolution V fractional factorial design with ten additional axial points run in a new block produced a central composite design, allowing for estimation of a second-order model. We simulated the second block of experimental runs in sequence as a continuation of the first 20 runs and used the same procedure to calculate run averages as in the first

Table 8. Run order, standard order of the runs, and average operating cost after removing the transition time at the beginning of each run. The "c" in standard order marks the center points.

Block 1: 2^{5-1}_{V}						*Block 2: Augmented plan*		
Run order	*Standard order*	*Operating Cost ($/h)*	*Run order*	*Standard order*	*Operating Cost ($/h)*	*Run order*	*Standard order*	*Operating Cost ($/h)*
1	9	163.66	11	17c	128.83	21	27	147.82
2	14	162.79	12	19c	126.96	22	22	135.91
3	12	155.84	13	3	144.00	23	21	126.96
4	10	175.84	14	13	175.24	24	28	189.13
5	7	127.38	15	2	180.51	25	29	168.99
6	18c	131.29	16	1	140.62	26	26	136.39
7	20c	123.26	17	16	159.84	27	24	117.51
8	6	145.13	18	8	136.36	28	30	163.25
9	5	151.53	19	11	158.39	29	23	147.95
10	4	129.90	20	15	136.09	30	25	140.13

Table 9. ANOVA and estimated effects based on the first 20 runs in Table 8. Third order and higher interactions are ignored.

Source	Sum of Squares	df	Mean Square	F Value	Prob > F	Estimated Standardized Effects ($/h)
Model	3941.46	7	563.07	29.65	< 0.0001	
A: Reactor Liquid Level	151.89	1	151.89	8.00	0.0164	3.08
B: Reactor Pressure	1360.21	1	1360.21	71.64	< 0.0001	-9.22
C: Amount of A in the reactor feed (y_A)	184.90	1	184.90	9.74	0.0097	-3.40
D: Amount of A+C in the reactor feed (y_{AC})	1093.39	1	1093.39	57.58	< 0.0001	8.27
E: Reactor Temperature	21.22	1	21.22	1.12	0.3131	-1.15
CE	225.63	1	225.63	11.88	0.0055	3.76
DE	904.21	1	904.21	47.62	< 0.0001	7.52
Curvature	*2017.86*	*1*	*2017.86*	*106.27*	*< 0.0001*	3.08
Residual	208.87	11	18.99			
Lack of Fit	174.46	8	21.81	1.90	0.3234	
Pure Error	34.41	3	11.47			
Cor Total	6168.18	19				
				R^2		63.90%
				Adjusted R^2		42.84%
				R^2 prediction		34.71%

Table 10. ANOVA and estimated effects for the augmented design using observations in both blocks. The model includes only those terms significant on a 5% significance level. Third order and higher interactions are ignored.

Source	Sum of Squares	df	Mean Square	F Value	Prob > F	Estimated Standardized Effects ($/h)
Block	0.49	1	0.49			
Model	9896.57	10	989.66	51.10	< 0.0001	
A: Reactor Liquid Level	188.15	1	188.15	9.72	0.0060	2.80
B: Reactor Pressure	1809.73	1	1809.73	93.45	< 0.0001	-8.68
C: Amount of A in the reactor feed (y_A)	159.56	1	159.56	8.24	0.0102	-2.58
D: Amount of A+C in the reactor feed (y_{AC})	1924.18	1	1924.18	99.36	< 0.0001	8.95
E: Reactor Temperature	37.30	1	37.30	1.93	0.1821	-1.25
CE	225.63	1	225.63	11.65	0.0031	3.76
DE	904.21	1	904.21	46.69	< 0.0001	7.52
C^2	160.68	1	160.68	8.30	0.0100	2.40
D^2	2772.06	1	2772.06	143.14	< 0.0001	9.95
E^2	2453.31	1	2453.31	126.68	< 0.0001	9.36
Residual	348.58	18	19.37			
Lack of Fit	314.17	15	20.94			
Pure Error	34.41	3	11.47			
Cor Total	10245.64	29				
					R^2	96.60%
					Adjusted R^2	94.71%
					R^2 prediction	89.49%

block. We did not impose any blocking effect in the simulations. The analysis of the 30-run augmented design gives the second-order model shown in the ANOVA table (Table 10). The residual analysis indicated that the 15th run (standard order #2) could be an outlier. However, since we did not find a reasonable explanation for this outlier, we chose to include it in the model despite a slight decrease in the R^2, R^2 adjusted, and R^2 predicted statistics. Table 10 thus presents the ANOVA table of the augmented design

Table 11. The suggested setting of the reactor set-points to obtain lowest operating cost.

Loop	Controlled variable	Suggested set-points setting
7	Stripper liquid rate (production)	Not in model (refer to Table 7)
9	Stripper liquid level	Not in model (refer to Table 7)
10	Separator liquid level	Not in model (refer to Table 7)
11	Reactor liquid level	70.37%
12	Reactor pressure	2701.30 kPa
13	Mole % G (product quality)	Not in model (refer to Table 7)
14	Amount of A in reactor feed (y_A)	63.67%
15	Amount of A+C in reactor feed (y_{AC})	52.25%
16	Reactor temperature	124.25 °C
Estimated process operating cost		117.07 $/h

in Table 8 (5% significance level). The non-significant lack of fit and the high values of the R^2 statistics indicate that the model fits the data well and has good predictive ability.

We then minimized the operating cost within the experimental design region spanned by the low and high levels of the factors in Table 7 based on the model in Table 10. The numerical optimization tool in the Design Expert® was used to search the design space, and Table 11 presents the settings of the reactor set-points that result in the lowest predicted cost.

Phase 3: Confirmation runs

Three additional confirmation runs were simulated in the TE process using the suggested set-points (Table 11). The average cost of these runs was 117.16 $/h. An average operating cost of 117.16 $/h represents a reduction of 30.44 $/h compared to the operating cost when starting set-point values are used, a reduction that we assume most production engineers would deem considerable.

Closing remarks

The sequential experimentation example illustrates how DoE methodologies can be explored in processes where engineering process control is present using the TE process simulator as a testbed. The example shows how a continuous process operating in closed-loop can be improved by shifting the set-points of the controlled variables. Experimental plans can help to explore the relationship between set-points and overall process performance indicators such as process cost or product quality. Note that the change in operating conditions invoked by the recommended change of the set-points may require re-tuning of the controllers in the system. We have not done that. That is, we assume that the control configuration and settings can still maintain the stability of the system in the new operating condition based on the new set-points. In our approach, we use DoE as a systematic solution to reduce the cost of the TE process based on an existing control system without redesigning it. As such, it resembles ideas in the so-called retrofit self-optimizing control approach from the engineering control domain described by Ye et al. (2017).

Conclusions and discussion

The TE process simulator is one of the more complex simulators available that offers possibilities to simulate a nonlinear, dynamic process and operates in closed-loop useful for both methodological research and teaching. In this article, we provide guidelines for using the revised TE process simulator, run with a decentralized control strategy, as a testbed for new SPC and DoE methods. In our experience, understanding the details of the TE process simulator and getting it to run may be challenging for novice users. The main contribution of this article is the flowcharts coupled with recommended settings of the TE process that will help a novice user of the simulator to get started. Another contribution is the suggested approach of how to induce random variation in the simulator. The possibility of introducing random variability in the simulator improves the usability of the TE process simulator in SPC and DoE contexts. This way, independent simulations can now be produced for SPC applications and independent replicates can be run in an experimental application.

In the two examples provided, we illustrate some of the challenges that an analyst normally faces when applying SPC and DoE in continuous processes operating under closed-loop control. We would like to reiterate that the illustrated examples are only examples of applications for which the TE process simulator can be used. We believe that the revised TE process simulator offers ample opportunities for studying other and more complicated scenarios that will mimic real-life applications.

SPC methods do not jeopardize the production or the product quality since these methods use observational data and require human intervention if out-of-control situations are indicated. For instance, in a real scenario, the process engineer may deem that the out-of-control situation is too marginal to stop the process for corrective actions but keep the disturbance in mind the next time the process is overhauled. However, when developing and testing SPC methods, the revised TE process simulator can quickly provide datasets with the desired characteristics as, for example, sample size, sampling time, or occurrence of a specific fault.

Unlike SPC methods, developing of DoE methods requires data from a process that was deliberately disturbed and getting access to such data could mean loss of product quality or risking the plant integrity. Consequently, the method developer will have trouble getting production managers to accommodate requests for disturbing the processes, just for the sake of developing new methods. Experimental campaigns in continuous processes tend to be lengthy and expensive. Therefore, simulators are particularly useful for developing DoE methods in such environments.

As a suggestion for further research, the possibility to develop other statistically based methods such as times series modelling or predictive analytics to be useful for a continuous process environment using the revised TE process in other applications on a wide variety of topics should of course be possible.

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PAPER D

On Monitoring Industrial Processes under Feedback Control

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On Monitoring Industrial Processes under Feedback Control

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Abstract

The concurrent use of statistical process control and engineering process control involves monitoring manipulated and controlled variables. One multivariate control chart may handle the statistical monitoring of all variables, but observing the manipulated and controlled variables in separate control charts may improve understanding of how disturbances and the controller performance affect the process. In this article, we illustrate how step and ramp disturbances manifest themselves in a single-input–single-output system by studying their resulting signatures in the controlled and manipulated variables. The system is controlled by variations of the widely used proportional-integral-derivative (PID) control scheme. Implications for applying control charts for these scenarios are discussed.

Keywords: engineering process control (EPC), statistical process control (SPC), control charts, proportional-integral-derivative (PID), disturbance signatures.

1. Introduction

Statistical process control (SPC) and engineering process control (EPC) have developed more or less independently, but with the same overarching goal of reducing process variability. SPC methods typically employ control charts to monitor that a product quality characteristic or important process variable remains close to a nominal value. If control charts signal a statistically significant change in the process mean and/or variability, the SPC methodology assumes that off-line process analysis will be able to identify sources of variation, so-called assignable causes. Given that the root-cause can be identified, problem-solving methods can then be used to remove or reduce effects of the variation sources. EPC, conversely, attempts to make a process insensitive to external disturbances by continuously adjusting a process input (manipulated variable) to ensure that an output variable (controlled variable) remains on target (the controller set-point).

The assignable causes in SPC usually arise from external disturbances. Such disturbances will increase probabilities for out-of-control signals in control charts. An out-of-control signal should trigger further investigation and corrective action and, given a successful remedial action, the reduced variability improves the process performance. The EPC controllers continuously adjust the process to minimize deviations of a controlled variable from its set-point due to various unexpected and/or unplanned external phenomena. The control action stems from the manipulation of a related and less sensitive variable thereby transferring the variability from the controlled variable to the manipulated variable. Knowledge of the causal relationships between such manipulated and controlled variables and of the process dynamics is therefore important to determine the required EPC adjustments. Athough the continuous adjustments of the manipulated variable may be able to keep the controlled variable at its set-point they may come at some increased cost that we would like to avoid.

The currently high and increasing level of automation leads to complex production environments where a combination of EPC and SPC may be needed to improve the processes, as for example, in semiconductor manufacturing (Janakiram and Keats 1998). Accordingly, there have been attempts to develop a unified tool for process improvement that concurrently uses EPC for process adjustments and SPC for process monitoring (Box and Kramer 1992; Box and Luceño 1997). MacGregor (1988) suggested that engineers could use control charts to monitor a process that was already under feedback control. For additional background and discussions, see, for example, Vander Wiel (1992), MacGregor (1992), Tucker et al. (1993), Fultin et al. (1993), Del Castillo (2002), and Vining (2010).

To apply SPC naïvely in a process under feedback control without considering how the implemented feedback control should affect the choice of variables to monitor is risky. A control chart applied to a tightly controlled variable in an EPC scheme will often result in a small "window of opportunity" or in a failure to detect out-of-control situations due to the continuous adjustments of the manipulated variable (Vander Wiel 1996). In the SPC literature, there are two basic recommended approaches to deal the potential masking effect that EPC may have on process disturbances. The first approach suggests monitoring the difference between the controlled variable and set-point value, i.e., the control error (Montgomery et al. 1994; Keats et al. 1996; Montgomery et al. 2000). Keats et al. (1996) showed that a control chart that monitors the control error detects sources of variation for which the feedback controller does not compensate. The study included integral (I), proportional-integral (PI), and proportional-integral-derivative (PID) control schemes. Montgomery et al. (1994; 2000) drew similar conclusions for feedforward control schemes.

The second approach is to monitor the manipulated variable itself (Box and Kramer 1992; Capilla et al. 1999; Capaci et al. 2018). Tsung and Tsui (2003) demonstrate that monitoring the manipulated variable may be more appropriate than monitoring the controlled variable for some processes and vice versa for others. Therefore, a combined approach that jointly monitors the control error and the manipulated variable (or the controlled and the manipulated variables) using a multivariate control chart is also possible (Tsung, Shi, and Wu 1999; Tsung 1999). A combined approach increases the chances that the control chart will issue an out-of-control signal. The out-of-control signal may be issued either when the controller fails to compensate for the disturbance completely or when the manipulated variable deviates from its normal (expected) operating condition.

The main aim of this article is to provide further insight and guidelines to an analyst who wants to apply SPC on a system under feedback control. We focus on outlining and illustrating what we in this article will call 'disturbance signatures' (e.g., mean shifts or trends) and how these will manifest themselves in the controlled and/or manipulated variables at steady-state for step and ramp disturbances. We limit our study to a single-input–single-output (SISO) system controlled by variations of the widely used proportional-integral-derivative (PID) control scheme. Step and ramp disturbances represent two general classes of disturbances and control engineers often use such disturbances to quantify feedback control systems in practice. The controlled and manipulated variables are also monitored using control charts. We argue that monitoring both the manipulated and controlled variables in separate univariate charts instead of using a combined, multivariate chart may increase understanding of the out-of-control condition of the process and also makes it possible to evaluate controller performance. We use two simulated examples of SISO systems in Matlab/Simulink® to illustrate the disturbance signatures in the controlled and manipulated variables and the implications for process monitoring.

2. Preliminaries on Engineering Process Control

Feedback control schemes mitigate unwanted deviations of a process variable by adjusting a related manipulated variable, i.e., a process input. These adjustments (the actuator signals) depend on the implemented control scheme and the output error fed back to the controller. The output error is the difference between the actual measured value of the process variable and its set-point. Feedback control systems are also referred to as closed-loop systems. Figure 1 shows a general block diagram of a closed-loop system (Romagnoli and Palazoglu 2012). Conventionally, the variables are expressed in the frequency domain through their Laplace transformed quantities:

- $y(s)$ is the controlled variable to be kept at its set-point value $y_{sp}(s)$,
- $u(s)$ is the actuator signal of the controller, i.e., the manipulated variable,
- $y_m(s)$ is the measured output variable,
- $e(s)$ is the output error, i.e., $e(s) = y_{sp}(s) - y_m(s)$, and
- $d(s)$ is the disturbance signal affecting the process.

By definition, all Laplace transformed variables are also in deviation form, i.e., each variable represents its deviation from a corresponding steady-state value.

The dynamics of the various elements in the feedback loop are defined through their transfer function models as,

- $g_p(s)$ is the transfer function of the process plant,
- $g_c(s)$ is the transfer function of the controller,
- $g_m(s)$ is the transfer function of the measuring element (e.g., a sensor) and,
- $g_d(s)$ is the transfer function describing how the disturbance influences the output.

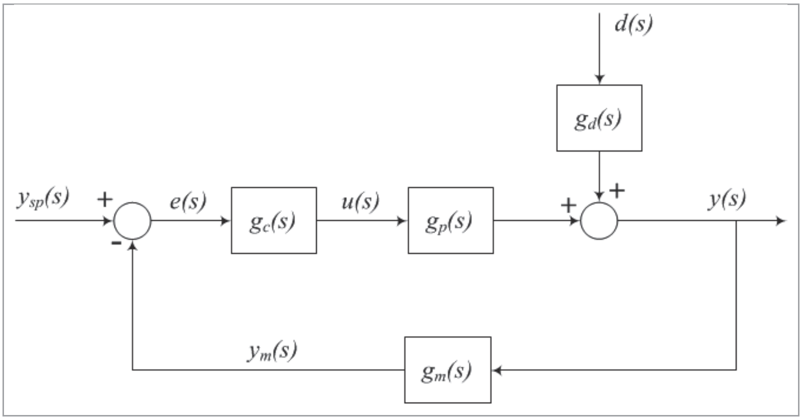

Figure 1. Block diagram of a closed-loop system subject to a disturbance.

2.1. Transfer Function of the Controller

The implemented EPC action defines the controller model (e.g., a transfer function model, $g_c(s)$). The outcome of the EPC action is evaluated considering several criteria such as closed-loop stability and performance. The speed of the response, the degree of overshoot and damping, as well as the ability of the control system to eliminate the steady-state error are often important aspects of controller performance evaluation (Romagnoli and Palazoglu 2012). Below, we briefly discuss the properties of the common PID controller.

The PID controller is typically deployed in one of three control modes - P, PI, or PID - depending on the system requirements. For convenience and ease of exposition, we will assume that the transfer function of the measuring element, $g_m(s) = 1$. We will thus have $y_m(s) = y(s)$.

Proportional (P) controller

The P mode is the simplest form of a feedback controller. The relationship between the manipulated variable and the control error is expressed proportionally as,

$$g_c(s) = \frac{u(s)}{e(s)} = k_c \tag{1}$$

where the constant k_c denotes the proportional gain. The P controller has the main advantage of having only one parameter (k_c) to tune. However, the P controller can produce a steady-state error. That is, a non-zero difference, $e(s) \neq 0$, between the set-point and measured output will remain indefinitely as long as the disturbance persists.

Proportional-Integral (PI) controller

The PI controller combines the proportional and integral control actions according to the transfer function:

$$g_c(s) = \frac{u(s)}{e(s)} = k_c\left(1 + \frac{1}{\tau_I s}\right) \tag{2}$$

where τ_I is the integral time. In the PI control mode, the integral part of the control action works to eliminate the steady-state error. However, tuning of τ_I is critical, as a too large value can lead to long settling times and a too small value can produce an oscillatory response of the controlled variable.

Proportional-Integral-Derivative (PID) controller

A PID controller combines the proportional, integral, and derivative control actions. The transfer function of this combined control action is given by,

$$g_c(s) = \frac{u(s)}{e(s)} = k_c\left(1 + \frac{1}{\tau_I s} + \tau_D s\right) \tag{3}$$

where τ_D represents the derivative time. A PID controller has the added advantage of balancing the aggressive integral action by providing an anticipatory element through the derivative action (Romagnoli and Palazoglu 2012).

2.2. Transfer Function Model of the Process Plant

One of the core components of a controlled system is the process plant model, representing the dynamic behavior of the controlled variable of interest in response to a specific input (manipulated) variable. The model of the process plant is usually expressed in the following general form,

$$g_p(s) = \frac{k_p\,(b_0 s+1)(b_1 s+1)\ldots(b_m s+1)}{(a_0 s+1)(a_1 s+1)\ldots(a_n s+1)} \tag{4}$$

where k_p is the process gain and the a's and b's can be viewed as time constants associated with the underlying physical phenomena. The constants m and n represent the order of the numerator and denominator polynomials and their difference denotes the relative order of the model. For causal systems, $m \leq n$.

2.3. Closed-Loop Systems Subject to a Disturbance

Closed-loop systems are designed to satisfy particular control objectives such as stability and performance while addressing two specific problems: set-point tracking and disturbance rejection. In this article, our focus will be on the disturbance rejection problem, and we will thus assume that the set-point is held constant. We will study the effect of external disturbances on systems controlled by variations of PID control modes and show that in some cases, even though the controller attempts to mitigate unwanted variations by adjusting the manipulated variable, the controlled variable may have a resulting steady-state error depending on the disturbance type. Therefore, steady-state analysis of both the controlled and manipulated variables in systems where EPC is implemented is relevant for understanding how SPC will work if applied to that system. Specifically, the steady-state analysis is important to understand how SPC can help detect the out-of-control signals that may result from disturbance signatures in the controlled and manipulated variables. In what follows, we focus on analyzing the steady-state behavior of the controlled and manipulated variables in closed-loop systems subject to a disturbance. We examine the effects of using P, PI, and PID controllers on the behavior of the controlled and manipulated variables for step and ramp disturbances. As most textbooks on process control provide the mathematical background, we give here only essential concepts for purposes of completeness. Appendix A provides a more detailed derivation.

2.4. Steady-State Response of Controlled and Manipulated Variables

The following assumptions are made:

- the set-point $y_{sp}(s)$ is constant over time, that is, $y_{sp}(s) = 0$,
- the set-point $y_{sp}(s)$ and the disturbance $d(s)$ are handled independently, and
- the closed-loop system is stable.

As shown in Appendix A, using the Final Value Theorem, the steady-state error e_{ss} and the steady-state values (the long-term value after the transient dynamics have settled) of the controlled and manipulated variables, y_{ss} and u_{ss}, are determined to be:

$$e_{ss} = \lim_{s \to 0} se(s) = \lim_{s \to 0} s\left[-\frac{g_d(s)}{1+g_p(s)g_c(s)}d(s)\right] \tag{5}$$

$$y_{ss} = \lim_{s \to 0} sy(s) = \lim_{s \to 0} s\left[\frac{g_d(s)}{1+g_p(s)g_c(s)}d(s)\right] = -e_{ss} \tag{6}$$

$$u_{ss} = \lim_{s \to 0} su(s) = \lim_{s \to 0} s\left[-\frac{g_d(s)g_c(s)}{1+g_p(s)g_c(s)}d(s)\right] \tag{7}$$

The steady-state values of the controlled and manipulated variables of a closed-loop system can be determined using Equations (5)-(7) if the implemented controller $g_c(s)$, the process plant model $g_p(s)$, the disturbance model $g_d(s)$, and the disturbance signal $d(s)$ are known. Again, for convenience, and without loss of generalization, we assume that $g_d(s) = 1$.

Scenario I: Step disturbance

In this first scenario, suppose that a step disturbance of magnitude $\bar{d}$ affects the system in Figure 1, that is, $d(s) = \bar{d}/s$. The steady-state values of the controlled and manipulated variables can now be determined for a given control mode - P, PI, or PID - using the process plant model in Equation (4) and Equations (5-7). Table 1 presents the steady-state error e_{ss}, and the steady-state values of the controlled and manipulated variables, y_{ss} and u_{ss}, when a P, PI, or PID control mode is in place and a step disturbance of magnitude $\bar{d}$ affects the system.

Table 1 shows that a P control mode produces a steady-state error e_{ss} proportional to $\bar{d}$ (magnitude of the disturbance) and inversely proportional to k_c (proportional gain). Even though the controller adjusts the manipulated variable continuously, ($u_{ss} \neq 0$), the controller cannot keep the controlled variable at the set-point.

Table 1. Steady-state error (e_{ss}) and steady-state values of the controlled variable (y_{ss}) and manipulated variable (u_{ss}) of a closed-loop system subject to a step disturbance when a P, PI, or PID control mode is in place.

Control Mode	Steady-state error	Controlled Variable	Manipulated Variable
	e_{ss}	y_{ss}	u_{ss}
P	$-\frac{\bar{d}}{1+\ k_c k_p}$	$\frac{\bar{d}}{1+\ k_c k_p}$	$-\frac{k_c\,\bar{d}}{1+\ k_c k_p}$
PI, PID	0	$0\ (= y_{sp})$	$-\frac{\bar{d}}{k_p}$

On the contrary, both the PI and PID control modes produce a steady-state error $e_{ss} = 0$, which means that both control modes are able to remove the step disturbance effect from the controlled variable by adjusting the manipulated variable ($u_{ss} \neq 0$). Note that for ease of discussion, we intentionally avoided adding a random component to the system. In the presence of a small amount of random noise, e_{ss}, y_{ss}, and u_{ss} also show the presence of noise, slightly fluctuating around their steady-state values. However, when the amount of random noise is not negligible, the control action design should also consider noise attenuation. Hereafter, we assume that the random noise affecting the system is small and that the controller can cope with it.

Scenario II: Ramp disturbance

In this second scenario, suppose that a ramp disturbance of a slope $\hat{d}$ affects the system, that is, $d(s) = \hat{d}/s^2$. Similar to the step disturbance scenario, the steady-state values e_{ss}, y_{ss}, and u_{ss} (given in Table 2) can be determined for the P, PI, and PID control actions when a ramp disturbance affects the system. Note that when a P action is in place, the steady-state values e_{ss}, y_{ss}, and u_{ss} do not converge to a finite value. It is thus evident that a P control mode is not suitable if ramp disturbances are expected. When a PI or a PID control action is in place, the steady-state value of the controlled variable y_{ss} converges to a constant finite value, although different from the set-point value y_{sp}, proportional to $\hat{d}$ (slope of the ramp) and τ_I (the integral time constant) and inversely proportional to k_c (the proportional gain of the controller). In summary, a PID control scheme cannot remove the steady-state error for a ramp disturbance.

Table 2. Steady-state error (e_{ss}) and steady-state values of the controlled variable (y_{ss}) and manipulated variable (u_{ss}) of a closed-loop system subject to a ramp disturbance when a P, PI, or PID is in place. Note that the signs of ∞ need to be changed to the opposite signs if $\hat{d} < 0$.

Control Mode	Steady-state error	Controlled Variable	Manipulated Variable
	e_{ss}	y_{ss}	u_{ss}
P	$-\infty$	$+\infty$	$-\infty$
PI, PID	$-\frac{\tau_I}{K_c K_p}\hat{d}$	$\frac{\tau_I}{K_c K_p}\hat{d}$	$-\infty$

3. SPC and EPC Used Concurrently

As mentioned earlier, the aim of EPC is to reduce variation by keeping the variable of interest around a set-point through continuous adjustments of another variable. SPC also aims at reducing variation, but in this case, the aim is the detection and subsequently the removal of the disturbance from the system that causes more than an expected amount of variation. In that regard, EPC can be seen as relieving the symptom (i.e., excessive variation) without necessarily identifying and removing the cause of the problem. Its prevalence has primarily been due to its ease of application at a low cost. However, continuous monitoring of the process via SPC can be more effective than EPC alone when the disturbance is persistent, for example when the resulting disturbance signature in the manipulated variable is a mean shift and adjustments are relatively costly.

SPC is by nature a real-time scheme. That is, process surveillance is performed as an on-going process. The idea is to focus on a variable of interest or a statistic directly related to the state of the process and based on its current value declare the process in-control or out-of-control. Hence, SPC can ultimately be seen as a decision-making scheme and as is the case with any decision made, two potential errors can occur: labelling a process out-of-control when in fact it is in-control (false alarm) and vice versa (delay in detection).

The probability of these errors happening can be calculated if the distribution of the statistic being monitored is known. In most cases, even if the distribution is identified, its parameter(s) needs to be estimated. For that, an off-line study (also called Phase I study) is performed where the data is collected following the data collection scheme set for the real-time monitoring and parameter estimates are estimated accordingly. These estimates can be used to calculate the probabilities of a false alarm or delay in detection for a given change in the distribution parameters. The uncertainties associated with the parameter estimation also affect the calculation of these probabilities, but this is beyond the scope of this article.

In SPC, the primary decision-making tool is a control chart on which the statistic of interest is plotted along with a threshold(s) (also called the control limits) within which the statistic is expected to be for an in-control process. The threshold is obtained through the probability distribution of the statistic. Akin to Type I and Type II errors in hypothesis testing, the decision errors (false alarm and delay in detection) compete leading to a choice of threshold where a balance between the probabilities of these two errors is established. Similarly, the commonly used performance measure for a control chart is its average run length (ARL), the expected amount of observations collected before an out-of-control signal is seen. For an in-control process (and assuming that the observations are independent), the ARL is the inverse of the false alarm rate, and for an out-of-control process, it is the inverse of the probability of detection. For further details on control charts, we refer the reader to Montgomery (2012).

3.1. Control Charts for Individual Observations

The Shewhart chart and the time-weighted control charts, such as the cumulative sum (CUSUM) control chart (Page 1954) or the exponentially weighted moving average (EWMA) control chart (Roberts 1959), are commonly applied univariate control charts for individual observations. In this article we elaborate on the CUSUM chart in somewhat more detail below as it performs well in detecting small shifts in the mean of a process, which we will encounter in the upcoming examples.

As the name indicates, the statistic for the CUSUM chart is obtained through the accumulated deviation from the expectation. Since in this work we mainly focus on the shift in the process mean, we apply CUSUM on the deviations of the observations from their expectation. To avoid scaling issues, we standardize the variable by taking its average out and dividing it by the sample standard deviation both obtained from the Phase I study. For the standardized CUSUM chart, the following two statistics are recorded for upward and downward shifts in the mean, respectively:

$$\begin{aligned} C_i^+ &= max\left[0, \frac{x_i - \mu_0}{\sigma} - k + C_{i-1}^+\right] \\ C_i^- &= min\left[0, \frac{x_i - \mu_0}{\sigma} + k + C_{i-1}^-\right] \end{aligned} \qquad (9)$$

where μ_0 is the target value and σ is the standard deviation of the process variable x estimated, respectively, using the average and the sample standard deviation, and k is the reference or slack variable. The slack variable is used to avoid excessive false alarms and often chosen to be halfway between the target mean (μ_0) and out-of-control mean (μ_1) that is of interest for fast detection. The shift is often given in standard deviation units

$\mu_1=\mu_0+\delta\sigma$. For the standardized variable, we then have $k = \delta/2$. Furthermore, the starting values are $C_0^+ = C_0^- = 0$.

The process is deemed out-of-control if either C_i^+ or C_i^- exceeds a critical value h. In most practical applications, $h = 5$ is often recommended as it provides a good average run length (ARL) to detect shifts of 1σ in the process mean. The reader is referred to Montgomery (2012) for further details about the CUSUM chart.

3.2. Disturbance Signatures in the Controlled and Manipulated Variables

Depending on the applied control mode, (P, PI, or PID), the steady-state error in the controlled variable due to a step disturbance can be eliminated partially or completely through continuous adjustments of the manipulated variable (see Table 1). Moreover, Table 2 shows that variations of the PID control scheme, at best, only reduces the steady-state error in the controlled variable that a ramp disturbance induces. Consequently, there are circumstances where the disturbance signature appears in both the controlled and manipulated variables. If control charts are applied to both the controlled and manipulated variables, then both may issue an out-of-control signal, albeit for different reasons. The choice of control mode will also influence how the two charts will signal for different types of disturbances. Moreover, the disturbance types and magnitudes, and the control chart and its parameters influence the charts' detection abilities. General recommendations of which control charts and control chart parameter settings are most appropriate for each variable in a process under feedback control are hard to give. However, if we know which control action is in place (P, PI, or PID), we would know a-priori in which variables a step or a ramp disturbance will manifest itself and what kind of signature to expect (mean shift or trend). Such knowledge can guide the choice of a control chart and eventually the disturbance identification during the monitoring phase (Phase II).

Table 3 indicates on which variables (manipulated and/or controlled) the signature of a step or ramp disturbance can be found depending on the control mode used (P, PI, or PID) and if this signature is of the type 'mean shift' or 'trend'.

Table 3. Signatures of step and ramp disturbances on the controlled and manipulated variables depending on the control mode (P, PI, or PID).

Control Mode	Step Disturbance		Ramp Disturbance	
	Controlled variable	Manipulated variable	Controlled variable	Manipulated variable
P	Mean shift	Mean shift	Trend	Trend
PI, PID	No signature	Mean shift	Mean shift	Trend

As shown in Table 3, the signature of a step disturbance can be found as a mean shift solely in the manipulated variable when the PI or PID control modes are used, whereas the signature of a step or ramp disturbance will be visible as mean shifts or trends in both the controlled and manipulated variables in the remaining cases. In the former case, a properly chosen and parameterized control chart applied to the manipulated variable should issue an out-of-control signal if the controller is working properly. In latter cases, control charts on both the controlled and manipulated variables can be expected to issue out-of-control signals. Consequently, the typical approaches of monitoring either only the manipulated variable or both the manipulated and controlled variables in one multivariate control chart are expected to result in an out-of-control signal for all cases in Table 3. However, it should be underscored that the multivariate chart in itself would be less informative as monitoring the controlled and manipulated variables separately allows for more insight, e.g., regarding how well the controller is performing, or if the controllers are malfunctioning as well as to offering clues of what type of disturbance may be affecting the system.

4. Example 1 – Heat-Exchanger with a proportional (P) controller

In this example, we will study how the disturbance signatures manifest themselves in the controlled and manipulated variables of a simulated SISO system controlled by a proportional (P) controller to exemplify some of the theoretical results presented in Tables 1-3.

4.1. Heat-Exchanger and Controller Transfer Functions

The model of the process plant, $g_p(s)$, obtained empirically by Romagnoli and Palazoglu (2012), represents a heat-exchanger where the input-output relationship between the exit temperature (°C) of the process stream and the steam flow rate (ml/s) is expressed as

$$g_p(s) = \frac{\text{Temperature}}{\text{Steam Flow Rate}} = \frac{2.58e^{-14.61s}}{33.73s + 1} \tag{10}$$

Here it is assumed that the heat-exchanger is operating in closed-loop with a P controller:

$$g_c(s) = \frac{u(s)}{e(s)} = k_c = 0.8315 \tag{11}$$

where the proportional gain, k_c, was tuned using the Ziegler-Nichols technique. The system was simulated in Matlab/Simulink® adding a random, normally distributed noise with zero mean and constant variance, $\sigma^2 = 0.002$.

4.2. Scenario I: Step Disturbance

A dataset including 840 samples of the controlled and manipulated variables was produced through simulation. A step-change disturbance of magnitude $\bar{d} = 0.25$ was introduced at the 440th observation and onwards.

Disturbance signatures in the controlled and manipulated variables

The left half of Table 4 provides the mean, standard deviation, and steady-state values of the temperature (controlled variable) and steam flow rate (manipulated variable) when no disturbance is present, $\bar{d} = 0$. The mean and the standard deviation were calculated by removing the start-up phase of the process that was deemed to be completed after 40 samples, creating a Phase I data set consisting of 400 observations. All theoretical steady-state values, y_{ss} and u_{ss}, were calculated using the formulas in Table 1.

As shown in the left half of Table 4, the theoretical steady-state values y_{ss} and u_{ss} are similar to the respective mean values of the controlled and manipulated variables. Differences from the theoretical steady-state values are due to the added random noise. As the mean temperature is close to zero, it is clear that the P controller is able to keep the controlled variable at its set-point when the process is running without any disturbance ($\bar{d} = 0$).

The right half of Table 4 provides the theoretical steady-state values y_{ss} and u_{ss} when the process is affected by a step disturbance of magnitude $\bar{d} = 0.25$ as well as the estimated means and standard deviations of the controlled and manipulated variables. The P controller is no longer able to maintain the temperature at the desired set-point value. The mean of the controlled variable when the disturbance is active is 0.090, close to the theoretical steady-state value. As outlined in Table 3, when a P controller is used a step disturbance results in a mean shift on both the controlled and manipulated variables.

Table 4. Mean, standard deviation, and steady-state values of the controlled and manipulated variables when $\bar{d} = 0$ and $\bar{d} = 0.25$ (step disturbance).

Variable	**Phase I: $\bar{d} = 0$**				**Phase II: Step disturbance $\bar{d} = 0.25$**			
	Mean	*Sd*	*Steady-state value*		*Mean*	*Sd*	*Steady-state value*	
Temperature [°C]:controlled	0.001	0.047	y_{ss}	0	0.090	0.045	y_{ss}	0.080
Steam flow rate [ml/s]:manipulated	-1.066	38.87	u_{ss}	0	-74.937	37.74	u_{ss}	-66.109

Figures 2 (a-b) provide the time series plots of the 800 observations of the temperature (controlled variable) and steam flow rate (manipulated variable). Both variables show a transient and then a clear, sustained shift after the introduction of the step disturbance. Hence, we do not provide control charts as any univariate control chart would be able to detect these apparent mean shifts in the variables quickly.

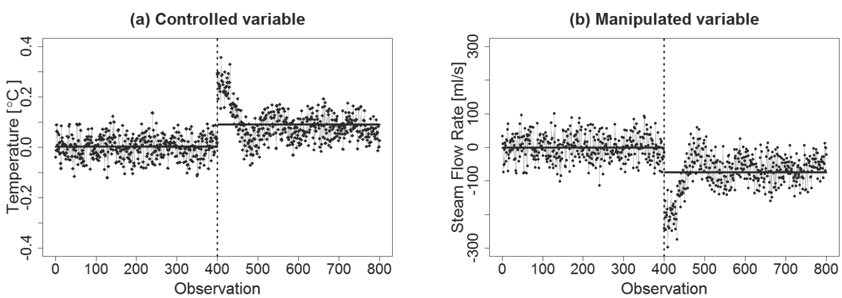

Figure 2. Time series plots of the controlled (a) and manipulated (b) variables. The step disturbance of magnitude $\bar{d} = 0.25$ occurs at the 400th observation as indicated by the vertical dotted line. The horizontal lines in the time series plots indicate the mean values of the controlled and manipulated variables in Phase I and Phase II (after the introduction of the disturbance).

4.3. Scenario II: Ramp Disturbance

A new dataset with 840 observations of the controlled and manipulated variables from the heat-exchanger example was generated. This time, a ramp disturbance with a slope $\hat{d} = 0.01$ was introduced at the 440th observation and onwards.

Disturbance signatures in the controlled and manipulated variables

Table 5 shows the mean, standard deviation, and the theoretical steady-state values of the controlled and manipulated variable without the disturbance ($\hat{d}$ = 0) and after the disturbance is introduced ($\hat{d}$ = 0.01). Again, the mean and the standard deviation when there is no active disturbance were calculated by removing the first 40 observations of the start-up phase. The theoretical steady-state values y_{ss} and u_{ss} are zero when $\hat{d}$ = 0 (see Table 1) and drawn from Table 2 when $\hat{d} = 0.01$.

Table 5. Mean, standard deviation, and steady-state values of the controlled and manipulated variables when $\hat{d} = 0$ and $\hat{d}$ = 0.01 (ramp disturbance).

Variable	**Phase I: $\hat{d} = 0$**				**Phase II: Ramp disturbance $\hat{d} = 0.01$**			
	Mean	*Sd*	*Steady-state value*		*Mean*	*Sd*	*Steady-state value*	
Temperature [ºC]: controlled	0.0004	0.045	y_{ss}	0	0.4244	0.044	y_{ss}	$+\infty$
Steam Flow Rate [ml/s]: manipulated	-0.3322	37.695	u_{ss}	0	-352.873	37.196	u_{ss}	$-\infty$

As expected, the simulation results summarized in Table 5 confirm those presented in Table 3. The P controller cannot keep the temperature at its set-point when the ramp disturbance is introduced, and the disturbance signature is visible on the mean values of both the controlled and manipulated variables in Phase II. Note that the theoretical steady-state values of the controlled and manipulated variables approach infinity as the ramp disturbance approaches infinity. That is, the values of the controlled (manipulated) variable keep increasing (decreasing) as long as the ramp disturbance continues to increase (decrease). Figures 3 (a-b) provide a graphical representation of this behavior where the temperature continues to increase and move away from its set-point while the steam flow rate keeps decreasing to counteract the disturbance. Similar to the previous case, these trends in both variables are apparent, so we do not provide control charts. Any univariate control chart would be able to signal an out-of-control situation in these variables quickly.

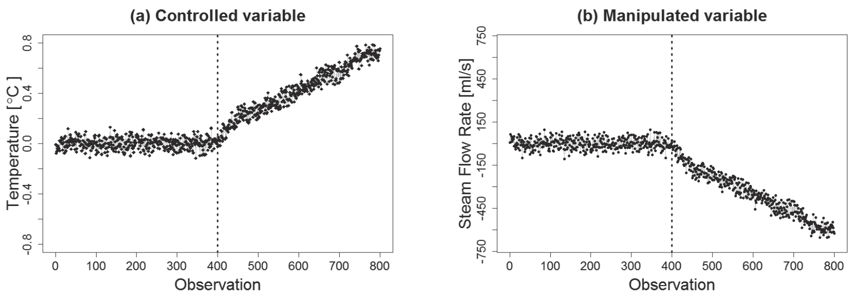

Figure 3. Time series plots of the controlled (a) and manipulated (b) variables. A ramp disturbance of a slope $\hat{d}$= 0.01 occurs at 400th observation as indicated by the vertical dotted lines.

4.4. Remarks on the Heat-Exchanger Example

The heat-exchanger example illustrates that for the P control mode, the adjustments of the manipulated variable at best reduces the effect of a step disturbance on the controlled variable while a ramp disturbance will affect the controlled variable with a continuously increasing difference between the controlled variable and its set-point over time. Consequently, the signatures of a step or ramp disturbance are present on both the controlled and manipulated variables for the P control mode. When introducing control charts to monitor a process controlled by the P control mode, it may suffice just to monitor the controlled variable in a univariate chart. Since the disturbance signal in the controlled variable may be a small mean shift, a robust choice may be to use a time-weighted control chart, such as a CUSUM chart to increase detection capability. Regarding diagnosing disturbances, note that the disturbance signatures on the controlled and manipulated variables keep their step and ramp characteristics in both cases. As we have illustrated, a step disturbance induces mean level shifts on both the controlled and manipulated variables for the P control mode whereas a ramp disturbance induces an increasing/decreasing trend in both variables. The analyst can thus use these known patterns to classify which type of disturbance is affecting the process, knowing that a P controller is governing it.

5. Example 2 – Steel Rolling Mill with a Proportional-Integral (PI) Controller

In this second example, we further illustrate the theoretical results presented in Tables 1-3 but now with a different example using the PI control mode.

5.1. Steel Rolling Mill and Controller Transfer Functions

Figure 4 depicts a steel rolling mill where steel bars pass through a pair of rolls to reduce their thickness. Each time a new bar engages the rolls, the load change produces a torque on the rolls that reduces their speed. This unwanted speed reduction can be avoided by designing a feedback control scheme that keeps the roll speed (the controlled variable) at the desired set-point (Dorf and Bishop 2011). The steel rolling mills are usually equipped with a DC motor and a speed controller to maintain the speed of the rolls. That way, the DC motor can convert the electromotive force (the manipulated variable) into rotational energy according to the error fed back to the controller. The resulting feedback control scheme has a block diagram like the one shown in Figure 1, where the torque on the rolls due to the load change can be interpreted as a (known) constant disturbance.

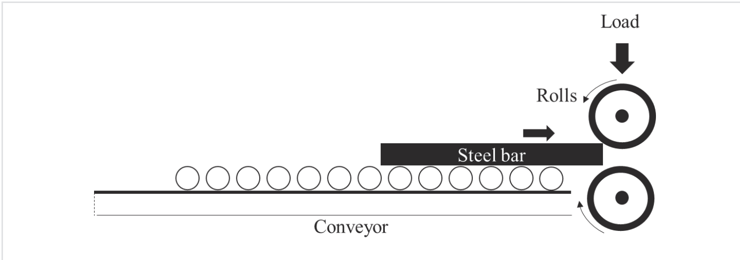

Figure 4. Steel rolling mill. Figure inspired by Dorf and Bishop (2011).

The described system was implemented in Matlab/Simulink®, introducing a normally distributed random noise with zero mean and constant variance $\sigma^2 = 6 \text{ x } 10^{-5}$ chosen subjectively to provide a realistic simulation. The variance level was picked by trial and error. The employed DC motor has the following transfer function,

$$g_{\mathrm{p}}(s) = \frac{\text{Speed}}{\text{Voltage}} = \frac{2.857}{(\tau s+1)} = \frac{2.857}{(0.086s+1)} \quad (12)$$

A Matlab model of the DC motor by Elshamy (2006) is available in the *Matlab central* file repository. For additional information about the transfer function and typical constants of the DC motor, see Dorf and Bishop (2011, pp.70-73).

A PI controller with the following transfer function

$$g_{\mathrm{c}}(s) = k_c\left(1 + \frac{1}{\tau_I s}\right) = 0.175\,(1 + \frac{1}{0.086s}) \quad (13)$$

was implemented to keep the roll speed at the set-point value. The controller parameters were tuned using the internal model control (IMC) rule by setting λ = τ/2, which indicates a twice as fast closed-loop response time compared to the open-loop. The reader is referred to Romagnoli and Palazoglu (2012) for additional information about the IMC rules for tuning PID controllers.

5.2. Scenario I: Step Disturbance

Observations of the roll speed (controlled variable) and the voltage (manipulated variable) were collected in sequence during a continuous simulation of the process. Again, 840 observations were generated. The first 440 observations were collected under normal operating conditions, that is, $\bar{d} = 0$. The first 40 observations were excluded to remove the start-up phase thus creating a Phase I data set of 400 observations. The last 400 observations constitute the Phase II dataset. A step disturbance in the torque of magnitude $\bar{d} = -0.0025$ was introduced at observation 100 in the Phase II dataset.

Disturbance signatures in the controlled and manipulated variables

Table 6 shows the mean, standard deviation, and theoretical steady-state values of the controlled and manipulated variables in Phase I and Phase II. The theoretical steady-state values y_{ss} and u_{ss} were calculated based on formulas in Table 1.

Table 6. Mean, standard deviation, and steady-state values of the rolls' speed and voltage in Phase I and Phase II (step disturbance of magnitude $\bar{d} = -0.0025$).

Variable	Phase I: $\bar{d} = 0$				Phase II: Step disturbance $\bar{d} = -0.0025$			
	Mean	*Sd*	*Steady-state value*		*Mean*	*Sd*	*Steady-state value*	
Speed [rad/s]: controlled	0.000	0.0079	y_{ss}	0	0.000	0.0082	y_{ss}	0
Voltage [mV]: manipulated	-0.093	1.380	u_{ss}	0	0.585	1.431	u_{ss}	0.875

From Table 6 we see that mean values of the controlled and manipulated variables in Phase I are the same or similar to the theoretical steady-state values y_{ss} and u_{ss} indicating stable process operation during which the PI controller is able to keep the controlled variable at the set-point. The mean value of the manipulated variable is close to the theoretical value, u_{ss}, and the small difference is due to the random noise. Table 6 also provides the theoretical steady-state values y_{ss} and u_{ss} in Phase II. Note that in a real process, these values are not known in advance since the disturbance types and magnitudes are unknown beforehand. However, in the specific situation that the analyst can assume that the disturbance is a step-change, formulas in Table 1 may actually be used to estimate the magnitude of the disturbance $\bar{d}$ using the mean of the controlled (or manipulated) variable in Phase II as an estimate of the steady-state value y_{ss} (or u_{ss}).

Table 3 as well as the mean values of Phase II in Table 6 suggest that for the PI control mode, the signature of a step-change disturbance should only be visible as a mean shift in the manipulated variable. This means that the PI controller is able to keep the disturbance from affecting the controlled variable and the disturbance signature is only identifiable in the manipulated variable.

Monitoring the controlled and manipulated variables in control charts

Figures 5 (a-b) show the time-series plots of the controlled and manipulated variables in both Phase I and II. A visual inspection of the time-series plots shows that the controlled variable does not exhibit a clear shift when the step disturbance is introduced. However, the time series plot of the manipulated variable seems to exhibit a slightly higher mean value after the step disturbance is introduced.

The Phase I and Phase II datasets with 400 observations each of the controlled and manipulated variables were used to create the control charts. Two CUSUM charts were applied to monitor the controlled and manipulated variables in Phase II, see Figures 5 (c-d). Note that in this example (as well as in the previous one) the observations in Phase I (no disturbance) are independent and normally distributed. Without active disturbances, the random variability of the controlled and manipulated variables comes from the added random, normally distributed noise. Throughout this example, we used the common choices of $k = 0.5$ and $h = 5$ for the CUSUM charts (Montgomery 2012). Other choices are possible, but here we are mainly interested in illustrating how commonly used univariate control charts can be applied to the controlled and manipulated variables, and not in optimizing the sensitivity of the charts. Under the assumption of time-independent observations, the selected CUSUM charts' parameters would result in an in-control average run length (ARL_0) of 465 observations (Montgomery 2012).

From Figure 5 (c), we see that the CUSUM chart for the controlled variable does not issue any out-of-control signal. However, the CUSUM chart for the manipulated variable issues an out-of-control signal as the CUSUM passes the control limit at the 543rd observation in Figure 5 (d). From the analysis of the control charts, it is possible to conclude that the controlled variable is in control operating close to or at its desired set-point and that the PI controller prevents the disturbance from affecting the controlled variable. The signature of the disturbance is instead displaced to the manipulated variable. The engineer may at this point undertake a root cause search for the disturbance if the sustained control action is causing unwanted costs or other negative consequences.

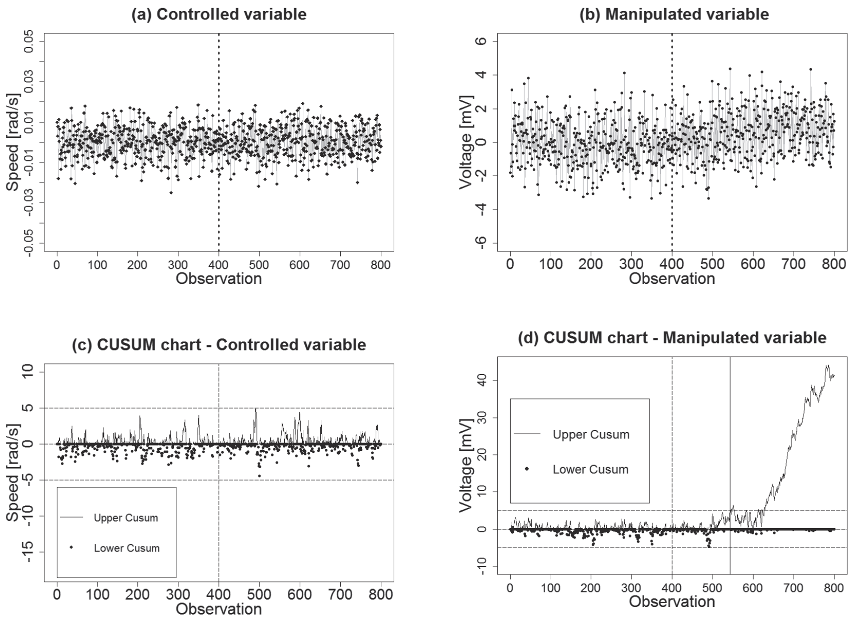

Figure 5. Time series plots of the speed (a) and voltage (b) variables. A step-change disturbance of magnitude $\bar{d} = -0.0025$ occurs at the 500th observation. The vertical dotted lines divides observations in Phase I and Phase II. (c) CUSUM chart for the controlled variable. (d) CUSUM chart for the manipulated variable. The vertical solid line indicates the out-of-control signal at the 543rd observation.

5.3. Scenario II: Ramp Disturbance

Another dataset of 840 observations was once again produced for both the controlled and manipulated variables following the same criteria of the previous step disturbance scenario. Again, the first 40 observations were removed and the Phase I dataset includes 400 observations. This time, a ramp disturbance with a slope $\hat{d} = -0.025$ was introduced at observation 100 in the Phase II dataset.

Disturbance signatures in the controlled and manipulated variables

Table 7 shows the mean, standard deviation, and theoretical steady-state values of the controlled and manipulated variables in Phase I ($\hat{d}$ = 0) and in Phase II ($\hat{d}$ = - 0.025). The theoretical steady-state values, y_{ss} and u_{ss}, are zero in Phase I whereas their values in Phase II were obtained using the formulas in Table 2.

Table 7. Mean, standard deviation, and steady-state values of the rolls' speed and voltage in Phase I and Phase II (ramp disturbance with a slope $\hat{d} = -0.025$).

Variable	Phase I: $\hat{d} = 0$				Phase II: Ramp disturbance $\hat{d} = -0.025$			
	Mean	*Sd*	*Steady-state value*		*Mean*	*Sd*	*Steady-state value*	
Speed [rad/s]: Controlled	-0.000	0.0074	y_{ss}	0	-0.003	0.0077	y_{ss}	-0.004
Voltage [mV]: Manipulated	0.029	1.2948	u_{ss}	0	4.478	1.3330	u_{ss}	$+\infty$

Monitoring the controlled and manipulated variables in control charts

Figures 6 (a-b) show the time-series plots of the controlled and manipulated variables. A visual inspection of the time-series plots shows that after the disturbance introduction (500th observation) there is an obvious increasing trend in the manipulated variable and a slight decrease in the mean of the controlled variable. In this example, the PI controller does a fair job of keeping the roll speed close to its set-point by rapidly increasing the voltage. Based on theoretical results summarized in Tables 2-3, the signature of a ramp disturbance should remain on both the controlled and manipulated variables, but a signature in the controlled variable is perhaps not evident from a visual inspection of Figure 6 (a). Therefore, we move on to analyze the control charts for the controlled and manipulated variables. Again, we used a CUSUM chart for both the controlled and the manipulated variables using the same control chart parameters as in the previous step disturbance scenario, see Figures 6 (c-d).

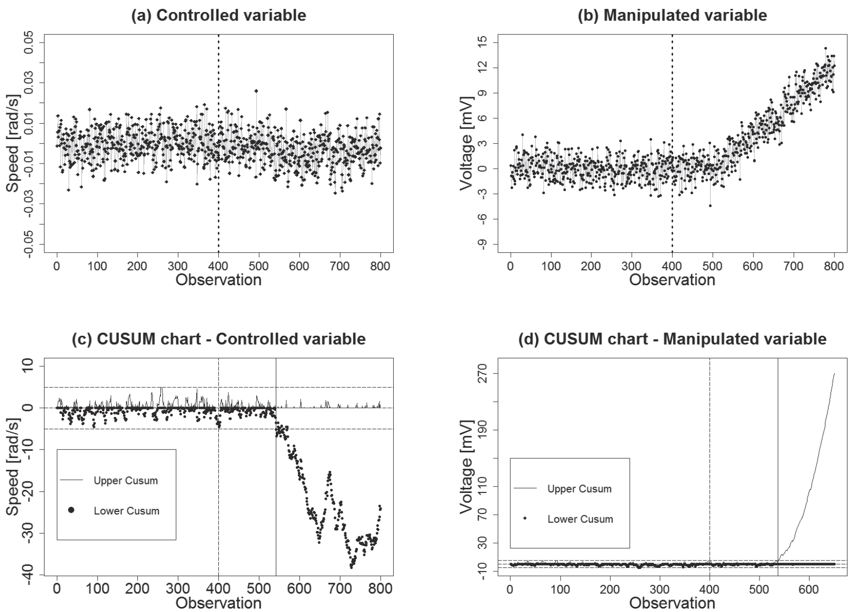

Figure 6. Time series plots of the speed (a) and voltage (b) variables. A ramp disturbance with a slope $\hat{d} = -0.025$ is introduced at the 500th observation. The vertical dotted lines divide Phase I and Phase II data. (c) and (d) are CUSUM charts for the controlled and manipulated variables, respectively. The vertical solid lines indicate the out-of-control signal at the 542nd observation for the controlled variable and at 537th observation for the manipulated variable.

The CUSUM chart for the controlled variable issues an out-of-control signal indicating a decrease in the mean of the controlled variable; see Figure 6 (c). Not surprisingly, the CUSUM chart in Figure 6 (d) for the manipulated variable also issues an out-of-control signal with an ever-increasing voltage. In a real-life scenario, however, the voltage would only be allowed to increase to a certain limit before the process would be shut down.

5.4. Remarks on the Steel Rolling Mill Example

The steel rolling mill example shows how for a given implemented control scheme and process plant, monitoring the controlled and manipulated variables separately may be crucial for understanding and interpreting out-of-control situations in a closed-loop system. Monitoring both the controlled and the manipulated variables in separate charts allows the analyst to evaluate the performance of the controller but also to develop an increased understanding of which type of disturbance is active in the system (step or ramp). For the PI (or PID) control mode, a step disturbance results in a mean shift signature in the manipulated variable only. However, a ramp disturbance induces a mean level shift in the controlled variable and an increasing or decreasing trend in the manipulated variable. In which of the variables a disturbance signal can be detected depends on the control mode used, the type of disturbance affecting the system, and the choice of control chart, as we have illustrated in the examples above and in Tables 1-3.

A generalization on the proper choice of control chart for a general EPC application is not self-evident. The Shewhart chart for individual observations would be fast to signal when a large shift occurs, such as a dramatic step-change. However, at times the remaining signals in the controlled and/or manipulated variables may be much smaller and time-weighted control charts, such as the CUSUM chart, would be needed for fast and effective shift detection.

6. Conclusions and Discussion

This article explores and discusses the concurrent use of EPC and SPC and more specifically the implications of monitoring variables from a system under feedback control through control charts. From an SPC perspective, the control action increases complexity and influences the behavior of the process variables when a disturbance affects the process.

The analyst may even fail to detect a disturbance affecting the system when monitoring only the controlled variable in an EPC scheme. This mistake may occur since the controlled variable in a feedback controller usually is “the” important process output that the naïve analyst may think warrants monitoring through SPC.

In this article, we provide formulas for calculating the theoretical steady-state values of the controlled and manipulated variables in a SISO system for the P, PI, and PID control modes, given that the system is affected by step or ramp disturbances. In the two simulated examples, we illustrate how step and ramp disturbance signatures manifest themselves in the controlled and manipulated variables for the above-mentioned control modes. The control mode used, the disturbance type, and the choice of control chart determine whether the disturbance signature can be detected in the controlled and/or manipulated variables. For step disturbances, PI and PID controllers can maintain the controlled variable on target by adjusting the manipulated variable thereby displacing the disturbance signature to the manipulated variable. For P controllers and for ramp disturbances combined with all tested control modes, the disturbance affects both the controlled and the manipulated variables.

Consequently, irrespective of the control mode applied, properly chosen and parameterized control charts monitoring the controlled and/or the manipulated variables should be able to signal out-of-control situations for step and ramp disturbances affecting the system. Our recommendation is to monitor both the controlled and manipulated variables when applying SPC on a process under feedback control. A combined study of the disturbance signatures in both control charts can also give important information on how well the controller is performing in terms of disturbance elimination as well as clues of what type of disturbance is affecting the system (step or ramp). Indeed, for the P, PI, and PID control modes, univariate control charts monitoring only the manipulated variable may also issue out-of-control signals for step and ramp disturbances. Another alternative is to use a bivariate chart based on both the controlled and manipulated variables. However, these choices would potentially be at the expense of gaining a deeper process insight. For example, if the control chart for the controlled variable is in control and the control chart for the manipulated variable is out-of-control, one can infer that the controller is performing satisfactorily in keeping the controlled variable at its set-point by transferring the disturbance (variability) from the controlled variable to the manipulated variable. The disturbance signature in the manipulated variable may, of course, be a lingering problem if the sustained adjustment incurs increased costs or other negative consequences. The goal of SPC in this case is to eliminate the assignable cause to cut potential unwanted costs of corrective adjustments by the controller. Moreover, if the control charts for both manipulated and controlled variables are out-of-control, we may conclude either that the controller is not working or that the controller is working but unable to counteract the disturbance completely. In this case, understanding and eliminating the assignable cause is even more important to reduce unwanted costs of waste, resource consumption, production of off-spec products, safety risk, or to consider potential changes on the controller design if, for example, the assignable cause occurs frequently.

This article focuses on SISO systems. Future research will explore multivariate systems and the potential of dividing controlled and manipulated variables in separate multivariate control charts for increased process insight.

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Appendix A

As shown in the block diagram of Figure 1, the effect of $y_{sp}(s)$ and $d(s)$ on the controlled variable can be expressed through the representation of the set-point tracking and disturbance rejection problems. This yields the additive output response as,

$$y(s) = \frac{g_p(s)g_c(s)}{1+ g_p(s)g_c(s)} y_{sp}(s) + \frac{g_d(s)}{1+ g_p(s)g_c(s)} d(s) \quad \text{(A.1)}$$

$$y(s) = g_{SP}(s)y_{sp}(s) + g_D(s)d(s)$$

where $g_{SP}(s)$ and $g_D(s)$ are the closed-loop transfer functions for the set-point response and the disturbance response, respectively. Since the set-point is assumed to be constant ($y_{sp}(s) = 0$), we are left with the expression,

$$y(s) = \frac{g_d(s)}{1+ g_p(s)g_c(s)} d(s) \quad \text{(A.2)}$$

The steady-state value of the controlled variable y_{ss} can then be determined using the Final Value Theorem:

$$y_{ss} = \lim_{t\to+\infty} y(t) = \lim_{s\to 0} s[y(s)] = \lim_{s\to 0} s[g_D(s)d(s)] \quad \text{(A.3)}$$

or, incorporating Equation (A.2) in Equation (A.3):

$$y_{ss} = \lim_{s\to 0} s \left[\frac{g_d(s)}{1+ g_p(s)g_c(s)} d(s)\right] \quad \text{(A.4)}$$

where the steady-state value of the controlled variable y_{ss} becomes a function of the controller, $g_c(s)$, the process model $g_p(s)$, and the disturbance model, $g_d(s)$ as well as the disturbance signal. If y_{ss} is non-zero, it represents the steady-state error. Similarly, the steady-state value of the manipulated variable is calculated as,

$$u_{ss} = \lim_{t\to+\infty} u(t) = \lim_{s\to 0} s[u(s)] = \lim_{s\to 0} s[e(s)g_c(s)]$$

Since the error term is expressed as,

$$e(s) = y_{sp}(s) - y(s)$$

This yields,

$$u_{ss} = \lim_{s\to 0} s\left[\frac{-g_d(s)}{1+ g_p(s)g_c(s)} d(s)\right][g_c(s)] = \lim_{s\to 0} s\left[\frac{-g_d(s)g_c(s)}{1+ g_p(s)g_c(s)} d(s)\right] \quad \text{(A.6)}$$

PAPER E

A Two-Step Monitoring Procedure for Knowledge Discovery in Industrial Processes under Feedback Control

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Submitted for Publication

A Two-Step Monitoring Procedure for Knowledge Discovery in Industrial Processes under Feedback Control

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ABSTRACT

Many modern production processes involve engineering process control as in the case of feedback controllers. Nonetheless, statistical process control remains valuable for detecting and eliminating assignable causes of variation. As feedback controllers continuously adjust manipulated variables to keep critical process outputs on set-points, monitoring only the controlled outputs may be ineffective. Controlled and manipulated variables can be also jointly monitored in the same multivariate chart(s) such as a Hotelling T^2 chart. However, this approach might hinder deeper process insight.

The aim of this article is to explore multivariate processes under feedback control, and to describe and illustrate a two-step monitoring procedure in which [1] the variables are pre-classified as controlled, manipulated, and measured variables and [2] a multivariate monitoring scheme is applied to each group of variables. Potential scenarios an analyst might encounter when applying the illustrated procedure are presented and knowledge discovery in terms of process and controller performance is discussed. The two-step monitoring procedure is applied using the Tennessee Eastman process simulator under a decentralized feedback control strategy. The results of two simulated examples are compared with the approach of monitoring the variables together in the same multivariate chart(s.)

Keywords: multivariate processes, multivariate statistical process control, engineering process control, latent structure methods, enhanced process understanding.

1. Introduction

Statistical process control (SPC) is a well-known, established methodology that uses control charts as the main tool to monitor whether a specified product quality characteristic or an important process variable remains near a nominal value. Many modern industrial processes currently operate under engineering process control (EPC), as in the case of feedback controllers. In industrial operations, EPC contributes to production plant safety, environmental impact reduction, and process and product optimization by keeping process variables of interest near desired target values.[1] Even though SPC and EPC appear to chase the same goal of reducing process variability, these methodologies rely on methods and concepts that are fundamentally different.

The core idea of the SPC methodology is to declare a process as in control, or out-of-control, by monitoring the process mean and/or variability with a real-time scheme, namely, a control chart.[2] A shift of the process parameters usually arises from external disturbances, responsible for unwanted sources of variability so-called assignable causes of variation. When a shift of the process parameters occurs, a control chart should give an out-of-control signal and analysts can seek ways to isolate assignable causes of variation. A reduction of the long-term process variability is thus achievable once the assignable cause(s) has been detected and removed. Additionally, feedback controllers attempt to make a process insensitive to external disturbances by continuously adjusting a process input (manipulated variable) to ensure that a process output (controlled variable) remains on target (set-point.) The control action stems from the manipulation of a process input, thereby transferring the short-term variability from the controlled to the manipulated variable. Typically, feedback controllers are utilized to keep critical process outputs on target. On the contrary, other outputs that might be difficult to adjust are not governed by feedback controllers, but are still measured and analyzed to assess the overall process performance. Such measured outputs are called measured variables.

Over the years, the concurrent use of SPC and EPC has been widely recognized and there is abundant research on the topic.[3,4,5,6,7] Statistical process control charts should be applied to an engineering controlled process to detect and remove assignable causes of variation rather than continuously compensating for them.[8] This way, an overall process improvement is achievable using the complementary capabilities of SPC and EPC to reduce long-term and short-term process variability, respectively.[9]

Naïvely applying a control chart to a tightly controlled variable in an EPC scheme will often fail to detect out-of-control situations due to the continuous adjustments of the manipulated variable [10,11]. SPC literature recommends two basic approaches to deal with EPC's potential masking of process disturbances. The first approach suggests monitoring the difference between the controlled variable and set-point value, (i.e., the control error.)[12,13,14] The second approach is to monitor the manipulated variable.[15,16] Monitoring the control error (controlled variable) or the manipulated variable alone might be ineffective.[17,18,19] Therefore, a combined approach that jointly monitors the control error and the manipulated variable (or the controlled and the manipulated variables), using a bivariate control chart is also used.[17,18] A combined approach increases the chances that the control chart issues an out-of-control signal when either the controller fails to compensate for the disturbance completely or the manipulated variable deviates from its normal (expected) operating condition[20].

The combined approach of monitoring the controlled and manipulated variables in the same multivariate chart(s) can be also extended to multivariate processes.[18,21] In this case, when an out-of-control situation occurs, the faulty variables need to be isolated to diagnose the assignable cause of the disturbance. Contribution plots are commonly used to identify which variables make the greatest contributions to push the monitored statistic(s) above the control limits.[8] However, in case of complex faults or complex processes, contribution plots suffer from a 'smearing effect' on non-faulty variables, which might make the isolation of the faulty variables challenging.[22,23,24] Classifying the process variables in 'blocks', representing for example a process unit or a section of a unit, might make the fault isolation task easier, as the process variables are analyzed in groups rather than all at once.[8,25] As alternative, the analyst can resort to the analysis of the univariate control charts but, treating the variables one at a time, as they were independent, often makes the interpretation and diagnosis difficult.[8] Although monitoring the controlled and manipulated variables in the same multivariate chart(s) usually allows detecting out-of-control process conditions, this approach might hinder deeper process insight. Monitoring the controlled and manipulated variables separately might be crucial for understanding out-of-control process conditions and controller performance. For example, Capaci et al.[26] explore single-input single-output systems under variations of the proportional-integral-derivative control scheme, and illustrate if and how frequently occurring disturbances (i.e., step and ramp disturbances) manifest themselves in the controlled and manipulated variables at a steady state. Capaci et al.[26] argue in favor of monitoring the manipulated and controlled variables in separate charts because the understanding of out-of-control conditions and controller performance might be improved.

The aim of this article is to explore multivariate processes (with multiple inputs and outputs) under feedback control and to describe and illustrate a two-step monitoring procedure in which [1] the variables are pre-classified as controlled, manipulated, and measured variables and [2] a multivariate monitoring scheme is applied to each group of variables. Potential scenarios an analyst might encounter when applying the illustrated procedure are presented and the gained knowledge of process and controller performance is discussed. The two-step monitoring procedure is applied using the Tennessee Eastman process simulator under a decentralized feedback control strategy. The results of two simulated scenarios are compared with the approach of monitoring all the variables together in the same multivariate chart(s.)

2. Statistical Process Control Charts for Multivariate Processes

This section provides a short theoretical background on multivariate control charts based on principal component analysis (PCA.) In section 4, Hotelling T^2 and Q charts based on dynamic PCA are utilized to present the results from the application of the two-step monitoring procedure to the Tennessee Eastman (TE) process.

2.1. Control Charts Based on Principal Components

When the number of variables, k, to monitor is large and the level of cross-correlation among the variables is high, a common approach for reducing the dimensionality of the variable space is to apply PCA.[27,28] PCA transforms a set of correlated variables into a new set of uncorrelated latent variables, principal components (PCs), or scores that are linear combinations of the original variables defined as

$$\boldsymbol{t}_i = \boldsymbol{p}_i'\boldsymbol{x} \qquad (i = 1, 2, \dots, k) \tag{1}$$

where $\boldsymbol{x}$ is an observations vector on k variables, and $\boldsymbol{p}_i'$ is the ith eigenvector of the covariance matrix of $\boldsymbol{X}$ subject to $\|\boldsymbol{p}_i'\| = 1$. The variance of the ith PC is the eigenvalue λ_i or $var(\boldsymbol{t}_i) = \lambda_i$ and the PCs are defined so that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_k \geq 0$. Thus, the proportion of variability in the original data explained by the ith PC is given by

$$\frac{\lambda_i}{\lambda_1 + \lambda_2 + \dots + \lambda_k} \tag{2}$$

One can determine how much variability is explained by retaining the first few $r < k$ PCs. Retaining only the first r PCs, a data matrix $\boldsymbol{X}$ of m observations on k variables can be decomposed as

$$\boldsymbol{X} = \boldsymbol{TP}' + \boldsymbol{E} = \sum_{i=1}^{r} \boldsymbol{t_i}\,\boldsymbol{p_i'} + \sum_{i=r+1}^{k} \boldsymbol{t_i}\,\boldsymbol{p_i'} \qquad (3)$$

where the first r PCs are assumed to represent variation of underlying events driving the process phenomena, while the last k-r PCs are representative of the noise and can be summed up in a matrix of residuals **E**. Note that PCA is scale-dependent and the variables are often mean-centered and scaled to unit variance prior to PCA implementation. A complete explanation of PCA is available, for example, in Jolliffe [27] and Jackson [28].

Akin to other SPC procedures, a PCA-based monitoring scheme involves two phases. In Phase I, a process dataset representing normal operating conditions is used to estimate the in-control PCA model. In Phase II, new multivariate observations are monitored online based on the in-control model from Phase I. The process-monitoring scheme requires two complementary control charts that rely on the assumption of time-independent observations.[29] The first is a Hotelling T^2 chart based on the r first retained PCs (rather than the k original process variables) to monitor the variability in the PCA model space. The second is a Q control chart on the last k-r PCs to monitor the squared prediction error (*SPE*) of the residuals of the new observations, that is, the residual variability not captured by the PCA model.

In Phase II, the T^2 statistic is plotted against time along with the lower and upper control limits

$$LCL_{T^2} = 0 \qquad (4)$$
$$UCL_{T^2} = \frac{r\,(m-1)(m+1)}{m^2 - mr}\, F_{\alpha,r,m-r}$$

where $F_{\alpha,r,m-r}$ is the upper α percentile of the F distribution with r and m-r degrees of freedom. Note that in Phase I, the upper control limit for the T^2 statistic is based on the beta distribution and is provided by Tracy et al. [30]

In both Phase I and Phase II, the Q statistic is plotted against time, along with the upper control limit provided by Jackson and Mudholkar [31]

$$UCL_Q = \theta_1 \left[\frac{z_\alpha \sqrt{2\theta_2 h_0^2}}{\theta_1} + 1 + \frac{\theta_2 h_0 (h_0 - 1)}{\theta_1^2} \right]^{\frac{1}{h_0}} \qquad (5)$$

where z_α is the $100(1-\alpha)$ percentile of the standardized normal distribution, $\theta_{j=1,2,3} = \sum_{i=r+1}^{k} \lambda_i^j$, and $h_0 = 1 - \frac{2\theta_1\theta_3}{3\theta_3^2}$. The lower control limit is 0 in Phase I and in Phase II. For further details on control charts based on PCA, see MacGregor and Kourti[8], and Kourti[32].

2.2. Control Charts Based on Dynamic Principal Components

Frequently, process data exhibit a high level of both cross-correlation and autocorrelation. To account for static and dynamic relationships in the data, Ku et al.[33] suggest applying dynamic PCA (DPCA), that is, applying the usual PCA method to an augmented data matrix $\boldsymbol{X}_{lag}$obtained by appending to the original matrix $\boldsymbol{X}$ its l time-shifted duplicates. Table 1 illustrates the procedure to determine the time-shifts or number of lags l. Alternative approaches are discussed in Rato and Reis [34], and Vanhatalo and Kulahci[35].

Table 1. Ku et al.'s procedure to select the number of lags *(l)* in DPCA.[33]

1.	Set $l = 0$.
2.	Form data matrix $\boldsymbol{X}_{lag} = \boldsymbol{X}_{(m-l)\text{ x }k(l+1)} = [\boldsymbol{X}_{m\text{ x }k} \quad \boldsymbol{X}_{(m-1)\text{ x }k,1} \quad \dots \quad \boldsymbol{X}_{(m-l)\text{ x }k,l}]$.
3.	Perform PCA on $\boldsymbol{X}_{\text{lag}}$ and calculate all the scores.
4.	Set $d = k \times (l+1)$ and number of linear relations $c(l) = 0$
5.	Determine if the jth component represents a linear relation. If yes, go to 6; if no, go to 7.
6.	Set $d = d - 1$ and $c(l) = c(l) + 1$; repeat 5.
7.	Calculate the number of new linear relations $c_{new}(l) = c(l) - \sum_{h=0}^{l-1}(l-h+1)\, c_{new}(h)$
8.	If $c_{new}(l) \leq 0$, go to 10; otherwise, go to 9.
9.	Set $l = l + 1$; go to 2.
10.	Stop.

After applying DPCA on an in-control process dataset, Hotelling T^2 and Q charts based on dynamic PCs can be used to monitor the process. Since the DPCA residual space is composed of PCs with small eigenvalues, the linear relationships among the process variables should be weak in the DPCA residual space. Consequently, the Q statistic, applied to residuals, assumed to be independent, can primarily monitor the process dynamics. Refer to De Ketelaere[36] for further details on PCA-based monitoring schemes for time-dependent data.

Note that in case of strongly auto-correlated data, DPCA still produces auto-correlated PCs and the control limits of the Hotelling T^2 and Q charts might need to be adjusted.[37]

3. A Two-Step Monitoring Procedure for Processes under Feedback Control

Engineering process control is extensively used in modern industrial processes to satisfy particular control objectives such as process stability and performance. In a process under feedback control, potential unwanted effects of external disturbances on a process variable (i.e., a process output) are mitigated by adjusting a related manipulated variable (i.e., a process input); see Figure 1. The required adjustments depend on the implemented control scheme (variations of the proportional-integral-derivative schemes) and the output error fed back to the controller. The output error measures the difference between the actual process output and the desired target value or set-point. Therefore, feedback controllers are also referred to as closed-loop systems.

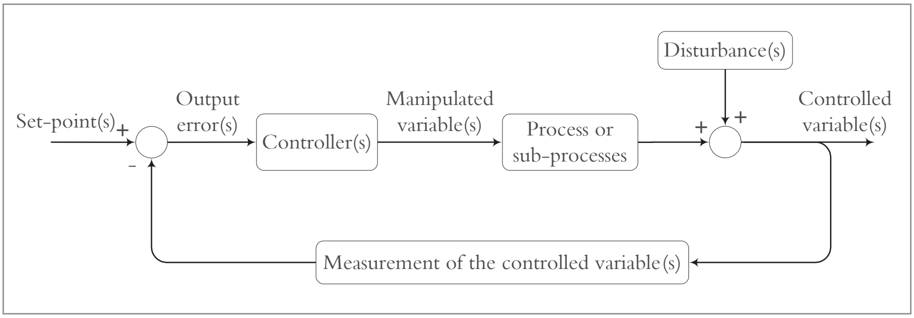

Figure 1. Compact representation of a process under feedback control subject to a disturbance.

The next section describes a two-step monitoring procedure for multivariate processes under feedback control in which [1] the variables are pre-classified qualitatively or quantitatively as controlled, manipulated, and measured and [2] a multivariate monitoring scheme is applied to each group of variables. Additionally, the next section presents potential scenarios an analyst might encounter when applying the suggested procedure, along with an understanding of process and controllers' performance.

3.1. Step 1: Classification of Process Variables

The first step of the suggested two-step monitoring procedure is to pre-classify the variables of a multivariate process under feedback control as controlled, manipulated, and measured variables. In processes with many inputs and outputs, the same set of control objectives can often be achieved via several control strategies. To determine the most appropriate control strategy, one of the most challenging tasks is the pairing between the (output) variables to be controlled and the (input) variables to be adjusted so that each controlled variable can approach the desired set-point.[1] Accordingly, control engineers first search for answers regarding potential causal relationships among process inputs and outputs, process dynamics, possible cross effects that the change of a process input might have on more outputs, and the interaction effects that the simultaneous change of more inputs might have on one output. Then, the pairing between the controlled and manipulated variables requires design decisions.[1] Control loops typically involve crucial process outputs that need to remain at the target values, for example, to maintain stable process operating conditions within equipment constraints for securing plant and personnel safety, and within quality-specification constraints.[1] On the contrary, other process outputs such as process operating costs, energy consumption, or product waste, are not usually involved in any control loop as they might be more difficult to adjust. These outputs are generally affected by the process operating conditions and are thus measured for assessing the overall process performance. The process outputs not involved in any control loop are called measured variables.

A qualitative or a quantitative approach can be used to classify the process variables as controlled, manipulated, or measured variables. A qualitative approach is feasible when existing knowledge about the variables' pairing of the process under feedback control and the implemented control strategy are known. For example, in a multi-loop strategy, multiple controllers are designed to control the whole process and each controller adjusts one manipulated variable to regulate one controlled variable. Other times, all or a subset of the manipulated variables can be used to govern simultaneously all or a subset of the controlled variables using a multivariable control strategy.[1] It is reasonable to assume that process engineers possess this kind of knowledge. Hence, a qualitative approach could often be pursued. Conversely, a quantitative approach is also possible. In this case, historical data and all the methodologies taking advantage of correlation and regression methods, such as partial least squares[32] or regression regularization methods[38,39,40], can be used to discover the hidden relationships among the process variables. An application of this approach can be found in Gao et al.,[41] who show how sparse principal component analysis regularized with a LASSO penalty can be used to discover the relationships among the process variables using simulated data from the TE process.

3.2. Step 2: Monitoring Each Group of Variables Separately

The second step of the suggested two-step monitoring procedure is to apply a multivariate monitoring scheme to each group of variables separately.

Monitoring controlled, manipulated, and measured variables in separate control charts provide additional knowledge on the process and controllers' performance. Specifically, the knowledge on where (on which group of variables) the disturbances manifest themselves supports understanding the severity of the out-of-control condition and the functioning of the controllers. Table 2 shows potential scenarios an analyst might encounter when monitoring the controlled, manipulated, and measured variables in separate multivariate control charts and summarizes the knowledge gained by analyzing the control charts.

Table 2. Potential scenarios and knowledge discovery regarding process and controller performance.

Scenario	*Controlled Variables*	*Manipulated Variables*	*Measured Variables*	*Knowledge Discovery*		
				Process Performance	*Controller*	
					Active compensatory control action?	*Performance*
1	In-Control	In-Control	In-Control	'Ideal' condition	No	N.A.
2			Out-of-Control	Not critically affected	No	N.A.
3		Out-of-Control	In-Control	Not critically affected	Yes	Well-functioning/full compensation for the disturbance
4			Out-of-Control	Not critically affected	Yes	
5	Out-of-Control	In-Control	In-Control	Critically affected	No	Malfunctioning and/or unable to counteract the disturbance
6			Out-of-Control	Critically affected	No	
7		Out-of-Control	In-Control	Critically affected	Yes	
8			Out-of-Control	Worst condition	Yes	

Note that the information in Table 2 should be thought from an SPC perspective. For example, in scenarios 3-4, the process is out-of-control although a fully operational control strategy that keeps the controlled variables on target is an in-control process from an EPC perspective. Moreover, the severity of the disturbance effect on the process performance (critically/not critically affected) is considered from a product quality standpoint. Since the controlled variables usually relate to quality characteristics of a product or of a process producing it, the process performance is deemed as critically affected by the disturbance if the controlled variables are out-of-control.

In scenario 1, the process operates at the ‘ideal’ condition as no disturbances affect the process. In scenarios 2–4, the process performance is not critically affected by the disturbance, as the controlled variables are in control. Conversely, in scenarios 5–8, the process performance is critically affected, as the controlled variables are out-of-control. Moreover, in scenarios 1 and 2, no relevant information about the controllers’ performance is available, but for different underlying reasons. In scenario 1, the process is not subject to disturbances and the analyst cannot make considerations about the controllers’ performance. In scenario 2, the process is subject to a disturbance but because this disturbance does not affect the implemented control strategy, no information is available to draw conclusions on the controllers’ performance. In scenarios 3 and 4, a compensatory control action successfully eliminates the effect of the disturbance on the controlled variables; hence, the controllers perform satisfactorily. Finally, in scenarios 5–8, the controllers are not performing satisfactorily as they are malfunctioning and/or unable to counteract the disturbance. Among the illustrated scenarios, scenario 8, in which all the variables are out-of-control, illustrates the worst process operating condition.

4. Two-Step Monitoring Procedure in the Tennessee Eastman Process

In this section, the two-step monitoring procedure is applied using the TE process under a decentralized control strategy.[42,43] The results of two simulated examples are illustrated and compared with the approach of monitoring all variables in the same multivariate chart(s.)

Data were simulated using the most recent version of the decentralized control strategy of the TE process simulator implemented by Bathelt et al.[43], as it allows for stochastic simulations, replications, and adjustments of the disturbances’ magnitude. The simulator works in Matlab/Simulink® and is available for download from the Tennessee Eastman Challenge Archive. [44] The analysis of the TE process data was conducted using the free R statistics software (the R Foundation for Statistical Computing) and the code is available upon request.

4.1. Step 1: Classification of Variables in Tennessee Eastman Process

The TE process simulator emulates a continuous chemical process composed of five major units: a reactor, a condenser, a vapor-liquid separator, a product stripper, and a recycle compressor. [45] The plant produces two liquid products from four gaseous reactants through four irreversible and exothermic reactions. It also produces an inert product and a byproduct purged as vapors from the system through the vapor-liquid separator. The TE process consists of 41 process outputs (XMEAS) and 12 process inputs (XMV) and can work in three operating modes (mode 1-3). In addition, the user can choose to activate 21 process disturbances (IDVs).

Ricker[42] devised the decentralized control strategy of the TE process. The decentralized control strategy partitions the plant into sub-units and designs a controller for each, with the intent of maximizing the production rate. Ricker identifies nineteen feedback control loops to stabilize the process and provides a comprehensive explanation of the implemented control strategy (control loops and pairing between the controlled and manipulated variables) and its design phases. Therefore, the classification of the TE process variables as controlled, manipulated, and measured variables can be accomplished using a qualitative approach.

Table 3 provides the control loops, the pairing between controlled and manipulated variables, and the measured variables for the decentralized control strategy of the TE process. As shown in Table 3, the classification has led to 16 controlled variables, 18 manipulated variables, and 25 measured variables.

Table 3. Controlled and manipulated variables in the 19 loops, and measured variables of the TE decentralized control strategy. The manipulated variables with codes such as F_p and r_7 come from the decentralized control strategy settings.[42] XMV(*i*) and XMEAS(*j*) are numbered according to the original article by Downs and Vogel.[45]

Loop	*Controlled variable*	*Code*	*Manipulated variable*	*Code*
1	A feed rate (stream 1)	XMEAS(1)	A feed flow	XMV(3)
2	D feed rate (stream 2)	XMEAS(2)	D feed flow	XMV(1)
3	E feed rate (stream 3)	XMEAS(3)	E feed flow	XMV(2)
4	C feed rate (stream 4)	XMEAS(4)	A and C feed flow	XMV(4)
5	Purge rate (stream 9)	XMEAS(10)	Purge valve	XMV(6)
6	Separator liquid rate (stream 10)	XMEAS(14)	Separator pot liquid flow	XMV(7)
7	Stripper liquid rate (stream 11)	XMEAS(17)	Stripper liquid product flow	XMV(8)
8	Production rate (stream 11)	XMEAS(41)	Production index	F_p
9	Stripper liquid level	XMEAS(15)	Ratio in loop 7	r_7
10	Separator liquid level	XMEAS(12)	Ratio in loop 6	r_6
11	Reactor liquid level	XMEAS(8)	Set-point of Loop 17	s.p. 17
12	Reactor pressure	XMEAS(7)	Ratio in loop 5	r_5
13	Mol % G (stream 11)	XMEAS(40)	Adjustment of the molar feed rate of E	E_{adj}
14	Amount of A in reactor feed, y_A(stream 6)	XMEAS(6)	Ratio in loop 1	r_1
15	Amount of A+C in reactor feed, y_{AC} (stream 6)	XMEAS(6)	Sum of loops 1 and 4 ratio	$r_1 + r_4$
16	Reactor temperature	XMEAS(9)	Reactor cooling water flow	XMV(10)
17	Separator temperature	XMEAS(11)	Condenser cooling water flow	XMV(11)
18	Maximum reactor pressure	XMEAS(7)	Production index	F_p
19	Reactor level override	XMEAS(8)	Compressor recycle valve	XMV(5)
Total	16		18	

Measured Variables	*Code*
Recycle flow	XMEAS(5)
Product separator pressure	XMEAS(13)
Stripper pressure	XMEAS(16)
Stripper temperature	XMEAS(18)
Stripper steam flow	XMEAS(19)
Compressor work	XMEAS(20)
Reactor cooling water outlet temperature	XMEAS(21)
Separator cooling water outlet temperature	XMEAS(22)
Reactor feed analysis (Component A, B, C, D, E, F)	XMEAS(23)-XMEAS(28)
Purge gas analysis (Component A, B, C, D, E, F, G, H)	XMEAS(29)-XMEAS(36)
Product analysis (Component D, E, F)	XMEAS(37)-XMEAS(39)
Total	25

4.2. Step 2: Separate Monitoring of the Controlled, Manipulated, and Measured Variables of the Tennessee Eastman process

In the second step of the illustrated procedure, controlled, manipulated, and measured variables of the TE process are monitored using a DPCA-based multivariate SPC scheme for each group of variables. First, data were collected by running the decentralized TE process simulator.

Data collection

The TE simulator was run twice to collect two datasets, one for each example. Values of the controlled, manipulated, and measured variables were collected in sequence during continuous simulation of the TE process and using the base-case values for operating mode 1. To realize the process dynamics and the full effect of the disturbances, Downs and Vogel[45] suggest a simulation time of 24–48 hours. The process exhibits a transition time of about 36 hours on startup. Thus, in both simulations, the process was run for 84 hours at normal operating conditions and then for further 48 hours, introducing a disturbance at 92 hours (see Table 4.) In the first simulation, the normal operating conditions were upset activating IDV(1), whereas in the second simulation activating IDV(4). IDV(1) mimics a step-change disturbance in the ratio between the chemical reactants A and C, that is, a quite realistic situation caused by substandard raw materials. IDV(4) emulates a step-change disturbance in the reactor cooling water inlet temperature, thus upsetting the process operational constraints.[45] Both disturbances were introduced with a scale factor of 0.50, that is, half of the maximum magnitude of the disturbance value. There are other possible choices, but in what follows, the focus is on the overall behavior of the controlled, manipulated, and measured TE process variables subject to a disturbance. Because the scale factor gives a scale replication of the variables' behavior, other choices of the scale factor are not expected to affect the points made here.

To create random simulations without overly distorting the results, the TE process was run with two active random disturbances, IDV(8) and IDV(13) with a scale factor of 0.10 and 0.25 respectively.[46] IDV(8) varies the composition of the components in stream 4 of the process whereas, IDV(13) deviates the coefficients of reaction kinetics. Moreover, the seed of the random numbers (second parameter of the TE model) was randomly selected and changed at the beginning of each simulation. That way, repeated simulations with the same starting conditions generate different values providing more realistic process data. Specifically, in the following examples, changing the seed of each simulation implies dealing with two different Phase I samples.

Table 4 summarizes the settings of the simulations and of the TE model parameters to produce the datasets for the two examples. Capaci et al.[46] include further details on how to use the decentralized TE simulator as a testbed for SPC methods, and Capaci et al.[46] and Bathelt et al.[43] provide information on the parameters' settings of the decentralized TE model.

Table 4. Settings of the simulations and of the TE model parameters to produce the datasets of example 1 and example 2.

Settings	*Example 1*	*Example 2*
Simulation:		
Sampling time	3 minutes	
Simulation time of which: • Transition time on process startup • Phase I • Phase II	132 hours: • 36 hours (720 observations) • 48 hours (960 observations) • 48 hours (960 observations)	
Step-change introduction at (from the simulation start)	92 hours (1840 observations)	
Step-change disturbance in Phase II, magnitude	IDV(1), 0.50	IDV(4), 0.50
Random disturbance 1 in Phase I and Phase II, magnitude	IDV(8), 0.10	
Random disturbance 2 in Phase I and Phase II, magnitude	IDV(13), 0.25	
Parameters of TE model:		
Parameter 1 (Initial conditions)	Default values for Mode 1	
Parameter 2 (Seed of the random generator)	8686	7746
Parameter 3 (Model structure flag)	194	

Example 1: IDV(1), Step-Change in the A/C Feed Ratio, B Composition Constant

The Phase I samples of the controlled, manipulated, and measured variables were produced by removing the observations during the transition time on process startup (see, Table 4.) Samples of the process variables during steady-state operations provide a more stable estimation of the covariance matrices and thus of the in-control models. Therefore, Phase I samples of the controlled, manipulated, and measured variables collected during 48 hours (960 observations) of normal operating conditions at steady state were used to estimate the in-control model for each group of variables. In addition, the Phase I sample composed by the controlled, manipulated, and measured variables was used to estimate the in-control model for all the variables together. The compressor recycle valve XMV(5) was excluded from the monitoring scheme of the manipulated variables as it had a constant value throughout the simulations. Thus, the group of manipulated variables resulted in 17 variables used for process monitoring.

Table 5 shows the minimum and maximum values of the autocorrelation coefficients at lag 1 for each group of variables in Phase I. Because the TE process variables exhibit moderate to high autocorrelation coefficients, a multivariate monitoring scheme based on DPCA was applied to monitor the controlled, manipulated, and measured variables, and the controlled, manipulated, and measured variables together.

Table 5. Minimum and maximum values of the autocorrelation coefficients at lag 1 for the controlled, manipulated, and measured variables, and for all the variables together in Phase I. Autocorrelation coefficients at lag 1 of the T^2 and Q statistics for each group of variables in Phase I.

Group of variables	*Autocorrelation coefficients at lag 1 in Phase I*		
	[Min, Max]	*T^2 statistic*	*Q statistic*
Controlled variables	[0.2833, 0.9966]	0.8367	0.3981
Manipulated variables	[0.1389, 0.9979]	0.9837	0.7907
Measured variables	[0.5394, 0.9976]	0.8911	0.6819
Controlled, manipulated, and measured variables	[0.1389, 0.9979]	0.8988	0.5452

Table 6 shows the number of lags (l), of variables, and of retained PCs, and percent of explained variance of the in-control DPCA models for the controlled, manipulated, and measured variables, and for the controlled, manipulated, and measured variables together. In each estimated model, the number of lags added to each group of variables was determined by applying the method by Ku et al.[33] (Table 1.) The retained PCs correspond to the number of PCs that provides the minimum absolute value of the difference between the cumulative variance explained by the PCs and the cumulative variance threshold value of 80%.

Table 6. Number of lags (l), of variables, and of retained PCs, and percent of explained variance of the in-control DPCA models for the controlled, manipulated, and measured variables, and for the controlled, manipulated, and measured variables together.

Group of variables	*No. of lags (l)*	*No. of variables*	*No. of retained PCs*	*Explained variance*
Controlled variables	1	32	9	80.29%
Manipulated variables	1	34	4	80.03%
Measured variables	1	50	6	79.26%
Controlled, manipulated, and measured variables	1	116	10	80.13%

The Phase II sample of each group of variables, 960 observations collected during 48 hours of simulation, was then used to build the Hotelling T^2 and Q charts based on DPCA for the controlled, manipulated, and measured variables (Figure 2 [a-f].) Moreover, the Phase II sample composed by the controlled, manipulated, and measured variables was used to build the Hotelling T^2 and Q charts based on DPCA for all the variables together (Figure 2 [g-h].) The theoretical upper control limits were based on the 99.73% confidence level. Under the assumption of time-independent and normally distributed observations, this choice of the confidence level generates only 27 false alarms out of 10,000 observations and corresponds to the typically used 3-sigma control limits.[2] The theoretical control limits could be adjusted due to the observed autocorrelation in both the T^2 and Q statistics (see

Table 5.) However, an adjustment procedure of the control limits is intentionally avoided here because the message to convey is still relevant using the theoretical limits.

The out-of-control signals issued by the Hotelling T^2 and Q charts applied to the controlled (Figure 2 [a-b]) and manipulated (Figure 2 [c-d]) variables indicate that the control action is not able to fully remove the effect of the disturbance on the controlled variables despite the compensatory control action of the manipulated variables. Furthermore, the control charts on the measured variables first issue an out-of-control signal near the disturbance introduction and then approach an in-control situation (Figure 2 [e-f].) The behavior of the measured variables might be most likely due to a cascade effect based on the directives generated by the controllers that indirectly affect the process variables not involved in control loops.

The illustrated example matches scenario 7 in Table 2. Hence, an analyst might draw the conclusion that some controllers are malfunctioning or that the implemented control strategy is unable to handle the disturbance. Because the controlled variables are out-of-control, the process performance is critically affected. Process engineers should immediately seek ways to remove the root cause of the disturbance to keep the production plant and the personnel safe, to avoid unwanted disruptions in the production plan, and to cut extra costs of the (in vain) control action. Note that the Hotelling T^2 and the Q control charts applied to the controlled, manipulated, and measured variables all together (Figure 2 [g-h]) promptly signal an out-of-control process condition, but do not provide any further insight on the process and controllers' performance.

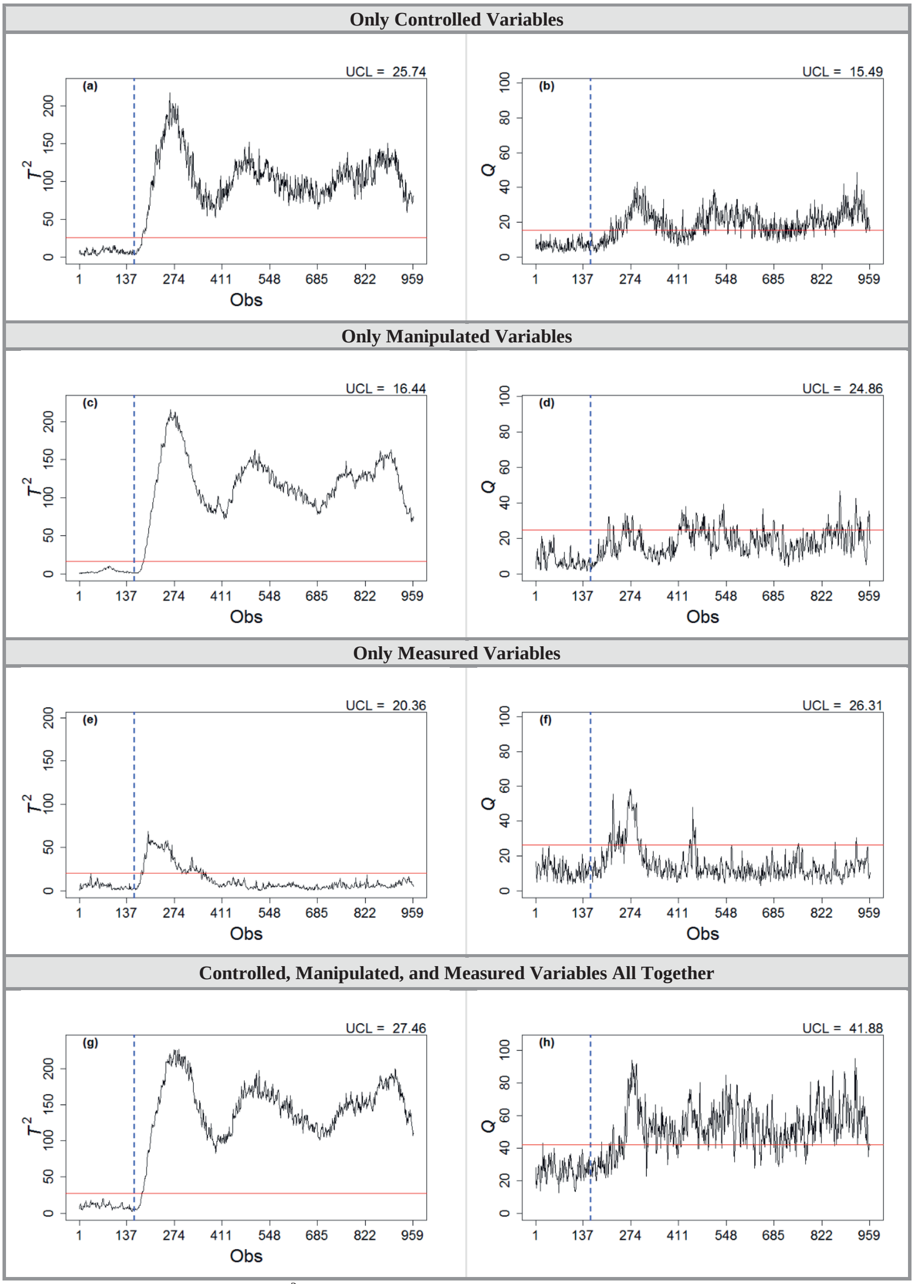

Figure 2. DPCA based Hotelling T^2 and Q charts in Phase II for the [a-b] controlled variables, [c-d] manipulated variables, [e-f] measured variables, and for the [g-h] controlled, manipulated, and measured variables together.

Example 2: IDV(4), Step-Change in the Reactor Cooling Water Inlet Temperature

Following the same criteria described above, the second simulated dataset was used to build the Hotelling T^2 and Q charts based on DPCA when IDV(4), a step change in the reactor cooling water inlet temperature, affects the TE process. Table 7 shows the minimum and maximum values of the autocorrelation coefficients at lag 1 for each group of variables in Phase I. Table 8 provides the number of lags (l), of variables, and of retained PCs, and percent of explained variance of the in-control DPCA model for each group of variables.

Table 7. Minimum and maximum values of the autocorrelation coefficients at lag 1 in Phase I and autocorrelation coefficients at lag 1 in Phase I of the T^2 and Q statistics for the controlled, manipulated, and measured variables, and for all the variables together.

Group of variables	**Autocorrelation coefficients at lag 1 in Phase I**		
	[Min, Max]	**T^2 statistics**	**Q statistics**
Controlled variables	[0.2691, 0.9968]	0.6312	0.3176
Manipulated variables	[0.1530, 0.9976]	0.9348	0.6822
Measured variables	[0.5257, 0.9968]	0.8394	0.5227
Controlled, manipulated, and measured variables	[0.1530, 0.9976]	0.8521	0.6600

Table 8. Number of lags *(l)*, of variables, and of retained PCs, and explained variance of the in-control DPCA models for the controlled, manipulated, and measured variables, and for the controlled, manipulated, and measured variables together.

Group of variables	***No. of lags (l)***	***No. of variables***	***No. of retained PCs***	***Explained variance***
Controlled variables	1	32	9	79.49%
Manipulated variables	1	34	4	80.14%
Measured variables	1	50	7	79.44%
Controlled, manipulated, and measured variables	2	174	13	79.99%

Figure 3 [a-h] shows the Hotelling T^2 and Q charts based on DPCA for each group of variables in Phase II. As shown in Figure 3 [c-d], the Q control chart on the manipulated variables issues an out-of-control signal indicating that a compensatory control action is working to counteract the disturbance. The prompt reaction of the controllers is also made apparent by the isolated out-of-control signals (indicated by the arrows in Figure 3 [a-b]) issued by the control charts applied to the controlled variables near to the disturbance introduction. The disturbance variability is then fully displaced from the controlled to the manipulated variables and both the Hotelling T^2 and Q charts on the controlled variables exhibit an in-control situation (Figure 3 [a-b].)

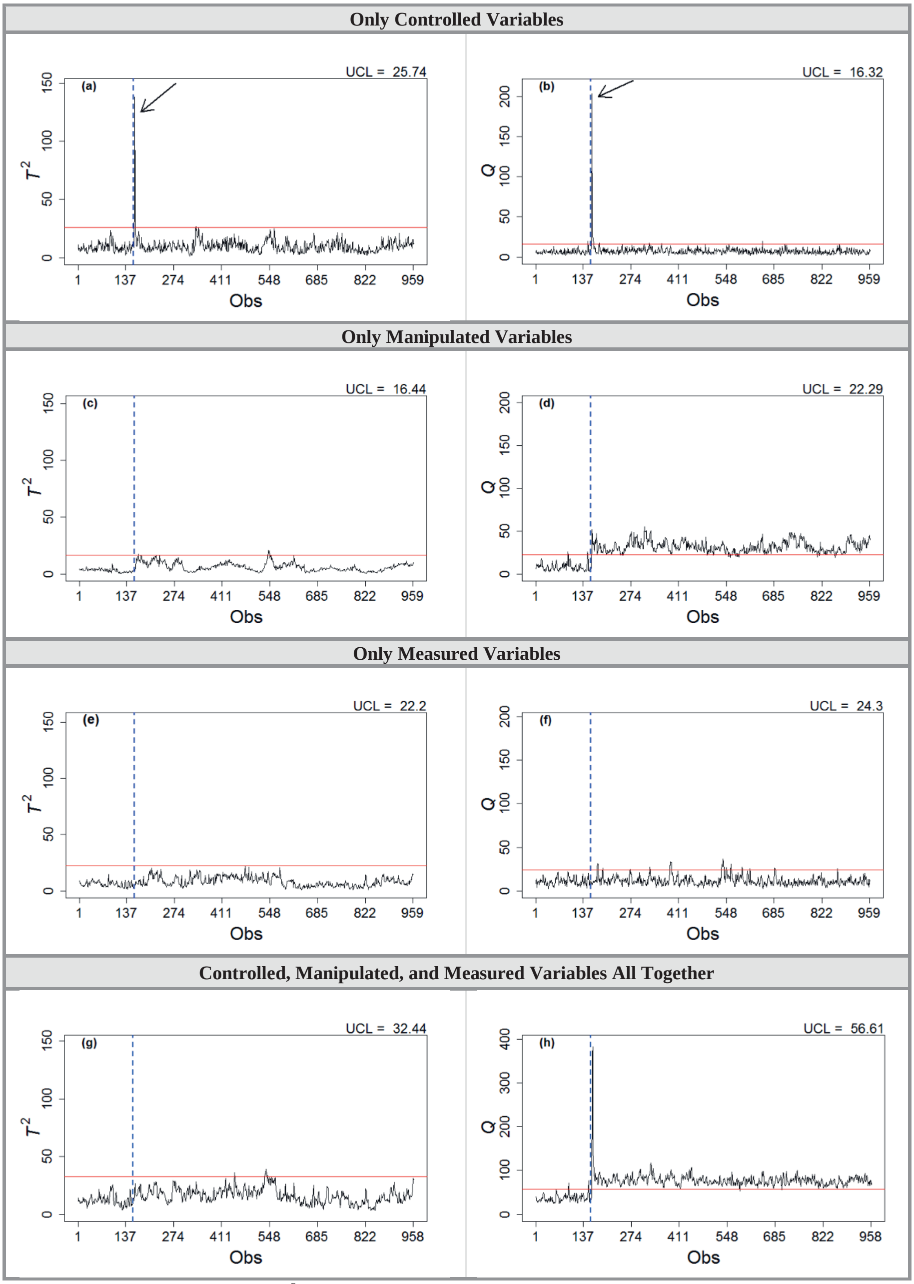

Figure 3. DPCA based Hotelling T^2 and Q charts in Phase II for the [a-b] controlled variables, [c-d] manipulated variables, [e-f] measured variables, and for the [g-h] controlled, manipulated, and measured variables together.

The measured variables are insensitive to the disturbance: both the Hotelling T^2 and Q charts seem to be in-control (Figures 3 [g-h]), except for a few sparse out-of-control signals issued by the Q chart that could most likely be explained with the underestimation of the control limits due to the autocorrelation of the Q statistic (see Table 7.).

The illustrated case matches scenario 3 in Table 2. Hence, a reasonable conclusion is that the control action is well designed to remove the effect of a disturbance, IDV(4), that could affect the process operational constraints. However, although the controlled and measured variables are on-target, an SPC analyst cannot deem the process to be in control. A more appropriate conclusion is that the process performance is not critically affected, as the controllers are fully compensating for the disturbance. Therefore, an overall improvement of the process performance can be achieved by detecting and removing the assignable cause that generates the unwanted costs of the compensatory control action. As in the previous example, it should be underscored that the Hotelling T^2 and Q charts applied to the controlled, manipulated, and measured variables all together clearly detect an out-of-control process condition (Figure 3 [g-h]), but once again at the expense of a more thorough understanding of the out-of-control situation.

4.3. Remarks

As many modern industrial processes operate under EPC, the usual approach of applying a control chart only on the process outputs might be ineffective because of the potential masking action of the controllers. Sometimes, a multivariate scheme that monitors process outputs and manipulated variables together in the same multivariate chart(s) is used. However, as shown in the above examples, this approach allows detecting out-of-control process conditions but does not provide additional knowledge on process and controllers' performance. On the contrary, monitoring controlled, manipulated, and measured variables in separate multivariate charts makes available information on process performance (severity of out-of-control process conditions) and controllers' performance (ability/inability to handle a disturbance or controllers' malfunctions) when a disturbance occurs.

5. Conclusions and Discussion

Due to the ease of application at low cost, many modern industrial processes involve EPC, as in the case of feedback controllers. Nevertheless, SPC remains valuable for detecting and eliminating assignable causes of variation.

This article explores the concurrent use of EPC and SPC in multivariate processes and illustrates how an analyst can use the information provided by the two complementary approaches in quality improvement efforts. EPC increases the process complexity and affects the process variables' behavior in different ways. Thus, an SPC analyst could enhance the understanding of the process and controllers' performance by classifying and monitoring the process variables in groups. This article illustrates a two-step monitoring procedure in which [1] the variables are pre-classified as controlled, manipulated, and measured variables, and [2] a multivariate monitoring scheme is applied to each group of variables separately. Potential scenarios an analyst might encounter when applying the illustrated procedure and the additional knowledge gained regarding process and controllers' performance is discussed. In general, the combined study of control charts on the controlled and measured variables provides information on process performance, whereas the combined study of control charts on the controlled and manipulated variables gives information on controllers' performance.

Through two simulated examples, the application of the two-step monitoring procedure to the TE process explores two potential (faulty) scenarios. In the first example, a disturbance critically affects the process performance. The compensatory control action of the manipulated variables is unable to remove the effect of the disturbance on the controlled variables. Thus, the critical nature of the out-of-control situation should trigger an immediate search of the assignable cause(s) and the implemented control strategy should be inspected. In the second example, a disturbance does not affect the process performance critically. The underlying assignable cause(s) will jeopardize neither the production plan nor the production plant, as the manipulated variables fully counteract the effect of the disturbance on the controlled variables. Hence, the control strategy is working properly but the elimination of the assignable cause might still be relevant to reduce the cost of continuous corrective adjustments.

It is worth emphasizing that the approach to analyze all the process variables in the same multivariate chart(s) still allows detecting out-of-control process conditions but at the expense of gaining deeper process insight. By contrast, the two-step monitoring procedure allows for knowledge discovery and deeper process understanding but with some added complexity in the analysis process. In the first step of the suggested procedure, experts' knowledge might play a crucial role, as the existing causal relationships among the process variables must be known or estimated. Furthermore, the second step of the procedure requires the concurrent building and monitoring of several control charts compared to the approach of monitoring the variables all together in one multivariate chart. However, when an out-of-control situation occurs, knowing on which group of variables (controlled, manipulated, and/or measured variables) the disturbances manifest themselves provides the analyst with a hint of the severity of the out-of-control situation and hence of the degree of urgency to search and remove the assignable cause of the disturbance. Moreover, the fault isolation task might be easier, as the analyst will need to analyze contribution plots for groups of variables rather than for all the variables together. Finally, the choice regarding the most suitable approach for monitoring a multivariate process should be left to the analyst who understands the process features and the consequences of frequently occurring disturbances on the process under study.

Future research on the topic should explore multivariate processes under feedback control to understand the 'signatures' or 'signals' that different disturbances (e.g. step and ramp disturbances) leave on the controlled, manipulated, and measured variables.

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