Department of Automation and Systems Technology

Added value of extended dynamic simulation in process design and operational planning

Jouni Savolainen

Aalto University

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Jouni Savolainen

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Abstract

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Abstract

Design of process industry plants and their automation is a challenging task, especially when cost-effectiveness pressures are ever increasing. This leads to challenges for engineers responsible for this work. This thesis investigates how those challenges could be alleviated by extended use of dynamic process simulation. The current trend of digital twins both calls for and enables this work. As this work relies on simulation models and is computational in nature, digital twins are an enabler. On the other hand, the digital twins call for approaches to extract added value from data, in the case of this thesis, simulation-generated data.

The present work consists of four case studies from the process industry. Dynamic process simulation is combined with a novel model comparison method, with global sensitivity analysis and with multiple objective optimization. By conducting a massive number of well-planned simulations and analysing the resulting data, it is shown that the challenges could be alleviated. The cases pertain to certain phases of a process industry plant's life cycle, namely early design and operation. Two cases, Paper production and Tower control, target the early design phases, while the Filtration and Bottleneck cases concentrate on the operation phase.

The Paper production case shows the utility of the proposed model comparison method. This led to the conclusion that it helps in gaining confidence in optimization results from simplified models, focusing the designer's attention as well as providing insight into the operation of the plant. The Tower control case, combining dynamic process simulation and global sensitivity analysis, highlights process areas where the control designer's attention should be focused. Similarly, the Bottleneck case shows where retrofit actions on an operational plant should be focused. Finally, the Filtration case shows the feasibility of combining dynamic simulation with interactive multiple-objective optimization in providing insight into the process operation. A synthesis of these contributing results then supports the main hypothesis of this thesis: Extended added value or utility can be extracted from simulation models when they are combined with other mathematical methods.

Keywords dynamic simulation, global sensitivity analysis, model comparison, multiple objective opimization

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Tekijä
Jouni Savolainen

Väitöskirjan nimi
Laajennetun dynaamisen prosessisimuloinnin lisäarvo prosessi- ja automaatiosuunnittelussa

Julkaisija Sähkötekniikan korkeakoulu

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Tiivistelmä

Prosessiteollisuuden laitosten sekä niiden automaation suunnittelu on haastava tehtävä, etenkin kiristyvien kustannustehokkuusvaatimusten johdosta. Tämä johtaa haasteisiin suunnitteluinsinööreille. Tässä työssä tutkittiin, miten näitä haasteita voitaisiin lieventää laajennetulla dynaamisella prosessisimuloinnilla. Tämän hetken ns. digitaalinen kaksonen-kehitys sekä kutsuu että tekee mahdolliseksi tämän työn. Koska tämä työ nojaa simulaatiomalleihin ja on luonteeltaan laskennallinen, on digitaalinen kaksonen nähtävissä työn mahdollistajana. Toisaalta, digitaalinen kaksonen-ajatus tarvitsee tapoja puristaa datasta, tässä tapauksessa simulaatiodatasta, arvokasta tietoa.

Työ koostuu neljästä prosessiteollisuuden tapaustutkimuksesta. Dynaaminen prosessisimulointi on liitetty uuden mallien vertailumenetelmän, globaalin herkkyysanalyysin ja monitavoiteoptimoinnin kanssa. Työssä osoitetaan, että suorittamalla suuri määrä suunniteltuja simulointeja sekä analysoimalla saatu data, edellä mainittuja haasteita voidaan lieventää. Tapaukset liittyvät tiettyihin prosessilaitoksen elinkaaren vaiheisiin, nimittäin esisuunnitteluun ja käyttöön. Kaksi tapausta, paperin valmistus ja tornien säätö, kohdistuvat esisuunnitteluun, kun taas suodatus- ja pullonkaulatapaukset keskittyvät laitoksen käyttövaiheeseen.

Paperin valmistus-tapaus osoittaa mallien vertailumenetelmän hyödyn. Päätelmänä on, että tällä voidaan saavuttaa luottamusta yksinkertaisilla malleilla saatuihin prosessioptimointituloksiin, fokusoida suunnittelijan huomio sekä tuottaa käyttövaiheeseen tietoa. Tornien säätö-tapaus, joka liitti dynaamisen simuloinnin globaaliin herkkyysanalyysiin, nostaa esiin säätösuunnittelun kannalta kriittisiä prosessialueita. Samoin, pullonkaulatapaus nostaa esiin prosessialueita, joihin jälkiasennus-työssä tulisi fokusoitua. Lopuksi, suodatustapaus osoittaa dynaamisen simuloinnin ja monitavoiteoptimoinnin hyödyllisyyden ymmärryksen saavuttamisessa prosessin käyttövaiheessa. Näiden osatulosten synteesinä saavutetaan työn päätulos: laajennetulla dynaamisella simuloinnilla on saatavissa lisäarvoa.

Avainsanat dynaaminen simulointi, globaali herkkyysanalyysi, mallien vertailu, monitavoiteoptimointi

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Preface

There road to this thesis has indeed been a long and winding one. It covers practically my whole career, so far, at VTT Technical Research Centre of Finland Ltd.. In the very early phases of that journey, I did not even realize I was on it. Gradually over the years, during numerous projects and interactions with colleagues and industry representatives, the thinking that culminates here, started to grow.

The actual work was conducted in projects co-funded by VTT, Metsäklusteri Oy / FIBIC Ltd., FIMECC Ltd., Digile Ltd., Tekes and the European Commission. Their support is gratefully acknowledged. Furthermore, I express my gratitude the multitude of companies that have participated in these research projects.

I would like to thank my supervisor, Prof. Arto Visala, for his insights and guidance in finalizing this work into an actual thesis. Dr. Tommi Karhela, my advisor, provided valuable guidance in earlier phases of the work, especially in the methodological and practical aspects of the work. For this, and for his insightful comments on the manuscript drafts, I express my warmest thanks. I also wish to thank the pre-examiners, Prof. Peter Palensky, and Prof. Kauko Leiviskä for taking the time to review my work and provide their encouraging comments. Finally, I am grateful for Prof. Erik Dahlquist for agreeing to be my opponent.

This work could not have been completed without my current and former co-workers and their support. Especially, I would like to thank all the co-authors of the publications. Dr. Olli Saarela provided valuable discussion and ideation sessions when working on the model comparison. Jari Lappalainen and Dr. Sakari Kaijaluoto have always been great companions when discussing process modelling and simulation. These interactions have greatly influenced the work presented here. Dr. Karthik Sindhya, Dr. Vesa Ojalehto, Dr. Jussi Hakanen and Prof. Kaisa Miettinen from the University of Jyväskylä multiple objective optimization group introduced me to this broad and interesting topic and I am happy to have collaborated with them. Dr. Hannu Niemistö has been a truly inspirational colleague, for which I am grateful. Finally, over the years, I have naturally worked with numerous other people, in fact too many to list here individually. Rest assured, you are not forgotten!

My warmest thanks go my friends for extracurricular activities that have and continue to be a balancing force in my life. Especially, Antti and J-P as well as their families have excelled in this. Dear Mom, Dad and Suvi: Thanks for always supporting me!

Finally, I thank my dear wife Maaria. Your example and unwavering support has made all this possible.

Espoo, April 17th, 2019
Jouni Savolainen

Contents

List of abbreviations

AF	Accumulation Factor
ANSI	American National Standards Institute
Apros	Advanced Process Simulator
ASM Consortium	Abnormal Situation Management Consortium
CP	Chemical Pulp
CV	Controlled Variable
DECU	Deculator
DF	Disc Filter
DGSM	Derivative-based Global Sensitivity Measure
DM	Decision Maker
DoE	Design of Experiments
DSR	Design Research Science
EPC	Engineering, Procurement, Construction
EWC	Energy and Waste Cost
FAST	Fourier Amplitude Sensitivity Test
FMI	Functional Mock-up Interface
GSA	Global Sensitivity Analysis
HAZOP	Hazard and Operability Analysis
HBX	Headbox
HENS	Heat Exchanger Network Synthesis
IEC	International Electrotechnical Commission
ISA	International Society of Automation
ISO	International Organization for Standardization
LCA	Life Cycle Assessment
MC	Machine Chest
MIDO	Mixed Integer Dynamic Optimization
MINLP	Mixed Integer Non-Linear Programming
MOO	Multiple Objective Optimization
MPC	Model Predictive Control
MV	Manipulated Variable
MVA	Material Value Added
ODE	Ordinary Differential Equation
OM	Optimization Model
PAROC	Parametric Optimization and Control
PCS	Process Control System
PDE	Partial Differential Equation

PI(D)	Proportional Integral (Derivative)
PM	Paper Machine
PSE	Process Systems Engineering
QC	Quality Control
ROI	Return On Investment
RQ	Reaction Quotient
SCM	Swiss Cheese Model
TMP	Thermomechanical Pulp
TVA	Total Value Added
VM	Verification Model
WP	Wire Pit

List of symbols

a	Tuning coefficient for filter fouling model
c_{feed}	Impurity concentration in filter fouling model
c_i	Control law coefficient i
c_{nom}	Nominal value of control law coefficient
$E(.)$	Expectation
EE_i	Elementary Effect of input i
F_i	Cumulative distribution EE_i
i,j,k,h	Indices
N_{var}	Number of comparison variables
p	Number of sampling levels of an input in Elementary Effects analysis
p_i	Tower level discretization limit i in control law
P^h	Decision maker preference information during iteration h of interactive MOO
$r_{filler,PM}$	Filler retention coefficient at paper machine
$S_{i,j}$	First-order Sobol' index from input i to output j
$S_{Ti,j}$	Total Sobol' index from input i to output j
t	Time
u_i	Controller output i
$V(.)$	Variance
V_i	Volume of paper mill tower i
w	Additive noise term to $r_{filler,PM}$
X_i	Input i of a model
Y_j	Output j of a model
$z^h{}_k$	k^{th} Pareto optimal solution shown to DM in iteration h
Δ	Increment to an input in Elementary Effects analysis
Δt	Time step
α	Experiment-wise significance level, Filtering coefficient for u_i
α_i	Comparison-wise significance level
μ_i	Mean of F_i
$\mu_i{}^*$	Mean of $\lvert F_i \rvert$
σ_i	Standard deviation of F_i
ξ	Pressure loss coefficient of a filter fouling model

List of publications

This thesis is based on the following publications, which are referred to in the text with Roman numerals I – IV.

I. Savolainen, J., Saarela, O., Lappalainen, J., Kaijaluoto, S., 2011. Assessment method of dynamic, stochastic process models with an application to papermaking. Nord. Pulp Pap. Res. J. 26, 336–348.

II. Savolainen, J., 2013. Global sensitivity analysis of a feedback-controlled stochastic process model. Simul. Model. Pract. Theory 36, 1–10.

III. Sindhya, K., Ojalehto, V., Savolainen, J., Niemistö, H., Hakanen, J., Miettinen, K., 2014. Coupling dynamic simulation and interactive multiobjective optimization for complex problems: An APROS-NIMBUS case study. Expert Syst. Appl. 41, 2546–2558.

IV. Savolainen, J., Lappalainen, J., 2015. Identification of process bottlenecks with global sensitivity analysis, an application to papermaking processes. Nord. Pulp Pap. Res. J. 30, 393–401.

Author’s Contribution

Publication I: In Publication I (the Paper production case), the author was responsible for the modelling work with the Apros® simulator in constructing the so-called verification models. The so-called optimization model referred to in the paper was constructed by Prof. Risto Ritala of Tampere University of Technology, while the major contribution of the Publication, the model comparison method, was ideated by the author with the aid of Dr. Olli Saarela. Implementation of the method, simulations and analysis of the results were done by the author.

Publication II: In Publication I (the Tower control case), the idea of applying global sensitivity analysis to the upper-level control law was conceived by the author. The control law under study was ideated by the author and Lic. Tech. Jari Lappalainen of VTT. The simulation model utilized is the same as the optimization model of Publication I. Implementation of the control law, definition of the sensitivity analysis problem, as well as conducting of the needed simulations and analyses are by the author.

Publication III: In Publication II (the Filtration case), the author was responsible for modelling the two-stage separation process and for defining the objective functions and decision variables. Furthermore, the author acted as the decision maker (DM) in the interactive optimization and provided engineering insights toward optimization progress.

Publication IV: In Publication III (the Bottleneck case), the author was responsible for ideating the utilization of global sensitivity analysis as a bottleneck identification method. The three simulation models were constructed by the author and problem definitions for the global sensitivity analysis were given by the author. Lic. Tech. Jari Lappalainen of VTT assisted the author in interpretation of the results and in the writing process.

1. Introduction

1.1 Background and motivation

The process industry in Europe represents over 450 000 individual enterprises with nearly seven million employees and a turnover of more than 1600 B€ (Tello and Weerdmeester, 2013). Still, it has been seen that the process industry has a clear need for improved efficiency and competitiveness, especially in Europe (Tello and Weerdmeester, 2013). This need affects all levels of a process industry company and its subcontractors, for example process and automation designers whose responsibilities often lie in the early phases of the plant's life cycle, including the physical processes which typically are designed to be quite long-lived: their lifecycle can cover decades. The life cycle of a process industry plant is linked to other life cycles relevant to an enterprise, relationships of which are shown in **Figure 1**.

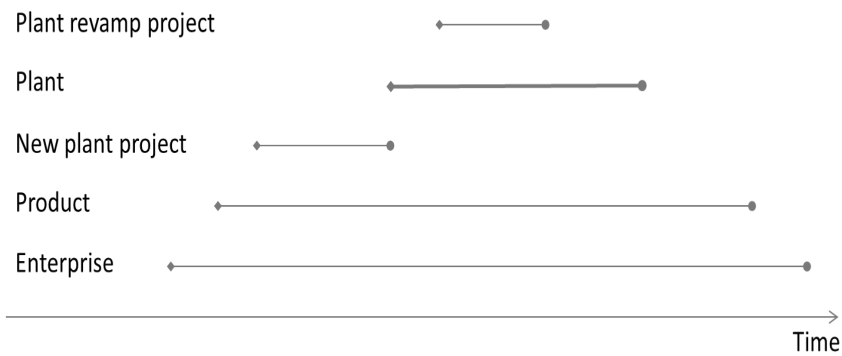

Figure 1 Other life cycles and their relation to the process industry plant life cycle, adapted from (Schneider and Marquardt, 2002).

The longest of these is the enterprise life cycle which can have several products. A product life cycle actually begins before the life cycle of the plant that produces it. Before the plant's life cycle there is the "new plant project" where the plant is designed and built. Moreover, inside a plant's life cycle there may occur one or more plant revamps or retrofits. Finally, here it should be noted that a plant's life cycle can include several products. This can lead to several revamp projects.

Design of a new plant actually begins quite early with the determination of needs and setting of design specifications/objectives. This pre-investment decision phase consists mostly of market and business oriented activities in which it is determined whether there are sufficient grounds to invest in a new facility. A capital investment project is a complex endeavour involving several stakeholders. One way of illustrating this is with a triangle with the three major parties depicted, see **Figure 2**.

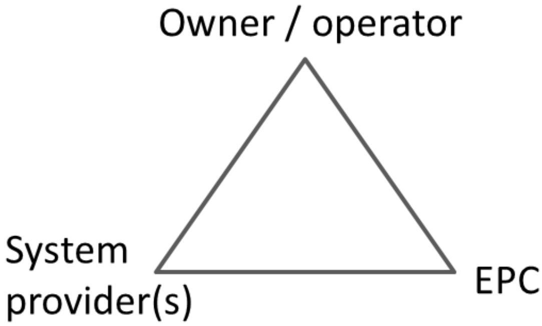

Figure 2 Main parties of a capital investment project.

On top is the plant owner/operator, which is the party investing in the new plant. Other corners of the triangle are the system provider(s) and engineering, procurement and construction (EPC) parties and their respective subcontractors. The system provider includes the process equipment provider, automation and instrumentation system providers, etc. The EPCs are, for example, responsible for plant layouts, cost calculations, purchasing, logistics, installation, coordination and commissioning.

If a decision to invest is made, the actual plant lifecycle, encompassing the three top levels of **Figure 1**, begins with conceptual design as depicted in **Figure 3**.

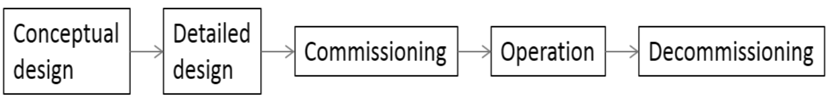

Figure 3 Phases of a process industry plant life cycle, adapted from the ISO-15926-1 standard (ISO, 2004).

The term life cycle here refers to the plant, even though the word “process” is sometimes used. This is also the situation on the original ISO-15926-1 standard. To clarify, a distinction should be made between **process design** and **plant design**. The prior deals with initial selection of the process to be used: flowsheets, equipment selection, specification, and chemical engineering design of equipment. The latter includes also detailed mechanical design of equipment, the structural, civil, and electrical design, as well as the specification and design of the supporting services, e.g. maintenance, firefighting, offices (Towler and Sinnott, 2013).

In the conceptual design phase, possible solutions to the needs and specifications are generated, evaluated and selected (Towler and Sinnott, 2013). This is typically done by an engineering or consultancy company and can even be done with rules of thumb and the experience of designers. A few process options are generated and then evaluated before passing to the next stage, and it is noteworthy that up to 98% of conceptual designs will not be built (Moran, 2015). The following detailed design phase, done usually by a contracting company, involves mainly detailed selection and dimensioning of equipment, instrumentation, etc. This stage is also called "design for construction" because a conceptually designed plant is not what is actually built. The contractors in many cases need to refine the conceptual design or even redesign parts the plant because they are the ones who give guarantees to the client (Moran, 2015). In this phase, alterations to the flowsheet, i.e. selection and topology of processing units, of the process are seldom made (Towler and Sinnott, 2013), if possible. In some texts, there is a step between the conceptual and detailed design phases called "front-end engineering design" which refines the conceptual design, analyses different process conditions, replaces bespoke unit operations with commercial standard units (wherever possible), and calculates costs based on quotes from suppliers. Also, between detailed process design and commissioning lies the construction of the plant. It has been noted, that in real-life, even having passed all previous stages, the plans may lack some details needed for construction or even contain errors. This requires redesign efforts and is referred to as site redesign (Moran, 2015).

The ultimate goal of a plant is to produce products profitably, which means that the business unit is heavily involved in the life cycle, mainly in setting the objectives and making decisions. Research parties typically produce new information that the process engineering's designers can utilize in their work. This work produces documents such as diagrams, which are used by the construction company to build the plant. This construction lies between the design and commissioning phases. In the commissioning phase the constructed plant is taken into use, which involves activities such as checking of the system configuration and instrumentation; cleaning and calibration of lines, vessels and instrumentation; dry, water and chemical tests and finally the handover to the plant owner (Killcross, 2012).

Plant operation begins after the handover, which takes place at the end of the commissioning phase. The transition to operation also marks a change in the stakeholder structure presented in **Figure 2**. Naturally, in this phase, the role of the operator party becomes important, but the EPC and system providers do not entirely fade away. They strive typically to have contracts relating to maintenance and other plant operation services. In addition to normal, steady operation, this phase also involves dealing with transients, either planned or unplanned. Operation or controlling of the plant, or an enterprise to be more general, is done on many levels. For example, the IEC 62264-1 international standard, which is an extension of the ANSI/ISA 95 standard, defines a functional hierarchy of control. On the top level (4) resides enterprise resource planning (ERP). The purpose of this is to handle production scheduling across several plants, operational management, etc. Thus, level 4 deals with not only one plant but also enterprise-wide business logistics. Below the ERP, on level 3, is the manufacturing execution system (MES) level, which is responsible, for example, for detailed production scheduling and maintenance. Level 2 is the process control system (PCS) used to keep the process stable and under control. Below this are levels 1 (sensors and actuators) and 0, the physical process equipment, e.g. pumps and valves (Panetto, 2007). This control hierarchy is illustrated in **Figure 4**.

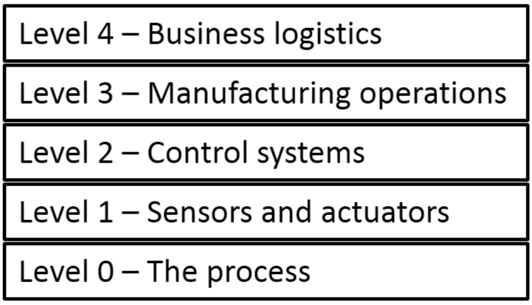

Figure 4 Control hierarchy.

Finally, during operation the plant will undergo maintenance and improvements or retrofits/revamps. Following the active operation phase of a process industry plant, decommissioning takes place and it is closed for an extended period of time, either due to a traumatic event or as planned.

In addition to the economic motivation described at the beginning of this chapter, another current trend motivated this work, namely digitalization. At the time of writing this thesis, digitalization is a much-hyped term and there seems to be multiple interpretations of it. One aspect is concerned with so-called digital twins. Simply put, a digital twin is a digital representation of a physical asset: a process, product or service. In the scope of this thesis, a simulation model could be seen as digital twin, or part of such, of a process industry plant. This model is constructed during the design phases and continues to evolve during the operation by gathering data from the actual process and adapting.

One way a digital twin is seen to bring value is via analytics of the gathered data. This ties it to the present thesis since the data can be used to help in construction of simulation models. The difference between this thesis and much of the digital twin hype is the modelling approach used. In this thesis, the simulation models are not purely based on data, but rather on first principles of physics because such models provide better extrapolation possibilities. This property of a first principles model is used extensively here to generate simulated data, which is then analysed with the extensions. This generation of simulated data ties the thesis to another aspect of digitalization: massive computation. Simulation in dedicated high-performance computational clusters has been an active field for a long time, but in recent years, flexible computational power has become easily accessible from cloud-based computing.

These two digitalization aspects seem to be trends that pave the way to more comprehensive up-take of also the approaches presented in this thesis. And vice versa, the approaches presented here enable better utilization of such resources.

1.2 Method

1.2.1 Case-based approach

This thesis consists of four computational case studies detailed in Publications I – IV, illustrating the potential of coupling dynamic process simulation with other mathematical methods. This number of cases is in line with suggestions by Voss et al., who state that a single case is problematic due to limited generalizability, while too many cases may reduce the depth of study (Voss et al., 2002). Although it is not possible to give a generally acceptable optimal number of cases, for example, Eisenhardt points out that four to ten cases seems to work well (Eisenhardt, 1989). Furthermore, the cases used in this thesis represent typical situations in the design and operation domain of process industry: The first two cases deal with early phases of process and automation design, the third with process operation and the fourth with analysis/improvement of an existing process. All such activities are typical in the process and design industry. Thus, we argue that the cases provide wide enough coverage of the plant life cycle and are indeed relevant to the process industry domain.

1.2.2 Design science research

Design science research (DSR) develops knowledge and solution(s) to practical problems by building and evaluating design artefacts. In contrast to natural sciences where the goal is understanding of reality, the objective in design science is creating things that serve a purpose. In natural sciences, the results are evaluated on the basis of explanatory power and truth, whereas in design science evaluation is more concerned with utility (March and Smith, 1995). Thus, DSR is quite engineering-like (Hevner et al., 2004) and has been chosen as the methodological framework in this thesis.

DSR provides a framework consisting of three major parts, the environment, research and the knowledge base (Hevner et al., 2004). The environment defines the problem to be solved (or “business need”) and contains people, organizations and technology, for example, the process design and plant operation engineers in their respective organizations. The problems that this environment defines are referred to in this thesis as challenges and are elaborated in chapter 3. In other words, the environment provides the next part, research, with relevance. The research part is further divided into the build and evaluate phases. In the build phase, concrete artefacts (e.g. software) are implemented and their utility to address the problem at hand is then evaluated. Typically, this design cycle is iterative. In this thesis, the artefacts are the pieces of software implemented in the cases and their utilization process in order to solve the identified challenges. Their evaluation was done by expert judgement of each case’s results (i.e. descriptive evaluation). Finally, the third part of the framework is the knowledge base providing foundations and methodologies. Foundations are the prior body of knowledge, e.g. theories, models and instantiations that are used in the build-evaluate phase and methodologies are guidelines for evaluation. The knowledge basis is said to provide rigor to the research part. In the scope of this thesis, the foundation consists of physics, mathematics, simulation models and computer simulators, especially when applied to chemical processes; a field also known as process systems engineering (PSE). This thesis provides additions to the knowledge base via the results obtained on the potential of extending dynamic process simulation.

March and Smith (1995) have focused on DSR of information systems and delved deeper into the artefacts' classification. They distinguish constructs, models, methods and instantiations, which in the scope of this thesis are summarised in **Table 1**. As this thesis deals with computer simulations, it seems natural to base the work in DSR for information systems.

Table 1 Artefacts of DSR in information systems.

Artefacts of DSR in information systems	**In this thesis**
Constructs, i.e. language to describe problem and solution	Mathematics, physics, chemistry, control
Models, i.e. representation of real world situation	Mathematical model
Methods, i.e. processes how to solve the problem	Extended dynamic computer simulation, expert judgement of results' utility
Instantiations, i.e. implementations demonstrating feasibility	The pieces of software produced. This means the combination of simulation tools, other mathematical software and the pieces of code connecting them.

Finally, Hevner et al. (2004) note that DSR must be distinguished from ordinary, routine design. The key is that DSR addresses unsolved problems in a unique / innovative way. We argue in chapter 3 that the challenges identified remain largely unsolved. Further, the proposed approach to solving them can be argued to be innovative since such extensions of dynamic process simulation were not found in the relevant literature.

1.3 Contribution of the thesis

In DSR the contribution arises from utility (Hevner et al., 2004). In accordance with this, the main contribution of this thesis is in demonstrating how extending dynamic process simulation with other mathematical methods can bring extended added value or utility to a process or automation designer.

More specifically, the contributions from the four Publications come from:

- demonstration of how coupling dynamic process simulation with certain other mathematical methods can provide added value in the form of insight to the process designer and plant operating personnel and thus alleviate some practical challenges

- development of a novel comparison method for hybrid stochastic-deterministic models in order to gain confidence that process optimization results obtained in early design phases with simplistic models are relevant also to real-life. The added value comes from the ability to trust and thus use optimization results.
- demonstration of how global sensitivity analysis can be used as bottleneck identification method. This adds value via being able to remove the bottleneck.

This thesis consists of an introduction and four publications. These publications and the author's contribution in them were summarised above in chapter Author's Contribution. There is a considerable body of work on this area in the literature, which is reviewed in chapter 2 and we do not claim that the approaches presented here are a once-and-for-all solution. Rather, this thesis proposes some additional tools to the designer's toolbox and aims to show their potential.

1.4 Scope of the thesis

This thesis deals with computational tools for process design and operation over its life cycle. The term process refers here to a chemical plant or more generally a process consisting of continuous fluid flows, and unit operations such as mixings, separations and reactions. Thus, processes such as manufacturing of discrete units, e.g. cars, are not studied here. Of the life cycle, the conceptual and early parts of detailed process design as well as plant operation phases are covered in this thesis (see **Figure 5**) while commissioning and decommissioning phases of the plant are not considered. The figure also positions the Publications in relation to the life cycle.

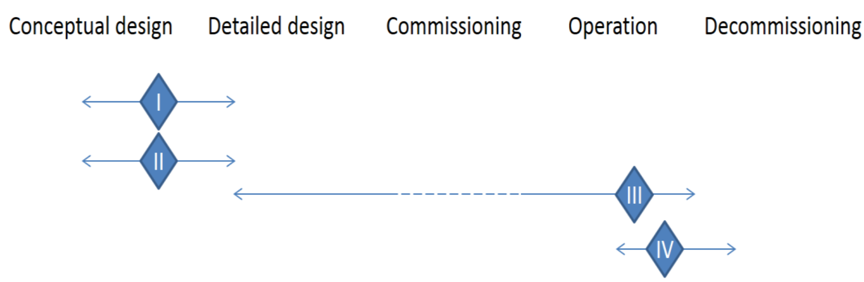

Figure 5 Relation of Publications to process industry plant life cycle.

It should be noted that nowadays it seems that the line between research and development (R&D) and design seems to be getting blurred. It is not always clear that the path from an idea through lab scale to industrial use follows a linear path of gradual upscaling. In this kind of development, the methods presented in this thesis may bring benefits, although the Publications do not explicitly address such pre-design phases.

1.5 Structure of the thesis

The structure of this thesis is as follows. Chapter 1 is an introductory section describing the practical starting points of the work as well as the methodological underpinnings. Chapter 2 reviews the related scientific literature, while chapter 3 leads the reader to the research questions via challenges faced by a process or automation designer. Chapter 4 then presents the main results of the thesis and how they stem from the case studies constituting the empirical work. Finally, in chapter 5 a discussion is provided and chapter 6 concludes the thesis.

2. Related research

2.1 Design phase

2.1.1 Traditional design approach

Design problems have been studied in the chemical engineering field for a long time (Nishida et al., 1976; Westerberg, 2004). Westerberg (2004) defined designing a process as an evolutionary approach where previous solutions are improved upon relying on guesswork, computations and experiments. The traditional chemical engineering approach, since the early 1900s revolved around the concept of unit operations and connecting them into processes (Sargent, 1991). Part of this discipline has in the decades since the 1960s diverged to Process Systems Engineering (PSE) (Grossmann and Westerberg, 2000; Westerberg, 2004). PSE has been defined as being “concerned with the improvement of decision-making process for the creation and operation of the chemical supply chain”. This goal of improvement has been addressed with development of systematic methods and tools, which tie PSE to the fields of mathematics, operations research and computer science (Grossmann and Westerberg, 2000). Furthermore, PSE strives to rethink the design process itself by, for example, bringing operational aspects into the design decision-making or by utilizing design models in the operation of the plant (Westerberg 2004).

Prior to any process design activity as such is initiated, investigation and economic analyses relating to such investments are made in a company (Biegler et al., 1997). After a decision to invest in a process industry plant, the actual design starts. Traditionally, the design of process industry plants has been a sequential procedure (Yuan et al., 2012). For example, Vega et al. (2014) illustrate this as a four-step procedure depicted in **Figure 6**.

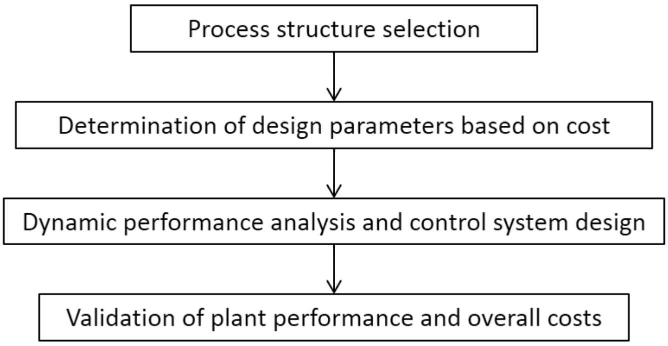

Figure 6 Traditional sequential design process (Vega et al., 2014).

This approach contains several subfields. Those closely touching this thesis are summarized in the following subchapters.

Flowsheet synthesis
The first step is also referred to as process flowsheet synthesis (Biegler et al., 1997), the goal of which is to discover the best combination of unit operations and their connections to accomplish a given production task (Siirola et al., 1971; Westerberg, 2004). This typically results in a process design in the form of process flow diagrams (PFD). A problem specification is made after which process concept(s) are generated. For example, a choice is made whether a well-proven, conventional process structure is used or whether an entirely new one is developed. After this, alternative designs are investigated, e.g. by searching for existing similar processes. The alternative designs are next analysed in order to see how they perform in the fulfilling of the goals set forth earlier. This analysis and evaluation typically involves balance and economic calculations and thus overlaps with the second step, where in addition to determination of design parameters, also the operating conditions of the process are determined. Sometimes controllability issues are already taken to be included in process synthesis (Biegler et al., 1997), but in **Figure 6** this has been divided as the third step where dynamics of the process are taken into account. It involves synthesis of control strategies to minimize product variability and to keep other key variables within acceptable ranges (Ricardez-Sandoval et al., 2009).

Flexibility analysis and control system design
Flexibility of a design refers to the plant being capable of operation in other steady states than the one used in its design (Biegler et al., 1997). The design variables include the fixed process structure and equipment dimensions, whereas control variables are those that are continually changing, e.g. flows. Constraints of feasible operation can be physical constraints or (product specifications) and examples of uncertain parameters are the raw material inlet concentrations. Thus, a more rigorous statement of flexibility is: given a design d, can the control variables z be adjusted in such a way that the constraints representing feasible operation are satisfied when faced with a change in uncertain process parameters (Halemane and Grossmann, 1983; Biegler et al., 1997)? On the other hand, flexibility analysis may strive to answer, not only

whether the design is flexible or not, but how much flexibility the design actually has (Swaney and Grossmann, 1985).

Moving from one steady state to another involves a transient, which is typically handled by an automatic control system. In a historical perspective Bennet (1996) traces development in automatic control back over two millennia, with early developments in controlling temperatures, pressures, liquid levels and rotation speeds (e.g. the Watt steam engine governor). Coming to modern times, in the so-called Pre-Classical Period (1900–1935) application of single-loop feedback control expanded while theoretical understanding and design methods lagged behind, although the first steps in understanding negative feedback were taken. The Classical Period (roughly 1935–1950) saw the advent of gain and phase margins, Nyquist stability criterion, Nichols chart, the Ziegler-Nichols tuning rules for PI and PID-controllers, block diagrams with use of Laplace transformations, root locus and control performance criteria. Coinciding with this period was the Second World War, which drove technological developments like radar. The era from 1955 onwards is called Modern Control in Bennet's classification. Major drivers during this period were the space race and the emergence of computers. Developments included the state-space approach, Bellman concept of optimality and dynamic optimization, Pontryagin maximum principle, optimal control, Kalman filter, systems engineering, and model predictive control. In general, control systems have been utilized in nearly all engineering areas but in this thesis, we shall focus on process control. The control systems in process control strive to keep essential quality variables at specified values, to minimize energy and raw material use while also providing the capability to make fast production or grade changes. The key concept here is the control loop in which a variable of the process is measured ("controlled variable, CV") and based on this feedback another variable ("manipulated variable, MV") is continually adjusted. A small process may have 20–100 of such loops, whereas large plants have thousands. This single loop control is still applied widely, especially on the lowest level of control, i.e. in the stabilizing controls of variables such as pressure and flows. Single loop control has as one major drawback: its poor ability account for interactions of many variables which has led to the development of multivariable control, see e.g., (Skogestad and Postlethwaite, 2005).

2.1.2 Integrated process and control design

Integration of process and control design strives to integrate systematic analysis of process dynamics into the design procedure (Vega et al., 2014) and has been a long-discussed subject going back to the 1940s (Ziegler, J., Nichols, 1943; Vega et al., 2014). The main driver in integration of process and control design is that the traditional sequential approach may lead several design iterations or poor plant operability, i.e. an optimally designed process may not function properly when faced with disturbances and uncertainties of the design model (Yuan et al., 2012).

In order to systematize integrated process and control design, frameworks have been studied and classified into two categories (Ricardez-Sandoval et al., 2009; Yuan et al., 2012). Firstly, there are the *indicator-based frameworks* that typically are used for screening of design alternatives. They utilize some sort of controllability index to characterize closed-loop performance of the system. The optimization approach in these frameworks has typically been cost minimization and they have been based on steady-state models (Ricardez-Sandoval et al., 2009). Examples of the used controllability indices are the relative gain array, condition number, disturbance condition number and integral error. Typically such problems result in mixed-integer non-linear programming (MINLP) optimizations (Hamid et al., 2010).

Secondly, there are the *dynamic optimization-based frameworks* for integrating process and control system design. The optimization in these relies on techniques of mixed-integer dynamic optimization (MIDO) and dynamic, non-linear models (Hamid et al., 2010). The effect of external disturbances and model uncertainties seems to have been a major concern in this field as several approaches have been suggested. Ricardez-Sandoval and co-authors (2009) list approaches such as dynamic worst-case-based design (Perkins and Walsh, 1996), matrix norms (Mohideen et al., 1997), parametric programming (Sakizlis et al., 2004), and the concept of back-off (Bahri et al., 1997). All dynamic optimization-based approaches suffer from high computational load. To alleviate this, the so-called robust approach has been researched over the last ten years. In these, the non-linear dynamic problem is replaced, at least partly, with an approximate linear problem which includes model uncertainty, see for example Chawankul et al. (2005).

Even though a considerable amount of research has been devoted to integrated process and control design there is still a lack of a generally accepted methodology (Pistikopoulos and Diangelakis, 2015). The PAROC framework they suggest, relying on tools such as gPROMS and Matlab, strives towards this goal. The workflow in this framework consists of construction of a high fidelity, dynamic simulation model, and its reduction to an approximate model, which is used in multi-parametric programming and validation of the optimization results with the original high-fidelity model. This approach closely resembles that which Ritala and co-authors (2013) reported as well. Hamid and co-authors (Hamid et al., 2010) have proposed the so-called reverse approach. In this approach, the vast design space is sequentially reduced to a small one from which the final solution is searched. The bounding of the search space is first done using thermodynamic and process insights. This is followed with further bounding based on process and controller design constraints. Once the final solution has been found, it is verified using rigorous simulation.

2.1.3 Other considerations

In the preceding chapters, we discussed general design of the process and its controls system, as they are the central areas to which the present work pertains. These fields have numerous sub-fields and considerations that we only briefly mention here, for the sake of completeness.

Heat exchanger network synthesis (HENS) was first proposed in the 1940's (Broeck, 1944) and it has been described as the "most commonly studied problem in process synthesis" (Furman and Sahinidis, 2002). The goal of heat exchanger network synthesis is to design a system that can optimally reuse released heat at appropriate places where it is needed making it an optimization problem, typically a mixed integer non-linear programming (MINLP) one. While the early works concentrated on synthesizing an entirely new network, retrofitting was taken into account by Linnhoff and Vredeveld (1984). Further reviews of this field can be found in Gundersen and Naess (1988), Furman and Sahinidis (2002) and Klemeš and Kravanja (2013).

Process safety focuses on prevention and mitigation of process accidents (fires, explosions and toxic releases), whereas the related field of occupational safety deals more with workplace hazards like trips, slips and falls. Methods and models utilized have been categorized as qualitative, semi-quantitative, quantitative and hybrid (Khan et al., 2015). Perhaps the most widely known qualitative hazard identification methods is HAZOP (Hazard and Operability Analysis) which was first applied in the 1960 and published in 1974 (Lawley, 1974). Since its publication it has been extended in numerous ways to include batch and electronic processes as well as human, management and organizational factors and also other methods like Failure Mode and Effects Analysis (FMEA) (see Khan et al., 2015). Another popular qualitative method is the standard risk matrix method (Garvey and Lansdowne, 1998) where the identified risks are placed in a two-dimensional array with impact and probability as the axes. In some applications, the risk matrix can be considered as a (semi-) quantitative method if numerical probabilities or impacts are used. Finally, the Swiss Cheese Model, originally proposed by Reason (1990), has gained both popularity and criticism since its publication and has also evolved since. A review of the evolution of and critique of the SCM model has been presented, e.g. in Reason et al. (2006).

Biegler and co-authors (1997) summarise the **economic considerations** of process design dealing with costs and revenues of the process. Costs are divided into fixed and variable costs, where the former include investments and overheads related to them, which are incurred at early stages of the process building project. Of main interest in process design are the capital investments, which can further be divided into fixed (buildings, equipment, land) and working capital (funds needed to operate the process until payments from the customers arrive). Variable costs, on the other hand, are incurred during the operation of the process continually, including raw material costs, credit, direct expenses (e.g. labour, utilities, maintenance, and supplies) and indirect expenses (e.g. depreciation, taxes, insurance). The profitability of a process can be estimated in several ways. Simple measures such as return on investment (ROI) and payback time can be used to give rough estimates, but their usefulness in comparison of alternative projects has been long acknowledged. The main drawback is that they do not account for time passing, i.e. schedule of payments and income, interest and inflation. To account for time passing, methods like net present value (NPV) of profit or costs, annualized payments, breakeven time and rate of return are used.

Typically, **environmental aspects** have been considered when evaluating alternative process candidate designs (Towler and Sinnott, 2013) in order to satisfy regulations regarding emissions and other damaging agents into the air, waterways and solid landfills (Biegler et al., 1997). Environmental and sustainability issues started to come gradually into the fore during the second half of the 20th century (Jacquemin et al., 2012). According to Young et al. (1997) the development began with a "reactive period" before the 1970s where environmental awareness was limited, few regulations existed and in general waste was not seen as an issue. The 1970s and 80s have been described as the "compliant period" where limited environmental awareness arose along with legislative controls on emissions and waste. In the following decade, all sectors and organizational levels became aware of environmental issues and the legislative situation became more stringent, while advances in process design methods, e.g. utilization of multiple objective optimization promoted sustainable process design (Bakshi, 2014). Also, environmental standards, audits and approaches such as life cycle assessment (LCA) came about. This decade has been dubbed as the "proactive period" while the 2000s is called the "progressive period" (Jacquemin et al., 2012), characterized with the generalization of LCA and its standardization into ISO 14040-14044, environmental process design tools (Carvalho et al., 2013), overarching environmental concepts (e.g. Design for Environment, Eco-efficient manufacturing, Industrial ecology) and evermore environmental policies (Jacquemin et al., 2012). In fact, design of environmentally benign processes was seen as one of the major challenges for process systems engineering of this period (Grossmann, 2004). All in all, the focus has shifted from early emission reduction activities of single plants to process (and product) life cycle thinking (Bakshi, 2014).

2.2 Process operation phase

2.2.1 Steady and dynamic operation

After the handover or commissioning the plant, operation begins (see **Figure 3**). Traditionally, steady operation of a chemical plant was seen to be the best way to go and this was reflected in its design, but it has been noted that in real-life plants do not operate in a steady state (Moran, 2015). Moreover, there has been a shift to operating plants, not in an isolated, steady manner, but as an integral part of the company and its dynamic environment, e.g. intermittent renewable power (Savolainen et al., 2016; Weiss et al., 2016). This means that plants cannot anymore be operated in a single operational point, but must also be able achieve good performance in exceptional operational points (Klatt and Marquardt, 2009). This needs to be reflected in the design phase of the plant as was mentioned when discussing flexibility and control system design.

2.2.2 Retrofits

In retrofits, part of the process is redesigned and built. One definition of a retrofit is of making minor changes to the process flowsheet and/or equipment sizes in order to significantly reduce operating costs, increase capacity, process new feed stocks and/or incorporate new technology (Fisher et al., 1987). The need for retrofits typically comes from the product market, for example in a case of limited demand, the retrofit goal could be to produce at the lowest cost (Simon et al., 2008). Other motivations for retrofits are typically higher product quality, improved safety, better energy efficiency, sustainability or waste reduction (Ben-guang et al., 2000; Simon et al., 2008; Lutze et al., 2010; Carvalho et al., 2013). The importance of retrofits is highlighted by Gundersen (1990) who has estimated that approximately 70% of process industry projects have been retrofits. Also, it has been noted that retrofit designs can be considered even more complicated than designs of new plants (Westerberg, 2004), since when evaluating retrofit alternatives, designing a new plant is always an option and it is desirable to re-use existing equipment as much as possible (Grossmann et al., 1987), which makes the design problem slightly different from a green field design. In designing new processes, equipment are dimensioned as a function of design variables like flow rates, whereas in retrofitting many equipment dimensions are, to a large extent, fixed already (Fisher et al., 1987). To address retrofitting, systematic procedures have been suggested in the literature.

Fisher and co-authors (1987) approached the issue with a “top-down, least commitment” strategy in which the idea is to terminate the retrofit study as early as possible, if there is not sufficient economic justification. This thinking is reflected also in the notion that retrofitting is a high-risk, high potential gain activity (Ben-guang et al., 2000). In Fisher’s approach, the analysis begins from the raw material and energy costs of the current flowsheet in order to determine the cost and material loss reduction possibilities related to them; e.g. if raw material savings are small compared to energy savings, then an energy focus is rational. In the second step, the option of building an entirely new process is quickly analysed, to provide a benchmark for retrofit options and process alternatives to consider. The alternatives are roughly screened to estimate order of magnitude of savings. Finally, the procedure involves equipment re-sizing in the existing or new process flowsheet as well as refining the calculations. Fisher et al. finally note that retrofitting can have an adverse effect on process controllability, e.g. by removing a manipulated variable, and on the process’s ability to handle disturbances. Thus, retrofitting also can benefit from integrated process and control design.

Simon and co-authors propose an indicator- and heuristics-based approach for batch processes. By indicators they mean numerical variables characterising the entire plant, a sub-process or a unit operation. Examples of these are equipment occupancy time, storage volume utilization, minimum driving force (e.g. temperature difference) or time rate of change of concentration. By heuristics they mean empirical process knowledge, which is used to link the indicators to retrofit actions. For example, “increase the driving force”. Finally, they note the usefulness of models in estimation of retrofit potentials in the process (Simon et al., 2008). This work is a continuation and adaptation of work by Uerdingen et al. (2003) where the focus was on continuous process retrofits. It relies on steady-state mass and energy balances as well as economic data such as raw material, utilities, waste and product prices. This approach is based on indicators, which in the original paper related to maximizing economic efficiency. Examples of such indicators are the material-value added (MVA), energy and waste cost (EWC), reaction equality (RQ), accumulation factor (AF) and total-value added (TVA). Identification of retrofit options is done by categorizing the component path flows and then applying generic retrofit actions. Such generic retrofit actions are reported in the paper but need to be adapted to each case. After identification of options, they are (qualitatively) evaluated, with a process designer's knowhow and finally cost impacts are calculated. The authors note that the presented framework is for screening of alternatives and due to simplifications made should be used as an order-of-magnitude estimate. A continuation of this work to extend the methodology to include safety and sustainability issues is presented in (Carvalho et al., 2008). The safety aspect is taken into account via the inherent safety index (ISI) of Heikkilä (1999), whereas sustainability issues come in through the works of Azapagic et al. (2002) and Cabezas et al. (1999). In Carvalho's study, sensitivity analysis of the indicators is used to set targets for retrofit design. In addition, sensitivity analysis is applied to identify which design variables (sizes, etc.) or operational variables (heat duties, etc.) have the largest effect on the targets. With this information, design alternatives are generated and finally evaluated with simulations. The authors talk about sensitivity analysis but it seems that what they mean by sensitivity analysis is not the same as in chapter 2.3.2 of this thesis. Rather, it seems that their sensitivity analysis consists of going through the calculated indicator values and selecting those that show the highest potential for improvements. These are then used to indicate the location of critical points of the process with respect to design or operational deficiencies.

Productivity increase retrofit is closely related to the concept of a bottleneck. In fact, it has been noted that retrofitting, aims solely to remove bottlenecks (Ben-guang et al., 2000). For batch plants Koulouris et al. (2000) have presented a simulation-based method for identifying bottlenecks. They defined a throughput bottleneck to be an equipment or resource that limits the amount of production and a scheduling bottleneck to be a unit or resource that limits the number of batches that can be produced per time period. In batch processes, the situation is complicated as attempts to increase production may result in scheduling conflicts for some units and such scheduling problems have been typically formulated as optimization problems. They emphasise the point that significant simplifications were necessary and that their simulation-based approach avoids this. Earlier, also Voudouris (1996) studied scheduling of a fine chemical plant using linear, discrete models. He raised three ways of utilizing such models in debottlenecking analysis: 1) simulating an existing production schedule and analysing its effects; 2) performing statistical analysis of manufacturing resource availability. Here the schedule is not fixed but rather generated statistically and Monte Carlo analysis is performed; 3) decision support tool. Of these, number 2) slightly resembles the work by Savolainen and Lappalainen (2015) in the choice methodological approach (Monte Carlo-type computations). The main difference is that in (Voudouris, 1996) the statistical approach was applied to a production schedule of batch units, whereas in (Savolainen and Lappalainen, 2015) the starting point was the equipment dimensions of a continuous plant. Furthermore, Voudouris did not pursue this approach further nor were there numerical results presented. Harsh, Saderne and Biegler approached the debottlenecking problem using MINLP optimization. They identify a bottleneck using violation of equipment performance inequality constraints as an indicator (Harsh et al., 1989).

Relating closely to the work presented in this thesis, Lucay et al. (2012) conducted sensitivity analysis of a mineral separation circuit. Their analysis used explicit expressions for output partial derivatives with respect to process parameters. This approach assumes that the analyst has access to the model equations, which may not be the case when using commercial simulators. In addition, the author relied heavily on graphical representations of the sensitivities and utilized the one-at-a-time approach. The sensitivity analyses works presented in this thesis do not make such assumptions. Continuing that work, Sepúlveda and co-authors (2014) have presented a study in which global sensitivity analysis was used to analyse mineral concentration circuits. In other words, the one-at-a-time limitation of Lucay et al. (2012) was overcome. The study, albeit of a more limited scope (smaller number of parameters and outputs; analysis only on Sobol' total sensitivity index), corroborates the main results of this thesis. In their work, they conclude that global sensitivity analysis can be of use in planning of retrofitting of mineral processing plants. Unfortunately, these papers do not present any argumentation on generalizability to other types of processes.

2.2.3 Other considerations

Similarly, to the design phase, in the operation phase process and automation engineers face other considerations than the ones mentioned above. Since they are not within the scope of this work, they are shortly mentioned here.

One major consideration during operation is **maintenance** of equipment or the entire plant (ISO, 2004), which aims at keeping the equipment, and more generally the whole plant, in operating condition. Maintenance has been divided into two categories: preventive maintenance and corrective maintenance, where the former aims to prevent equipment failures, whereas the latter deals with repairing failed equipment. This field has been and is an active research area but as this thesis is not concerned with maintenance, further discussion is omitted.

After operation of a plant has ceased, it will be run to a shutdown condition for a transition period. During this period, plans for the ultimate **decommissioning** can be made and needed data gathered. The decommissioning includes steps such as dismantling of process equipment and building, reusing the site, handling of chemicals left behind at the site in soil or groundwater (Hurme and Rahman, 2005). Decommissioning can actually be divided into several categories. A short shut down is referred to as idling, where systems are kept running in order to facilitate quick start-up. Mothballing refers to a long-term closure of a plant where systems are shut down for an undefined period. Starting up from a mothballed state may be non-trivial. Finally, scrapping refers to the complete dismantling of the plant (Briggs et al., 1997). As decommissioning is not in the focus of this thesis, we do not delve further into the literature on it.

2.3 Relevant mathematical methods

2.3.1 Modelling and simulation

Computer simulations

Computer simulation has its origins in the Manhattan Project in World War II and has developed in conjunction with the development of computers (Winsberg, 2015). While Winsberg (2015) notes that actually there is no single definition of computer simulation, a narrow definition by Humphreys is: “any computer-implemented method for exploring the properties of mathematical models where analytic methods are not available” (Humphreys, 1991). This definition is narrow in the sense that computer simulation is not only used when there are analytically unsolvable equations present (Winsberg, 2015). Furthermore, this definition relies on what is currently possible to solve analytically and fails to account for possible future advances in analytical techniques. More broadly speaking, Winsberg defines computer simulation as the process of studying systems, with steps of choosing a model, implementing it on a computer, calculating the outputs of the algorithm and visualizing the results (Winsberg, 2015). On a high level, the purposes of simulation can be divided into three categories (Winsberg, 2015). Firstly, computer simulation can be used as a heuristic tool in communication with other people and also with oneself. In science, such use can be applied to help arrive at new scientific hypotheses for further investigation (Parker, 2008a). On a more applied side, a clear application of this category is for operator-training simulators. Secondly, there is the prediction category. Prediction of the value of a certain variable at a given future time instant is referred to as point prediction, while in so-called range prediction no single point-type value is given. This kind of prediction may take a probabilistic form, e.g. the temperature will increase by 2–5 degrees in one hour with a probability of 0.66. Thirdly, qualitative predictions are possible. With these no point or ranges for variables are produced, but question such as “Is the system stable?” can be answered. The third category for use of computer simulations is in understanding of data. In other words, if one has experimental data, simulation can be used to understand how that data may have come about. Questions such as “How did things actually occur?” or “How could things have gone” fall under this category. Parker (2008a) also notes that computer simulation can be used as an evidential resource, i.e. to provide evidence for hypotheses about real-world target systems. In this aspect, computer simulation can be seen as another way of experimental science.

Modelling and simulations are the basic tools of design but also other process industry plant life cycle phases can benefit. Simulation models can act as a shared repository of and knowledge from R&D, design and operation. In fact, simulation can be placed as a unifying method between research and development, design and operation according to **Figure 7** (Dimian et al., 2014).

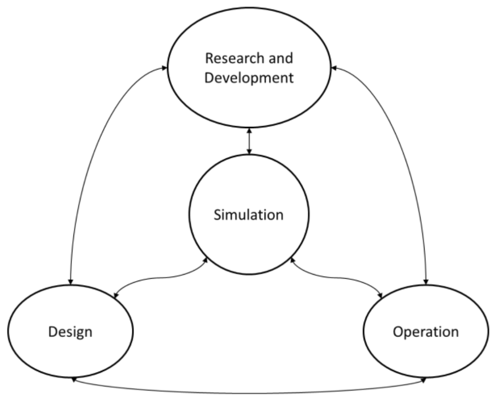

Figure 7 Simulation at core of R&D, design and operation (Dimian et al., 2014).

In R&D, simulation models can be validated with experimental data and then be used to substitute further, possibly expensive experiments. Such models are usable in the design of processes and their automation; especially since currently, processes have to operate at high material and energy efficiency, flexibly, safely and cleanly. During operation model-based process control is common, but also areas such as maintenance and supply chain management can be benefit (Dimian et al., 2014).

Model characteristics

The term model can refer to a great many things. In a very general sense, a model is any assumed relationship between variables of a system under study. This relationship can be phrased in many ways, not all mathematical (e.g. mental models, graphical models, i.e. plots, tables,...) (Ljung, 1987). In this thesis, we shall concentrate on mathematical models, i.e. descriptions of variables' relationships in terms of mathematical expressions. Such expressions or sets of equations are solved analytically or, as is the more usual case, using a computer to simulate them. Since the set of such models is very large, models have been classified according to several criteria. For example, Hangos and Cameron (2001) present a classification in five ways:

1. Mechanistic vs. empirical
   A mechanistic model, or first principles/white box model, takes such basic physical laws as conservation and transport of mass, energy and/or momentum as the starting point and builds the equations from there. In contrast, an empirical model, or a black box model, relies on

measured data from experiments and attempts to find a mathematical relation that describes the data best. Typically, the models used in process engineering are a combination of the two. Such models are sometimes referred to as grey box models (Hangos and Cameron, 2001).

2. Deterministic vs. stochastic
A deterministic model does not have randomness in it, i.e. the model output is fully determined by the values of its parameters and initial conditions. In contrast, a stochastic model or part of it contains an element of randomness and even the same parameter and initial conditions will produce different outputs. In deterministic models, the output is a number (scalar or vector) whereas in stochastic models the output is represented by a distribution. A model can have also hybrid characteristics, for example, it may contain both stochastic and deterministic parts.

3. Lumped vs. distributed parameter
Lumped parameter models refer to a class of model in which the spatial position is neglected, while distributed parameter models have this included. An example of a distributed parameter model is a partial differential equation.

4. Linear vs. nonlinear
Linearity of a model is that the superposition principle applies, i.e. that the response of the model caused by two or more inputs is equal to the sum of individual responses to the inputs. If this principle does not apply, the model is non-linear.

5. Continuous vs. discrete
In continuous models, the mathematical equations are continuous. Discrete models do not possess this continuity and are many times written as difference equations.

Another way of classifying models is the distinction between steady state and dynamic models. Dynamic models are used to describe the delayed or inertial characteristic of the system. This means that when the value of a model input is changed, the output does not immediately change to its new value. Rather, the output may at first not react at all (pure delay) or it may begin to move gradually towards its final value (inertia). Steady-state models do not possess this character. These characteristics are summarised in the following **Table 2** (Hangos and Cameron, 2001).

Table 2 Forms of model equations (Hangos and Cameron, 2001).

Type of model	**Examples of equation types** Steady-state	Dynamic
Deterministic	Nonlinear, algebraic	Ordinary differential equations (ODE) / Partial differential equations (PDE)
Stochastic	Algebraic/difference equations	Stochastic ODEs / difference equations
Lumped parameter	Algebraic equations	ODEs
Distributed parameter	Elliptic PDEs	Parabolic PDEs
Linear	Linear algebraic equations	Linear ODEs
Nonlinear	Nonlinear algebraic eqns.	Nonlinear ODEs
Continuous	Algebraic equations	ODEs
Discrete	Difference equations	Difference equations

In chemical/process engineering, the utilized models can be seen to have two major components: the part characterising the equipment and the part characterising the flowing material, i.e. material properties (Westerberg, 2004). The level of detail in equipment characterization can vary considerably. In steady state, mass and energy balance calculations a separation unit may be described only with constant separation coefficients. In a more detailed description, a characteristic dimension of a device may be included, e.g. the area of a heat exchanger. In an even more detailed model the entire 3D geometry of the device, e.g. a furnace, is used. The more detail used in a description, the more input information needs to be gathered and fed into the model. Also, the computational load will increase as a function of the detail level. Characterization of the flowing fluid or estimation of physical properties is a considerable task, since the sheer number of different pure fluids is enormous and when pure fluids are mixed, the physical properties are not always simple averages of the pure fluid properties, which makes the situation even more challenging.

Simulators

Computer simulation is conducted by specialized computer programs, referred to as simulators. In process systems engineering or chemical engineering they are called process simulators. There are numerous tools available, both open-source and commercial, running on different operating systems and concentrating on different applications, e.g. power plants, distillation, thermodynamic analyses, operator training, reactions, generic flowsheeting. For example, Wikipedia lists 58 chemical process simulators (Wikipedia, n.d.). The list seems to exclude many modelling-oriented programming languages such as Modelica® (Modelica, n.d.) and Matlab® ("MATLAB, The Language of Technical Computing," n.d.) and commercial software like Balas (VTT, n.d.), JADE (GSES, n.d.) and Flowmaster V7 (Mentor, n.d.). Simulators can be classified in many ways, but one of the most common is to distinguish between equation-oriented and agent-based simulators (Winsberg, 2015), with the prior more common in physical sciences, including engineering. In such simulators, the underlying theory is formulated in the form of equations, which the simulator numerically solves. Agent-based simulators are more common in social sciences and the system under study is represented by discrete, individual entities (agents) with their own behavioural rules (Winsberg, 2015). It should be noted that the term "equation-based" or "equation-oriented" has also another meaning. In this case, it refers to process flowsheet simulators and the way the calculation is conducted. In such "equation-based" flowsheet simulations, all the equations describing individual unit operations and their connections are collected and solved simultaneously. This is to be contrasted with the so-called "sequential-modular" simulators where the simulator moves from one unit operation to another and solves the equations describing one unit operation at a time (Biegler et al., 1997).

2.3.2 Global Sensitivity Analysis

One of the mathematical methods used in this thesis is global sensitivity analysis (GSA). In sensitivity analysis the goal is to quantify how a model's inputs or parameters affect its outputs or "the study of how uncertainty in the output of a model (numerical or otherwise) can be apportioned to different sources of uncertainty in the model input" (Saltelli et al., 2008). The "traditional" way of doing this has been to calculate the partial derivative of an output, Y_j, with respect to different inputs, X_i, either analytically or by finite differences around a given nominal point, $X_{i,o}$, as shown in **Figure 8**.

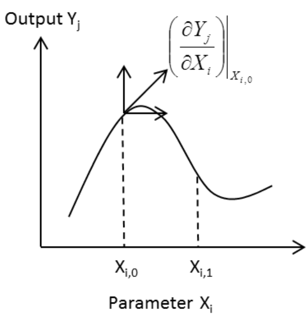

Figure 8 Local sensitivity of Y_j with respect to X_i at $X_{i,0}$.

The drawback of this approach is that it is local, i.e. it gives information only on how Y_j depends on X_i around $X_{i,o}$. This information may be inaccurate or even misleading at another point, say $X_{i,1}$ in **Figure 8** when the relationship is not linear. Global sensitivity analysis strives to overcome this locality problem. Below we give short descriptions of three global sensitivity analysis methods, although others do exist.

In conjunction with global sensitivity analysis the question of what exactly the analysis is used for is raised. Typically, two settings have been presented:

parameter screening and parameter ranking (Saltelli et al., 2008). In parameter screening setting, a large set of parameters are analysed with the intention to identify those parameters that do not have a major effect on the output of interest. In other words, these parameters are screened out. The rest, which hopefully form a small subset of the original parameter set, are the important ones. This is where the screening setting ends, i.e. it does not tell which is the most important parameter, which is the second most important, etc. Such results can be obtained with the parameter ranking setting. Needless to say, parameter ranking is more computationally expensive than parameter screening.

Morris method

One method of global sensitivity analysis is the Morris or elementary effects method (Morris, 1991) which is a screening method. In this method, for each input X_i the so-called elementary effect EE_i is calculated as:

$$EE_i = \frac{Y_j(X_1,\ldots,X_{i-1},X_i+\Delta,\ldots,X_k) - Y_j(X_1,\ldots,X_k)}{\Delta} \tag{1}$$

This resembles the definition of a partial derivative, but the difference is that X_i now takes multiple values from {0, 1/(p-1), 2/(p-1), ..., 1} where it has been assumed that $0 \leq X_i \leq 1$. The variable p is the number of levels at which X_i is sampled and Δ is a fixed multiple of 1/(p-1). The Morris method samples the parameters X_i and computes the elementary effects (EE_is) which form a distribution F_i, i.e. $EE_i \sim F_i$. To assess parameter X_i's effect on Y_j, the sample mean (μ_i) and standard deviation (σ_i) of F_i are computed and plotted as shown in **Figure 9**. The plot can be interpreted so that parameters with negligible effect are close to the origin. Those with a significant, but linear, effect are on the right and close to the horizontal axis ($\sigma_i << \mu_i$). Finally, those with a large non-linear effect or interactions with other parameters are towards the top right of the plot with σ_i and μ_i having the same order of magnitude (Iooss and Lemaître, 2014).

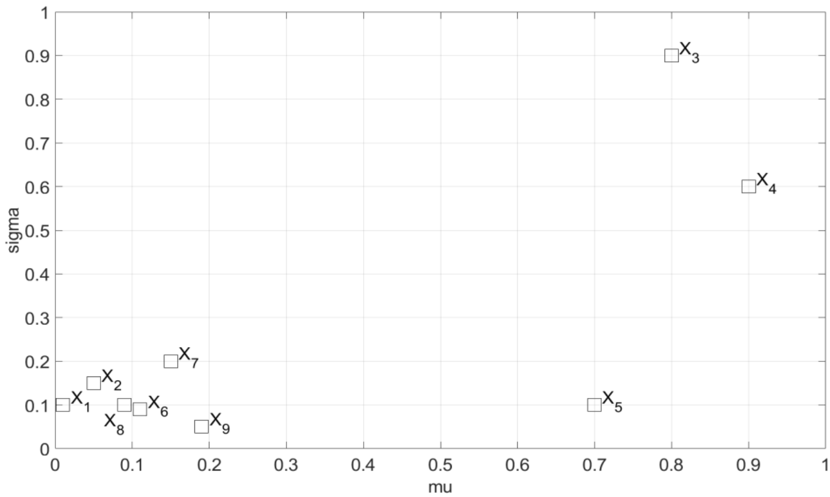

Figure 9 Example of a (μ,σ) plot of the elementary effects method.

The original method of Morris has been extended since its publication. The first extension is that instead of calculating the mean of the EE_is, a modified measure μ^* is calculated as the sample average of $|EE_i|$ and no σ is calculated. A second extension is a new parameter sampling strategy alleviating the original method's coverage of the input space, which was non-optimal. Finally, progress has been made with working with groups of parameters, i.e. to produce a sensitivity measure relative to a group of parameters. Such developments are summarised in (Campolongo et al., 2007).

Variance decomposition

Another approach to global sensitivity analysis is the variance-based method. Historically the first studies on variance-based methods were published as the Fourier Amplitude Sensitivity Test, FAST (Cukier, 1973; Cukier et al., 1978). Nowadays the Sobol' method (Sobol', 1993; Saltelli et al., 2008) seems to have gained popularity.

A variance-based method, as the name suggest, uses the variance of the model output, $V(Y_j)$, as the starting point for developing sensitivity measures. This variance arises from the parameters, which are varied in the analysis. The output's variance is decomposed into first- and higher-order effect of the inputs and from those the so-called first-order and total sensitivity indices are calculated. The first step is to ask how $V(Y_j)$ would be affected if parameter X_i were to be fixed to a value x_i while allowing the other parameters, denoted by $X_{\sim i}$, to vary according to their distributions. The variance of Y_j under this condition is denoted by $V_{X\sim i}(Y_j \mid X_i)$. If the output variance was clearly reduced by fixing X_i then it can be deemed as an important parameter with respect to Y_j. At this stage, the method is still a local one since X_i has been fixed to only one value. The next step is to take the expected value of the conditional variance as x_i changes: $E_{Xi}[\ V_{X\sim i}(Y_j \mid X_i)\ ]$. Now, the unconditional variance is decomposed as

$$V(Y_j) = E_{X_i}\left[V_{X_{\sim i}}\left(Y_j \mid X_i\right)\right] + V_{X_i}\left[E_{X_{\sim i}}\left(Y_j \mid X_i\right)\right] \qquad (2)$$

The first-order sensitivity index of output Y_j with respect to parameter X_i, $S_{i,j}$, is defined as

$$S_{i,j} = \frac{V_{X_i}\left\lfloor E_{X_{\sim i}}\left(Y_j \mid X_i\right)\right\rfloor}{V(Y_j)} \tag{3}$$

and the total index, $S_{Ti,j}$, as

$$S_{Ti,j} = 1 - \frac{V\left\lfloor E_{X_{\sim i}}\left(Y_j \mid X_{\sim i}\right)\right\rfloor}{V(Y_j)} \tag{4}$$

The first-order index measures a parameters linear effect on the output, while the total index is used to measure the effect of any degree, including interactions with other parameters. A more thorough treatment of the Sobol' and elementary effects method can be found for example in (Saltelli et al., 2008) and a recent review of variance-based methods from (Iooss and Lemaître, 2014).

To numerically calculate the first-order and total Sobol' indices Monte Carlo (Saltelli, 2002) simulations are conducted. Traditional random Monte Carlo simulations require a considerable number of simulations and thus quasi-random samples, such as Halton and Sobol' LP_τ sequences, are commonly used (Saltelli et al., 2008). In addition, the derivative-based approach, which is presented next, has been developed to alleviate computational load.

Derivative-based approach

The above discussion approached global sensitivity indices from the variance-decomposition point-of-view. The subject has also been approached from derivative-based global sensitivity measures (DGSM) point-of-view, see e.g. (Kucherenko et al., 2009; Sobol and Kucherenko, 2009; Kucherenko and Iooss, 2015), which can be seen as a generalization of the Morris method. This approach starts from the partial derivative $\partial Y_j/\partial X_i$ and uses functionals of it as sensitivity indices. For example, the modified Morris measure μ^* is an approximation of the functional

$$\mu^* \approx \int \left|\frac{\partial Y_j}{\partial X_i}\right| dX \tag{5}$$

and the total index $S_{Ti,j}$ is related to the functional

$$S_{Ti,j} \approx \int \left(\frac{\partial Y_j}{\partial X_i}\right)^2 dX \tag{6}$$

On the upside the approach is that it is computationally more efficient than the variance-based approach or Morris method (Kucherenko et al., 2009). On the downside it assumes Y_j as a differentiable function of the X_i's and as is demonstrated in (Sobol and Kucherenko, 2009), this can lead to false conclusions on parameter ranking of highly non-linear functions.

2.3.3 Multiple objective optimization

Traditionally, optimization in process engineering has been conducted as single objective optimization, while in the real world one quickly encounters several conflicting objectives. With conflicting objectives one means that not all objectives reach their optima at the same point (Hakanen, 2006). Thus, in multiple objective optimization, the concept of a solution has to be extended to the so-called Pareto optimal solution. A solution is Pareto optimal if no criterion can be improved without impairing some other criterion at the same time. For a given multiple optimization problem there may be several such solutions and they are in fact mathematically equivalent. Thus, to pick the final solution, a DM who can express preference information not encoded in the problem formulation, is needed (Hakanen, 2006). Optimization in chemical engineering is not always a straightforward task because the design spaces and even objective functions are not always clear to the designer (Westerberg, 2004). Nonetheless, optimization techniques have been used in process design at least from the late-1950's in the oil-refining industry starting with linear programming (Westerberg, 2004). Other techniques such as sequential quadratic programming, mixed integer optimization and multiple objective optimization have also been utilized. For further details, the reader is referred to (Biegler and Grossmann, 2004) for a review of methods and their application domains in process systems engineering. Also, future visions by the same authors are presented in (Grossmann and Biegler, 2004).

It has been noted that in process engineering one can find two kinds of optimization problems (Biegler et al., 1997; Hakanen, 2006). The first, parameter optimization, is used when the structure of the process is fixed and the operational parameters are used as decision variables in the optimization. The second, process synthesis, strives to find the process structure by using optimization. Typically, parameter optimization problems lead to continuous optimization problems, while in synthesis one quickly ends up with mixed-integer problems. For example, Psaltis and co-authors (2016) present a study where a distillation and heat exchanger network synthesis problem is formulated as a mixed integer non-linear programming (MINLP) problem. Their approach to solving it is by generating computationally efficient surrogate models by using more rigorous and computationally intensive models, an approach applied also by Savolainen et al. (2015). In relation to this thesis, it is noteworthy that Psaltis et al. also use sensitivity analysis in selecting input variables for their surrogate models; they used the one-at-a-time approach.

2.3.4 Hypothesis testing

Hypothesis testing, in the statistical sense, was employed in the model comparison method developed in Publication I, in order to determine if two models differ. The comparison is conducted by using several so-called comparison variables, which are chosen by the analyst. Originally, they are time series, but are then averaged over time. As the models in question contain a stochastic element, several simulation replications are performed necessitating the use of statistical methods. One needs to compare distributions, rather than just scalar values. This is done using the two-sample Kolmogorov-Smirnov test, which compares two cumulative probability distributions. The test statistic used is the largest vertical distance between these distributions, as shown in **Figure 10** below. In the figure two cumulative probability distributions, A and B, are shown along with the test statistic D.

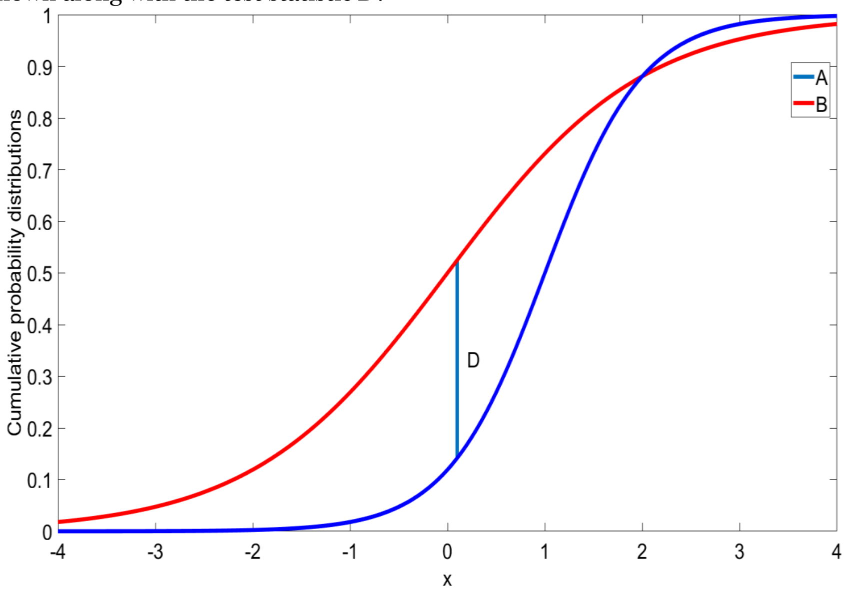

Figure 10 Example of two-sided Kolmogorov-Smirnov test.

In the model comparison method several comparisons on the same data are performed which is why the Bonferroni correction is included (Milton and Arnold, 1995). In this, the significance level for one comparison variable, α_i, is the experiment-wise significance level, α, divided by the number of comparisons, N_{var}.

3. Research questions

Westerberg (2004), citing the work of Bucciarelli (1996), argues that designing a plant is in itself a social process which includes meetings, discussions, etc., reflecting social values and knowledge. The design work's social aspect is typically handled with defining workflows, which prescribe, e.g., documents to be produced. This approach assumes that design work can be formulated as a sequence of clear steps, an assumption that Bucciarelli and others have shown not to be true. Rather, solving design problems involves moving back and forth from one part to another in order to gain an understanding of the problem (Westerberg, 2004). It could be then argued that gaining a better insight into the problem at hand can provide added value to the designer. As briefly referred to above, the tightening environment sets challenges for the designers and operating personnel of processes. In the following, we present a non-exhaustive list of such challenges as a motivation for the research questions. While this thesis does not directly address them, there are numerous other challenges faced by the designers and plant staff. Such challenges include management of abnormal situations, predictions, scheduling of maintenance activities as well as fault detection and diagnostics.

3.1 Finding the right focus

A process industry plant's objective is to deliver products satisfying quality requirements while achieving economic benefits at a minimal cost. On the design side, the early phases of a plant design project may not incur major expenses but can contribute significantly to cost-reduction opportunities and can have a significant impact on life cycle costs (Marquardt and Nagl, 2004). In fact, Dimian et al. (2014) suggest that design phases take approximately 15% of the total design and construction project (until end of commissioning) cost while representing nearly 45% of cost-reduction possibilities. Furthermore, they note that erroneous decisions made in the early phases can incur high costs later during plant operation, due to reduced production and a need for corrective actions. In addition, during operation the product demand, quality and raw material feed, are bound to change, which leads to challenges to the operation of the plant as it must be both flexible and controllable (Vega et al., 2014). Flexibility here refers to the plant's capability to operate in different (desirable) steady-states (Grossmann and Morari, 1983), whereas controllability is concerned with dynamic operation (Vega et al., 2014), e.g.

change situations from one operation point to another (Biegler et al., 1997). This demand for flexibility and controllability also poses challenges to the process designers whose process and control design should meet these targets (Vega et al., 2014). The challenges are exacerbated by the requirements that the design itself be performed cost-efficiently. For example, a study by Hussain and Wearne identified time as the second greatest problem in project management in the process industry (Hussain and Wearne, 2005). This then leads to a need to **focus the designer's attention on the most critical parts** of the process already in the early phases of the life cycle.

3.2 Limited knowledge

As Grossman and Morari (1983) state, practical engineering problems are more loosely defined than scientific ones since the prior contain uncertainties in, e.g. computational models, market forecasts, raw material and prices. Moreover, sometimes the designer is even faced with a situation where the (true) goals and the space of possible designs are not well specified (Westerberg, 2004). Also, it may occur that different parts of the process are developed or designed by different companies. For example, one company may have developed and patented a process concept, which is then licensed and adapted to a certain plant by a separate design company. While in an ideal world this would not be a problem, sometimes the information provided to the designers in early phases of design may be incomplete, either due to trade secrets or even due to limited knowledge of the provider. Furthermore, design consultants possess expertise in design work but may lack operational knowledge, while client companies possess operational data and expertise but usually no real design experience (Moran, 2015).

Moreover, it seems that the division between conceptual and detailed design is getting blurred and the traditional waterfall project model is being replaced with fast-track/unstaged design or collaborative contracting (e.g. the alliance model) (Suprapto, 2016). Reasons for this reorganization of work can be numerous, but it seems that the major driver has been the recognized budget and/or timetable overruns of large capital projects (see (Suprapto, 2016) and references therein). Such ways of organising the design work lead to a need for quick and accurate information exchange between parties, e.g. the design consultant(s) and the customer. This has proven to be a challenge, as exemplified by founding of the DEXPI group (www.dexpi.org). It can be argued that this leads to the fact that **design decisions need to be made with limited knowledge or under uncertainty** (Schneider and Marquardt, 2002) which is also tied to the previous challenge in that reducing the uncertainties requires time and money and should be worth the effort.

3.3 Multiple conflicting operational objectives

Traditionally, process design has been separated into two distinct parts: process and automation/control design (Vega et al., 2014). Nowadays, the operational aspects of automation design are being taken into consideration in earlier phases of design, typically involving multiple, conflicting goals or objectives (Ropponen, 2013) originating from the economic and dynamic performance objectives set forth by the customer. When striving to use mathematical optimization as a tool in solving such problems, a single objective function or a weighted sum has been typically the minimized criterion (Ropponen, 2013). This formulation has drawbacks that may result in loss of information about the relevant characteristics of the problem, interdependencies between factors and uncertainties (Hakanen et al., 2013), thus hindering learning and gaining insights. This leads to the need to **account for multiple objectives**, a situation also present in the designer's work.

3.4 Main hypothesis and research questions

Based on the discussion above, the main hypothesis of this thesis is that extending dynamic simulation with other mathematical methods can bring extended added value to a process or control designer. This added value comes from alleviating the challenges identified above. Here, the term extended added value refers to the fact that simulation alone typically brings added value, when used properly. Now, extending dynamic simulation with the other mathematical methods also extends this added value. The main hypothesis and results contributing to it from four case studies are summarized in **Figure 11**. A detailed description of the cases and their contributing results is given in chapter 4. The cases are numbered in the same order as the publications of this thesis. The figure also summarizes the extensions to dynamic simulation, which were used in the studies. Finally, in the figure, the industrial domains of the cases are presented. The three dots on the right-hand side of **Figure 11** indicate that this list is by no means exhaustive and can be seen as a topic for future work.

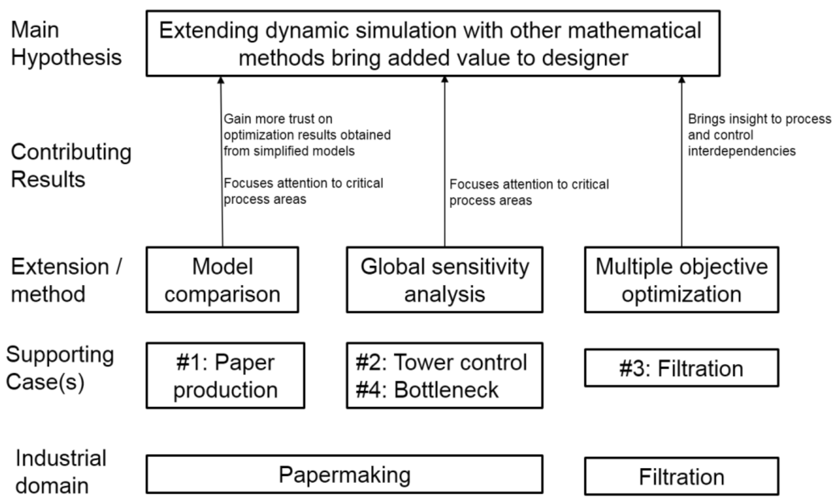

Figure 11 Thesis main hypothesis, contributing results, extensions, cases and industrial domains.

Finally, we formulate the research questions of this thesis as: How can coupling of process simulation and other mathematical methods (introduced in chapter 2.3) be

1. used to focus the designer's attention on the most critical parts of the process, even with limited knowledge?
2. used to provide insight into an operational plant's personnel?

To address question 1, a model comparison method was developed and its potential in early phase process optimization was shown. Also, combining global sensitivity analysis with process simulation was investigated and shown to be useful in attention focusing on preliminary process and automation design.

To address question 2, the potential of combining dynamic process simulation and interactive multiple objective optimization in design of operational practices was studied. In addition, a combination of global sensitivity analysis with dynamic process simulation as a method of identifying bottlenecks of a process was studied.

4. Results and empirical work

This thesis utilized three extensions to support the main hypothesis. The four cases used had certain common characteristics. Firstly, they all utilized dynamic simulation models. Building of the models followed a quite traditional iterative, step-wise approach, for example summarised in (Hangos and Cameron, 2001). The studies used as modelling environments Matlab ("MATLAB, The Language of Technical Computing," n.d.), Apros ("Apros," 2010) and Simlab ("SimLab - Sensitivity Analysis," 2010). Secondly, in all cases the models were simulated in a Monte Carlo-like fashion (Law, 2007). In essence, a model was run several times with different inputs or parameter values generating a large set of data. This data was analysed to draw the conclusions. Thirdly, all cases are tied with some stage of a process industry plant's life cycle as summarised in chapter 1.1.

In the next chapter, the supporting case studies and their contributing results are described in more detail.

4.1 Paper production case

The Paper production case study addressed concurrent process dimensioning and control design of a paper mill. The problem was approached with a two-level optimization, where on the lower level the operation of the mill was optimized for a given process dimensioning. This dimensioning was derived from the upper level of the optimization. The optimization problem formulation and results can be found, e.g. in (Ropponen, 2013) and the references therein. The initial motivation to apply a sophisticated mathematical approach to this rather traditional process (shown schematically in **Figure 12**), is the inherent difficulty of controlling (and designing controls for) certain aspects of it.

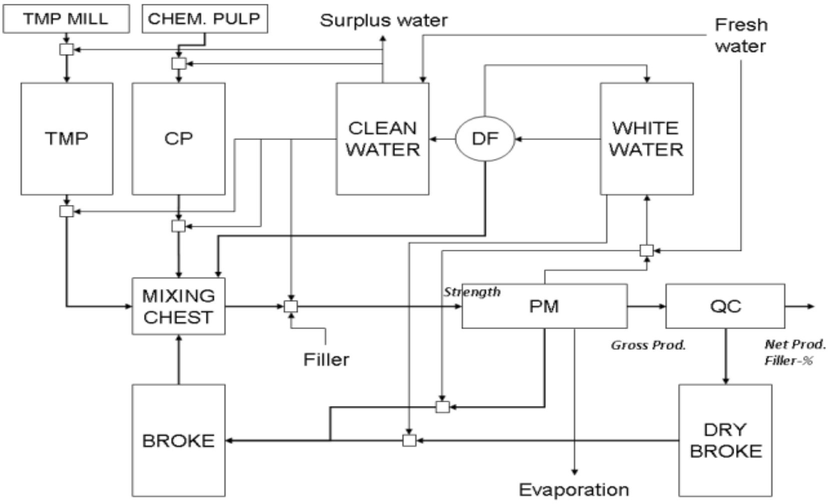

Figure 12 Schematic of the paper mill process utilized in the Paper production case.

When the process runs normally, the paper machine (PM) is fed a mixture of solid raw materials suspended in water. Part of the raw materials, such as thermomechanical pulp (TMP) and chemical pulp (CP), come fresh from their respective production units, but there also exists a recycling stream of so-called broke. Broke is produced in abnormal situations, called web breaks, at the PM in which all the produced paper is rejected and stored in the broke tower. In order not to waste this material, broke needs to dosed to the feed mixture, which has proven to be challenging. Namely, if too much broke is dosed, the quality (e.g. strength properties) of the mixture reaching the PM is compromised as the paper fibres have undergone operations that weaken their properties. This in turn increases the possibility of a new break and could lead to a vicious cycle. On the other hand, dosing very little broke could lead to overflowing and/or aging problems in the broke tower. Filler, which is typically a mineral substance and cheaper that TMP or CP, is fed to the mixture and it is desirable that as much as possible is retained at the PM and ends up in the paper. In the optimization model the retention was assumed to be constant, but as it is neither ideal or constant in real-life, some filler is recycled via the water system (simplified in **Figure 12** to consist only of a white water tower, a disc filter (DF) and a clean water tower). This brings another challenge to the process operation since filler tends to decrease paper strength, increasing the probability of breaks. Also, the customer buying the paper cannot tolerate too much filler in the paper, which means that the filler content, measured at the quality control (QC), needs to be controlled. On the fibrous raw material (TMP and CP) side, the qualities, e.g. with respect to strength, do not remain constant in real-life since in the preceding processes may experience upsets.

Thus, there exists a potential application of optimization to determine both the dimensioning and operation of the process. This needs to be done with limited knowledge (chapter 3.2) and in the face of multiple conflicting operational objectives (chapter 3.3). It is fairly evident that such two-level optimization involves a considerable amount of simulations necessitating use of a very fast model. This in turn has the effect that the model needs a considerably simplified description of the real-life process. In addition, this very simple model is necessitated by the fact that if such optimization is conducted in early phases of design, not much information might be available, which is one of the challenges identified in chapter 3. A natural question then is whether the results obtained with this optimization model (OM) are trustworthy and this aspect is the empirical work considered here. The work consisted of developing and applying a novel method to compare the optimization model with a set of increasingly realistic models, called verification models (VM). The idea is that if the optimization model and verification models are equivalent and the verification models are adequate descriptions of real-life, then the results obtained with the optimization results can be trusted.

The case utilized a Matlab-based dynamic model of a paper mill as the optimization model and eight different verifications models which were implemented with the Apros® Paper simulator. Each verification model contained some modification to the detail level of the optimization model. These modifications were chosen to reflect the non-idealities outlined above. The modifications are summarised in **Table 3**.

Table 3 Modification in the verification models of the Paper production case.

Verification model	Modification
1	None
2	Variable filler retention at PM
3	Bad-quality TMP from the TMP mill
4	New tank (white water) between PM and white water tower and disc filter.
5	Variable filler retention at PM and bad quality TMP from the TMP mill together
6	Variable filler retention at PM and new tank together
7	Bad-quality TMP from the TMP mill and new tank together
8	All modifications together

The "Variable filler retention at PM" modification was implemented with the following equation

$$r_{filler,PM} = 0.5 + w \tag{7}$$

where the value 0.5 was the original filler retention.

The modification comes through the noise term w which is a random variable distributed normally with zero mean and variance of 2.0. To avoid too large changes in the simulation, $r_{filler,PM}$ was further filtered with a time constant of 15 min. This value was then fed to the PM model of **Figure 12**.

The second modification, "Bad-quality TMP from the TMP mill" affected the flow from the TMP mill. For each 10-minute step of simulation, the model determined whether the TMP flow was of "bad quality" or not. This determination was implemented with a two-state model shown in **Figure 13**, where the arrows indicate transitions from one state to another and the associated numbers the probability of that transition.

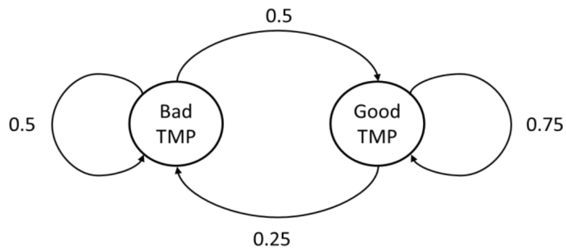

Figure 13 Two-state model for producing bad TMP.

The bad TMP then flowed through and mixed with other materials in the process, finally reaching the PM. There it affected adversely the paper's strength and in doing so increased the probability of a web break.

Finally, the "New tank" modification involved adding a new, ideally mixed tank between the PM and white water tower and disc filter. This tank, shown in **Figure 14**, is typical in real-life processes. The tank acts in this modification as a primary source of water for the needs of the process, while the white water tower is a reserve which can absorb excess water (overflow) or provide makeup if needed.

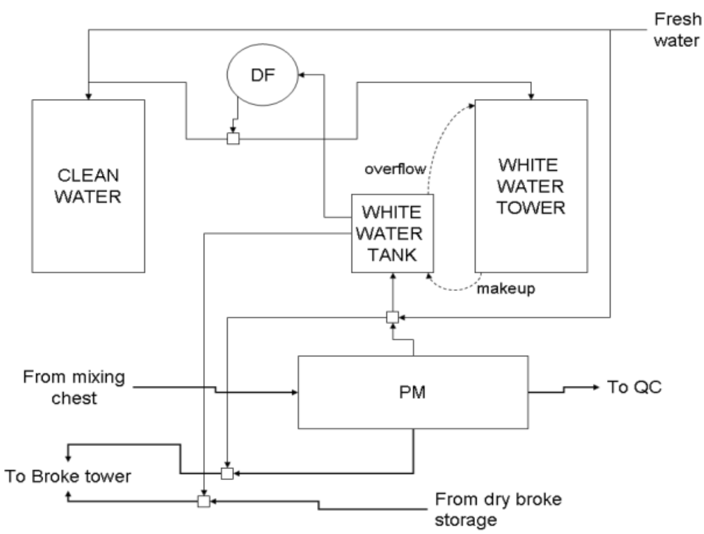

Figure 14 Addition of a white water tank.

The models in the Paper production case were hybrid models combining both deterministic and stochastic parts, which necessitated the development of a novel comparison method to distinguish differences arising from stochastic fluctuations from real differences. This hybrid nature of the models arose from the fact that in the preliminary process design phase solid information on the process may still be scarce and some parts of the process need to be modelled stochastically. In this case, the stochastic parts were the breaking of the paper web at the paper machine and the production of dry broke. Thus, the model comparison method needed to distinguish between two potential sources of model difference: stochastic fluctuations and fundamental model differences. To quantify the former a VM was compared with itself, with the only difference being the random numbers fed into it. This information was then utilized when comparing the OM vs. a VM. Comparison of the models was done with 16 variables relating to the product, behaviour of the control law (see the Tower control case for details) and overall operation of the plant. These are listed in **Table 4**.

Table 4 Comparison variables of the Paper production case.

Nr.	Description	Location in Figure 12
1	Filler content squared deviation from its target	"Filler-%" at QC
2	Gross production squared deviation from its target	"Gross prod." between PM and QC
3	Strength squared deviation from the target value	"Strength" at PM
4	Cumulative number of breaks	PM
5	Net production rate (PM gross production - dry broke)	Net Prod. after QC
6	Broke dosage	Between broke tower and mixing chest
7	TMP/CP ratio at the mixing chest	Between TMP and CP towers and mixing chest
8	TMP flow to its tower	Before TMP tower
9	CP flow from to its tower	Before CP tower
10	Disc filter input flow	From white water tower to DF
11	The pulping rate of dry broke	From dry broke tower to broke tower
12	The intake of fresh water to the clean water tower	From fresh water to clean water tower
13	Pulp consistency (dry matter %) into the TMP tower	Before TMP tower
14	Pulp consistency into the CP tower	Before CP tower
15	Disc filter filtrate recirculation flow	From DF to white water tower
16	Fraction of time that at least one tower under- or overflows	All the towers

To assess long-term average behaviour the resulting time series were averaged over the simulation time. In addition to this, also variability of the process behaviour was studied by using the coefficient of variation. The comparison was repeated for each of the modifications in the verification models. For each verification model, 500 simulations were executed resulting in 4000 simulations. The simulations were executed on a dedicated calculation server.

Contributing results

In the Paper production case, the specific goal was to develop a model comparison method to increase confidence that process design and operational optimization results obtained using rather simple models can be trusted. The developed method was designed to be used with hybrid deterministic-stochastic models. The case showed that the average behaviour of the models was mostly the same while differences were seen on the variational side. This is summarized in **Table 5**.

Table 5 Comparison results of the Paper production case.

Modification	Average	Variations
None	same	same
Variable filler retention at PM	same	different
Bad-quality TMP from the TMP mill	same	same
New tank (white water) between PM and white water tower and disc filter.	same	different
Variable filler retention at PM and bad quality TMP from the TMP mill together	same	different
Variable filler retention at PM and new tank together	same	different
Bad-quality TMP from the TMP mill and new tank together	same	different
All modifications together	different	different

Naturally, there were no differences when there were no modifications added to the verification model. As **Table 5** shows, on the average column none of the modifications alone made the optimization and models differ. In addition, combining any two modifications was not enough to drive the models apart but when all of the modifications were present, there was a significant difference. On the variational side, the situation was quite different as differences were seen quite often. The above results are believable since two of the three modifications were variational in nature, namely variable filler retention and bad-quality TMP. As process control typically is used to handle transient situations, i.e. variations, of the process, one can deduce that applying such model comparison would benefit optimization-based control design.

Thus, by utilizing the method the designer can i) gain understanding of how far the simple optimization model can be trusted and ii) focus possible future analyses on the most critical parts of the process. Thus, this approach contributes towards the main hypothesis of this thesis, as indicated in **Figure 11**.

4.2 Tower control case

In the Tower control case, the same stochastic-deterministic hybrid Matlab simulation model as in the Paper production case was utilized, but the focus now was on its tower level control law and its effect on the early phase, concurrent process and control design. Traditionally, the tower level control has been left to the plant operators, as fully automatizing it has proven to be difficult, which was already highlighted in the previous case's discussion of broke dosage, which involves multiple conflicting operational objectives (chapter3.3). Additionally, the large towers bring dominating dynamics to the system and can incur high investment costs. Thus, control of the tower levels should be considered early on when designing the process and finding the right focus (chapter 3.1), even with limited knowledge (see chapter 3.2), becomes important. In this case, the control law was formulated to mimic the actions of an operator of a paper mill in the form of lookup tables. The control law had seven manipulated variables and referring to **Figure 12** the control law contained the input-output matchings shown in **Table 6**.

Table 6 Control loops of the Tower control case.

Control loop	Measured variable(s)	Manipulated variable
1	Broke tower level, break state	Broke dosage
2	White water tower level	Disc filter input flow
3	Broke and dry broke tower levels, break state	Dry broke pulping rate
4	Broke tower level, break state	TMP/CP ratio at mixing the chest
5	Clean water tower level	Intake of fresh water to the clean water tower
6	TMP tower level	TMP flow to its tower
7	CP tower level	CP flow to its tower

Each manipulated variable, u_i, was calculated with

$$u_i(t) = \alpha\, c u_i^{nom} + (1-\alpha)\, u_i(t-\Delta t) \tag{8}$$

In equation (8), α is a filtering constant, while c's are coefficients obtained from look-up tables of the control law. In these tables the measured variables were divided into ranges, which were used to determine the value for the coefficient c for each manipulated variable u_i at any given tower level and break state. This could be exemplified for control loop 1 verbally as:

"if break is ON and broke tower level is between 75% and 100%, then coefficient c for broke dosage is 2".

In total, 36 parameters (p_i's) were used to define the ranges while the number of c-coefficients was 45. Thus, the structure, which is described in more detail in Publication II, was characterized by 81 parameters whose effects were initially analysed using the elementary effects method and finally with variance decomposition-based Sobol' sensitivity indices (Saltelli et al., 2008).

In the sensitivity analysis, operational and product quality points of view were taken into account when defining its four outputs (denoted by Y_j below). The operational aspects were characterised by the time until one of the towers experienced an undesirable under- or overflow situation, while the end product was characterised with deviations from desired strength, filler content and production rate, which are shown in italics in **Figure 16** below.

The hybrid nature of the model resulted in a large number of simulations. The initial analysis consisted of 1760 simulations and the actual Sobol' analysis of 2816 parameter samples, each sample being simulated with 100 replications to account for the stochastic parts of the model. The parameter sample generation and calculation of the sensitivity indices were conducted with Simlab software. The simulations were executed using parallelization on an eight-core calculation server.

Contributing results

In the Tower control case the goal was to demonstrate how combining dynamic simulation with global sensitivity analysis could be used to gain insight into preliminary phase process and especially control design. This was achieved with a case analysis of the control law of six connected storage tower levels of a paper mill. The analysis procedure was able to identify process areas whose control was important from operational and end product points of view. This identification is deduced from the sensitivity indices received by the different parameters: if one or more parameter located in a certain process area received a high index value, then this process area was deemed important. In the following **Figure 15** we show the results. Each of the four columns corresponds to one output variable:

Y_1: Time until first tower over- or underflow
Y_2 Time-average squared strength deviation
Y_3: Time-average squared filler content deviation
Y_4: Time-average squared gross production deviation

On the top row are shown the first-order indices (Equation (3)) and on the bottom the total indices of Equation (4). As can be seen, parameter c_{10} is by far the most important in six of the eight figures. For Y_2 the situation is less clear, with several parameters with relatively similar index values.

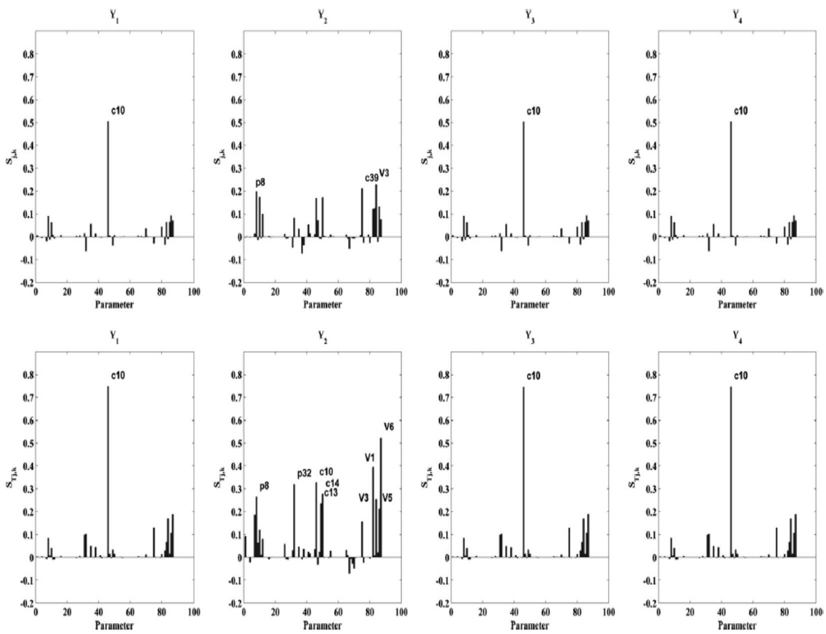

Figure 15 Sensitivity indices of the Tower control case (figure from Publication II).

As c_{10} relates to level control of the white water tower, a direct result is that this process area should receive the focus of the designer. Since this level is controlled by the flow to the disc filter and another parameter relating to it (p_8) is present, control of the disc filter seems to be of importance. Control of the broke and TMP towers were raised as the most important parts relating to the strength properties via parameters V_6 (clear water tower initial volume, providing dilution for TMP), V_1 (TMP tower initial volume), V_3 (broke tower initial volume) as well as p_{32} and c_{39} (related to inflow to TMP tower). These results, shown in red ovals in **Figure 16**, give the designer indications of where to focus additional design efforts. Thus, the Tower control case contributes to the main hypothesis of this thesis, as indicated in **Figure 11**.

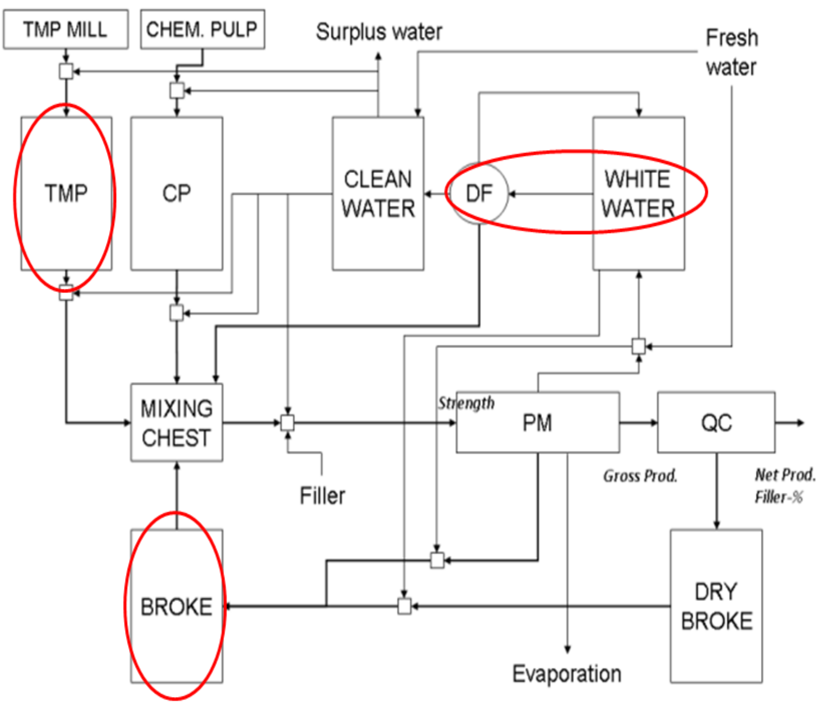

Figure 16 Process flow sheet of the two first cases. Red ovals indicate areas to focus on in the Tower control case.

4.3 Filtration case

The Filtration case dealt with operations planning of a two-stage filtration process shown in **Figure 17**.

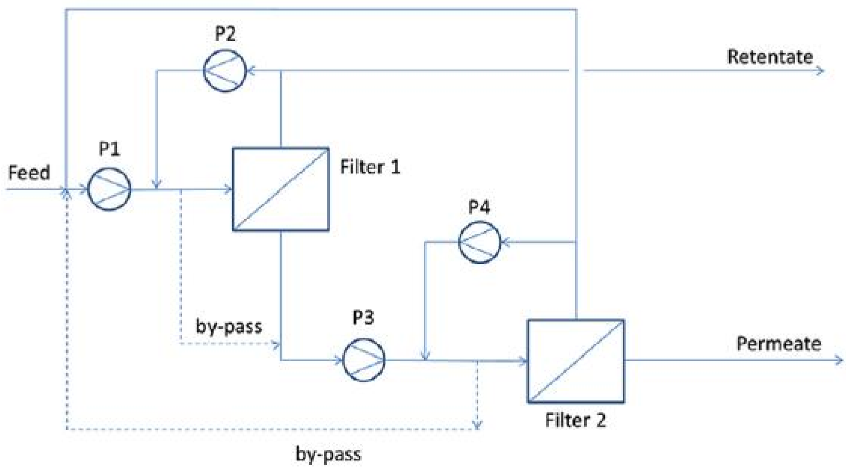

Figure 17 Flowsheet of the Filtration case process.

The process is used to filter impurities from the feed flow by two filters connected in series. The flows in the system are driven by four pumps, whose energy consumption should be kept to a minimum. Both filters produce two output streams, the permeate and the retentate. Of these, the retentate is the one into which the impurities should be concentrated while permeate is desired to be clean. As can be seen from **Figure 17**, both filters contain a local retentate recycle as well as an outer recycle to the feed of the process. The target here was to determine when each of the filters needs to be shut down for cleaning since the feed impurities tend to foul the filters. The fouling has the effect that it increases the flow resistance over the filter's membrane, between the feed and permeate streams. This in turn has the effect of either decreasing the permeate flux (flow per unit area of membrane) or increasing the required pumping power. In this case, fouling was modelled with a semi-empirical model, which increased the form loss coefficient, ξ, of the permeate flow line as a function of the accumulated amount of impurity on the membrane:

$$\xi(t) = a\int_0^t c_{feed}(t)dt \tag{9}$$

where c_{feed} is the impurity concentration of the inlet flow to the filter and the coefficient a is a tuning coefficient.

When a filter is washed, its associated loss coefficient is reset to zero and during this time, the filter cannot process any feed, which results in a lower amount of permeate. Furthermore, when filter 1 is being washed, the feed coming to it is directly by-passed to filter 2. In such times filter 2 receives dirtier-than-normal feed which results in dirtier permeate, an unwanted situation. This process is similar to the one studied in (Noronha et al., 2003), where the effect of varying filter-wise permeate recovery (flow rate of permeate divided by feed flow rate) was analysed with stationary models. They analysed energy consumption, permeate quality and permeate flow rate, but the analysis did not formulate the case as a mathematical optimization problem, nor did they utilize actual MOO solvers. Nonetheless, the authors note that even such a small process exhibits multiple optimization criteria and such interactions that simulation can make substantial contributions. In the case presented here, we continue their work by connecting the Apros® simulator with an interactive multiple objective optimization solver IND-NIMBUS (Miettinen, 2006) and formulating the case into an interactive MOO problem. Here the task was to derive an optimal washing schedule for the two filters as well as optimal rotation speeds for the four pumps over an eight-hour operating window using the following three objectives:

1. Maximize the permeate amount
2. Minimize the impurity amount in the permeate
3. Minimize the energy consumption of the pumps

This situation naturally lends itself to coupling of multiple objective optimization and dynamic process simulation to aid the process operations planning engineer who is faced with the challenge of multiple conflicting operational objectives (chapter 3.3). Furthermore, the case contained major modelling uncertainties in the form loss function presented above as well as in the cleaning efficiencies (or “impurity rejections”) of the filter, which were taken to be constant. Thus, the case also dealt with the challenge of limited knowledge (chapter 3.2).

The Apros-IND-NIMBUS combination, running on 3.4GHz Intel® Core™ i7-2600 computer, produced a set of candidate solutions, which were presented over e-mail to the decision-maker. He then analysed them and communicated his preferences for the direction in which the next optimization iteration should proceed.

Contributing results

In the Filtration case it was shown that a combination of interactive multiple objective optimization and dynamic simulation was able to provide insights in two aspects. Firstly, exploring trade-offs of conflicting operational requirements with the combination deepened the DM’s understanding of the problem at hand, as indicated in **Figure 11**. In the beginning of the interactive optimization the DM did not have clear preferences regarding which of the three objectives were the most important to him. While performing the optimization, the DM’s preferences became clearer and in looking back at the process it seems that the DM was mostly interested in improving two of the objectives (energy consumption and permeate cleanliness) while being willing to relax the remaining one (production amount of the permeate). This exploration of trade-offs is seen in **Figure 18**, which shows how the interactive optimization proceeded.

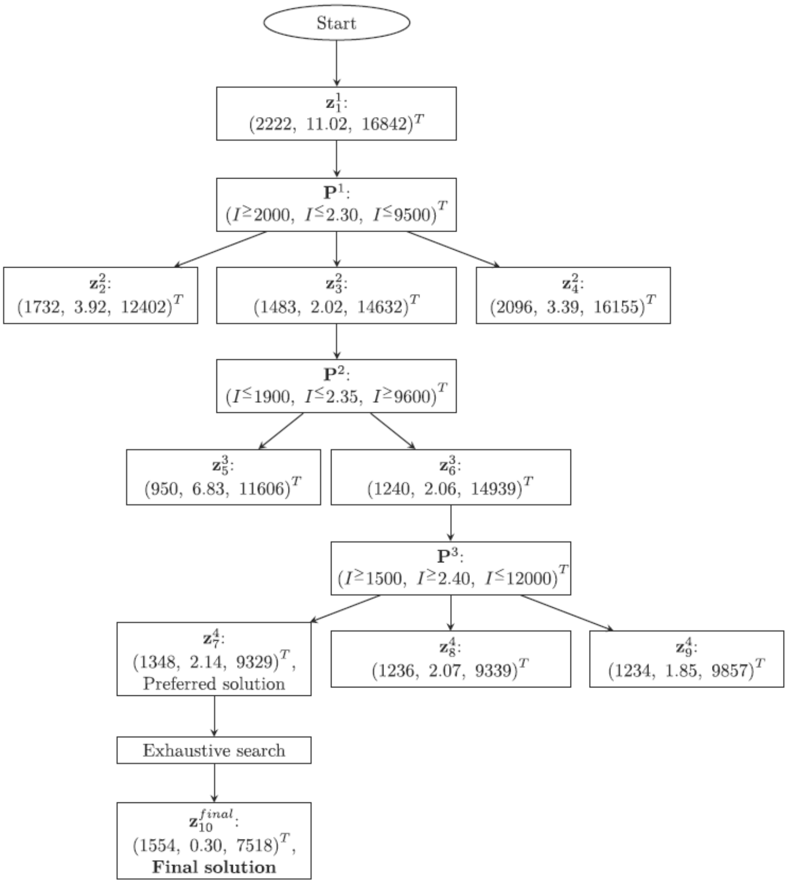

Figure 18 Solution procedure of the Filtration case (figure from Publication III).

In **Figure 18** the z's refer to Pareto optimal objective function values presented to the DM and P's are the DM's preference information which were passed to IND-NIMBUS. For example, P^1 is read so that objective function 1 could be impaired until 2000 while striving to improve objective 2 towards 2.3 and objective 3 towards 9500. The way the DM altered the preferences of improvement and impairment of objectives showed the learning process of the DM while working towards the final solution z_{10}^{final}. This is summarized in **Table 7**.

Table 7 Evolution of DM's preference in the Filtration case.

Iteration	**Objective 1**	**Objective 2**	**Objective 3**
P^1	allow to impair	improve	improve
P^2	improve	improve	allow to impair
P^3	allow to impair	allow to impair	improve

Secondly, it was shown that coupling of dynamic simulation with multiple objective optimization could be used in detecting modelling errors and thus in focusing the modeller's attention to critical parts of the process. This was exemplified by the frequent washing of the filters in z_{10}^{final} which indicated that the fouling model was in need of improvement. This in turn is an indication to the process and automation designers of a critical part of the process, i.e. how to handle or prevent filter fouling. Finally, some implementation-oriented issues on connecting a dynamic process simulator and an interactive MOO solver were detected. For example, the amount of pre- and post-processing code needed to make such an approach feasible is quite large. In pre-processing of the scheduling optimization, encoding of decision variables was seen to be a not straightforward task. On the post-processing side, processing of the simulation raw data into a form usable for the decision maker was seen to be in need of supporting tools such as advanced scripting languages.

4.4 Bottleneck case

Finally, the Bottleneck case relates to the operation phase and retrofit planning of a process industry plant. The challenge, which this case addressed, was finding the right focus (chapter 3.1), or in other words identifying which part of a process is its bottleneck from the production amount point of view. The simulator utilized here was Apros, which was coupled with global sensitivity analysis. To investigate how this coupling can be used as bottleneck identification, three different process models were used. The two first models, the so-called Simple Models in Publication IV, were test models to ascertain that a combination of dynamic simulation and global sensitivity analysis could be utilized as a method to detect process bottleneck. The models were formulated in such a way that the bottleneck could be determined solely with engineering expertise. These two models are shown schematically in **Figure 19**.

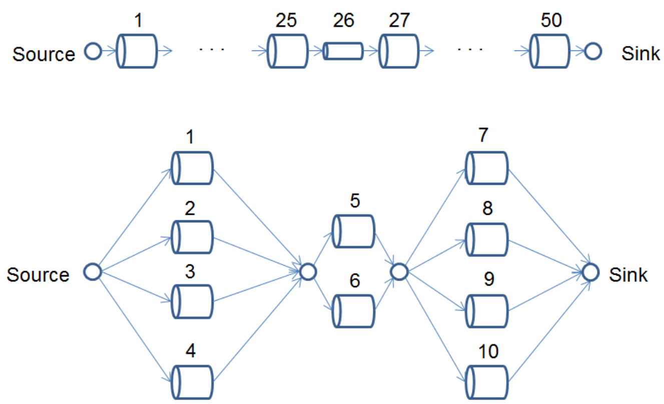

Figure 19 The Simple Models of the Bottleneck case.

On the top is shown a simple pipeline which is discretized lengthwise into 50 segments. Segment number 26 is much smaller than the others and is evidently the bottleneck with respect to mass flow through the pipe. On the bottom is a slightly more complex pipeline with 10 equal segments. In this flow setup, it is clear that the bottleneck is the middle part with segments 5 and 6. These Simple Models were subjected to a Sobol' global sensitivity analysis with the segment dimensions as the inputs and the flowrates through the systems as outputs. In the analysis of the first model 52224 simulations were conducted and with the second model 45056. All the simulations were executed on a dedicated computational server with eight parallel Apros simulators.

Finally, in the Bottleneck case a third, more realistic model of a paper mill's short circulation was utilized. This is shown in **Figure 20**. In the process, a feed stream is pumped from the machine chest (a tank with constant liquid level) through consecutive cleaning equipment to the paper machine's headbox. The cleaning consists of two screens, called the pressure and machine screens as well as a deculator tank. This tank is kept in low pressure which causes any air in the feed stream to boil and thus be removed. At the headbox, the one-dimensional pipe flow is spread on to the paper machine's former section. Here water is removed either with gravitation or with under-pressure suction and recirculated into the wire pit. This wire pit water is used to dilute the feed stream also. After the former section, the moist paper is subjected to mechanical pressing to remove even more water from it. Once mechanical separation cannot remove any more water, the paper is brought into contact with steam-heated metal cylinders of the drying section to reach the final moisture content. Typically, the flow into the head box contains 99.5% of water while the paper produced to the reel contains approximately 7%. This means that a considerable amount of water is being circulated in this area and investments in de-bottlenecking should be carefully planned. Thus, it can be argued that correct identification of the production bottleneck is of significance.

This model was also subjected to a global sensitivity analysis with the production amount, in tons per hour, at the reel as the interesting output. The analysis was on 25 input parameters describing the dimensioning of the short circulation equipment and summarised in **Table 8**.

Table 8 Input parameters of the paper mill short circulation model of the Bottleneck case.

i	Process part	Parameter	Nominal value	Min	Max
1	Pressure screen feed pump	Nominal head, m	20	15	25
2	Pressure screen feed pump	Nominal volumetric flow, m^3/s	1.5	1.125	1.875
3	Headbox feed pump	Nominal head, m	30	22.5	37.5
4	Headbox feed pump	Nominal volumetric flow, m^3/s	1.5	1.125	1.875
5	Furnish feed line	Diameter, mm	250	187.5	312.5
6	Pressure screen feed line	Diameter, mm	1000	750	1250
7	Pressure screen accept line	Diameter, mm	1000	750	1250

8	Machine screen feed line	Diameter, mm	1000	750	1250
9	Headbox feed line	Diameter, mm	1200	900	1500
10	Wire water channel	Diameter, mm	1000	750	1250
11	Deculator overflow line	Diameter, mm	500	375	625
12	Wire pit dilution line	Diameter, mm	500	375	625
13	Paper machine	Width, mm	8000	6000	10000
14	Paper machine	Speed, m/s	16	12	20
15	Former	Chemical pulp retention	0.85	0.6375	1.0
16	Former	Thermomechanical pulp retention	0.85	0.6375	1.0
17	Former	Filler retention	0.5	0.375	0.625
18	Former	Dewatering coefficient	0.02	0.015	0.025
19	Wet press	Nip 1 load, kN/m	30	22.5	37.5
20	Wet press	Nip 2 load, kN/m	30	22.5	37.5
21	Wet press	Nip 3 load, kN/m	30	22.5	37.5
22	Pressure screen reject line	Diameter, mm	100	75	125
23	Machine screen reject line	Diameter, mm	100	75	125
24	MC outlet pump	Nominal head, m	30	22.5	37.5
25	MC outlet pump	Nominal volumetric flow, m^3/s	0.3	0.225	0.375

A sample of 53248 input realizations was simulated with the model on eight parallel instances of Apros simulator. With all three models, the input samples were generated and the outputs analysed with Simlab software.

Contributing results

The result of this case was that a combination of dynamic process simulation with global sensitivity analysis could be used as a method of detecting bottlenecks of a process. The case utilized three models, which showed that process parts/equipment forming the process bottleneck could be identified with an appropriately formulated sensitivity analysis study. In the paper mill short circulation model, the analysis raised three parameters above the rest: X_{17}, X_{24} and X_{25}. Their locations in the process flow sheet are highlighted in **Figure 20**.

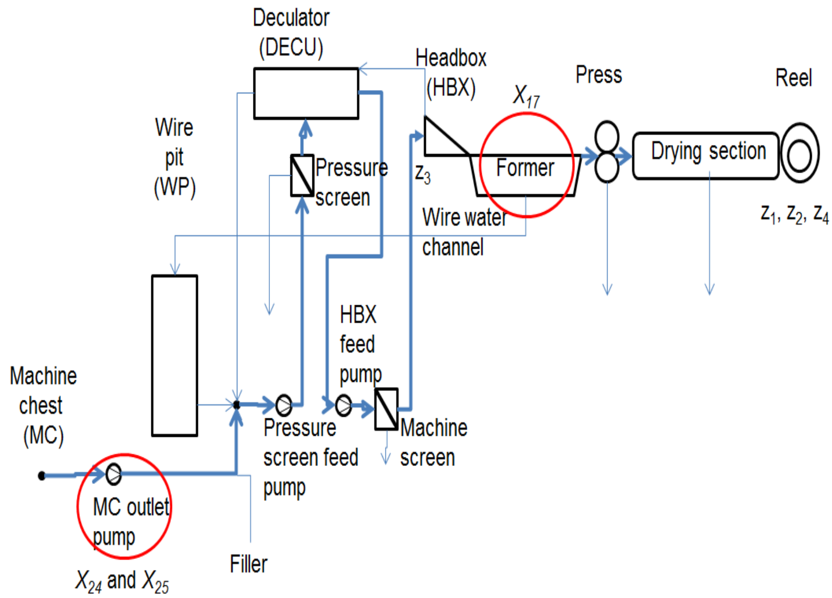

Figure 20 Paper making process with bottlenecks highlighted in red.

Two of these parameters were related to one piece of equipment, the machine chest outlet pump, giving a strong indication that this was where the bottleneck was located. Since this pump feeds raw material to the system, it is easy to agree that it is a bottleneck. This is also the situation with the third parameter, filler retention on the paper machine former section. Filler is one of the major raw material components of the end product and a parameter describing how well it is retained in the paper coming up in the analysis is clearly understandable. The effect of these parameters was finally validated with separate simulations. The end result was that this type of study would typically fit well when planning retrofits for a process industry plant under operation. A contribution to the main result of the thesis comes clearly from drawing the engineer's attention to critical parts of the process.

4.5 Summary of results

As stated in chapter 3, the research questions were: "How can coupling of process simulation and other mathematical methods be

1. used as a tool to focus the designer's attention to the most critical parts of the process even with limited knowledge?
2. used to provide insight into an operational plant's personnel?"

To answer these questions four specific goals were set. Their relation to the research questions as well as results are summarised in **Table 9**.

Table 9 Summary of case results and how they contribute to the research questions.

Research question	Specific goal	Result
1 and 2	To develop and investigate the functionality of a model comparison method as well as determine its potential in early-phase process and operational optimization.	The method was developed and utilized in analysis of a paper production process optimization problem (the Paper production case). The method was able to provide guidance for the analyst in the applicability of the process optimization results. As the optimization dealt with design and operation of a paper production process, the result pertains to both research questions.
1	To combine global sensitivity analysis with process simulation and investigate its usefulness in preliminary process and automation design.	In the Tower control case, combination of process simulation with global sensitivity analysis was able to highlight areas of the process to which the analyst should concentrate his/her efforts. Thus, the results answers research question 1.
2	To provide information on the potential of combining dynamic process simulation and interactive multiple objective optimization in design of operational practices.	The combination was realised and tested in the Filtration case. The results showed feasibility of the combination and provided insights to the decision maker on the process' operational characteristics, thus pertaining to question 2.
1 and 2	To investigate the combination of global sensitivity analysis with dynamic process simulation as a method of identifying process bottlenecks.	Applicability of global sensitivity analysis as a bottleneck identification method was shown in the Bottleneck case. As the task of debottlenecking is a design task, the result answers question 1, but also since this task is performed on a running plant, it also can be seen to contribute to question 2.

Combining the contributing results from the cases now gives support to the main hypothesis of this work: extending dynamic simulation with other mathematical methods can bring extended added value to a process or control designer.

5. Discussion

5.1 Practical implications

This thesis aimed to bring added value by alleviating certain challenges of a process/automation designer or an engineer dealing with a running process. The results presented above in chapter 4 show that combining dynamic simulation with other mathematical methods can be used in finding the right focus, alleviating limited knowledge and help dealing with multiple conflicting objectives. In doing so, the approach entails certain practical implications.

The first implication is related to the tools used since, obviously, the approach requires the user to master the tools, at least to some extent. The user may not have to be able to understand all the detailed mathematics of the tools but what is important is to understand the limitations of the tools. For example, the simulation models always are simplifications of the real world, the global sensitivity analysis depends heavily on the choice of its input parameters and their distributions and optimization results reflect the formulation of the problem. In addition, such tools typically also have their own, specific quirks and oddities, which may require quite a bit of detailed knowledge to overcome when implementing such combinations as presented here. Making existing tools more amenable to such co-use seems to be an active research topic, which is promising. Software tools integration approaches such as FMI (https://www.fmi-standard.org/) and Simantics (https://www.simantics.org/) in the field of co-simulation, the work on simulation-based optimization (Yang et al., 2014) and model-independent global sensitivity (Saltelli et al., 2008) are examples. Related to the tools, is also the execution of the massive number of simulations needed. This requires computing power and suitable ICT solutions to be cost-effective. Execution on dedicated high-performance computational clusters is one possibility. Second, perhaps an even more enticing option is the utilization of cloud computing which provides flexibility on the needed computing power. Furthermore, such technologies as Docker (Docker, 2018) pave way to its use in the presented approach.

The second implication relates to the scope of the analysis. Defining a large scope for the analysis may be able to include, in theory, all relevant aspects but becomes easily practically impossible to handle as it leads to computationally heavy situations. While computing power is nowadays readily and cheaply available, this issues should not be forgotten. For example, when conducting sensitivity analyses the computing power requirement may grow exponentially as a function of the number of parameters. On the other hand, a too-narrow scope leads to results that are not useful or could have been obtained otherwise. After the computations, all the results need interpretation and should be looked into with a critical eye and evaluated for practical significance.

Thirdly, application of the approach may even require a larger revamp of the design work practices. It may be that new roles, specializing in utilization of such tools, will emerge in the design companies. It has even been suggested that new organizations may emerge due to the new approaches and tools. For example, in (Ritala, 2013) a new element called "optimization and modelling organization" has been introduced to existing engineering organizations. Rise of such new roles and organizations will probably be a gradual, even slow, change since, as Moran has noted, the academic and practical chemical engineering/plant design have drifted quite far apart and the current, sophisticated methods developed in academia are not much used in practice (Moran, 2015). Thus, it seems that there remains a considerable amount of practically oriented work to be done here.

As briefly mentioned in chapter 1.3 the line between R&D and design is sometimes quite blurred. This is the case of course in situations where a new type of equipment or process concept is built the first time. It seems that the approach presented here could be especially suitable in such cases rather than in cases where the design work is mainly minor adjustments to tried-and-true process concepts. Now, coming back to **Figure 5**, it could be argued that the detail design phase may not benefit as much from the presented approach. This is because this phase typically tends to involve routine design tasks since the broad process concept is already fixed. This does not mean that the detailed design phase could not benefit from other advanced methods though. For example, optimization can be used to design the detailed routing of pipelines within the constrained physical area of the site or dynamic simulation is used to test the automation solution prior to commissioning.

In summary, to be useful this approach seems to require development of certain expertise in the tools and in defining the scope. How this expertise is obtained is not analysed in this thesis in detail but it seems that it is no different from other types of expert knowledge/ability. Thus, it seems conceivable that approaches to expertise development could be applicable and indeed needed here.

5.2 Validity of the research

Validity of research typically refers to two things: internal and external validity. The internal validity of research measures whether the used data, methods and results justify the claims. External validity on the other hand deals with the extent to which results can be generalized.

5.2.1 Internal validity

Validity of the research process

The object of this research is designing processes, their automation and operations, which is a practical thing and as such the motivation for the research has been derived from the practice. This practical starting point has affected the choice of how the research work was organised. As presented in chapter 1.2, the research of this thesis follows the DSR approach. It was chosen as the methodology since while it strives to uncover scientific knowledge, it also is closely tied to solving practical problems and providing utility via research. More specifically, the present work is based on the application of DSR on information technology systems (March and Smith, 1995). This is well suited for this thesis because of its quite practical aims and the computational approach used. Thus, the choice of research methodology favours the internal validity of the research.

Validity of the results
The main claim of this thesis is that coupling dynamic simulation with chosen mathematical methods can act as a tool to focus process designer's attention and to provide insight into operational personnel of the plant and thus bring added value (or in other words utility). To investigate this claim, data was gathered from four case-based, computational studies. Justification of the case-based approach was given in chapter 1.2 on methodology. The tools and computer simulation models used will be analysed in the next chapter. From the case results, support for the main hypothesis, as summarised in chapter 3.4, was derived and argumentation for generalizability of the results will be given in a later chapter. Putting these together finally gives support to the validity of the results.

5.2.2 External validity

Validity of the chosen computational tools and models
Parker has argued that validity of computer simulations' results deals mainly with external validity – their being indicative of what is true of the target system (Parker, 2008b). The obvious and best way of ensuring validity of the computer simulations' results is to compare them with measurements from a corresponding real-life process. Since a direct comparison of simulation results and measurement data is not always possible, Parker further analysed how the strategies employed by experimentalists to build confidence in their results could be employed in the domain of computer simulation. Here a distinction was made between model evaluation and code evaluation. The former, sometimes called model validation, is concerned with how well the model describes the phenomenon under study. The latter, sometimes called model verification, deals with quality of code implementation to solve the model equations, regardless of whether they actually describe the phenomenon. In order not to use the term validity in different meanings here, we shall utilize the term model evaluation henceforth.

Approach to tool evaluation
Next, each tool and simulation model is evaluated in more detail. This is done following the approach of Parker (2008b) who points out that a so-called

Sherlock Holmes strategy may be employed. Basically, it says: “Show that plausible sources of significant error can be ruled out”. It has the following conditions of successful application:

1. Make a thorough and good-faith attempt to **identify** all plausible sources of error and alternative explanations of the results.
2. Do not make the situation such that there is little clue how to answer the questions raised previously.
3. Make a thorough and good-faith attempt to uncover any indications that the simulation **did go wrong** in the ways identified above.

To argue the validity of the tools we next employ the Sherlock Holmes strategy in code evaluation, i.e., tools used here and in model evaluation, i.e., the simulation models used here.

Code evaluation

In code evaluation, the most obvious source of errors is programming mistakes and it pertains to all of the used tools. This can cause instability of the programs, spurious and/or non-physical simulation outputs, or otherwise clearly wrong results. Regarding Apros, the utilized unit operations models and solvers are well tested, some having over 30 years of development and successful utilization. This is done with a set of 24 validation simulations that are run before every new software version release. In addition, several other less-formal test are conducted. Similarly, the other tools (Matlab, Simlab and IND-NIMBUS) are results of a long period of development and have been quite extensively utilized. Thus, we may argue that programming mistakes are probably not problematic here. A more detailed source of code error is possible numerical instability of the simulators’ time integrations scheme. This would lead to non-physical (unstable) or oscillatory behaviour of model states and outputs, error messages and even halting of simulations. In Apros, a variable-step time integration scheme was applied to alleviate this error source, although it did not eliminate the problem entirely. In fact, some simulations did halt. This small set was removed from the data set. Similar problems may occur due to erroneous spatial discretization of the model. In this case, no such problems were encountered once the models had been iteratively built and tested. A final common possible source of error for all of the tools is a hardware malfunction. One detectable indication of this is the complete crashing of the simulator tool. In fact, in simulations of Publication I, this error source occurred in the form of a forced operating system update, which terminated all simulations. After this, the simulations were restarted with saving of intermediate results enabled so that the effect of possible future occurrences of this error source were removed.

Model evaluation

Next, we turn to evaluating the simulation models utilized in the case studies. This is done in **Table 10** for all of the models presented in chapter 4.

Table 10 Model evaluation

Model	Identified error sources	Indications that something went wrong during the simulation	Answer
Optimization model Publication I	Model equations inadequate for their purpose	Mass flows, liquid levels, concentrations either un-physical or not realistic.	The optimization model equations describe conservation of mass and are thus constructed using well-confirmed theoretical assumptions. Model was equipped with checks (e.g. mass balance checks). No un-physical or not realistic results were seen. It should be noted that the strength and web break probability models were not based entirely on a well-confirmed theoretical background. Clearly, this is a limitation but since they were constructed by subject matter experts utilizing plausible assumptions, the project team deemed the models adequate for their purpose.
	Parameter values tower sizes retentions (wire and disc filter) break and strength model parameters	Erroneous tower sizes may lead to faster dynamics than expected. Errors in retention parameters would show as unrealistic concentrations around the process. Erroneous break and strength model parameters would	Tower sizes were determined by a higher-level optimization, which had realistic bounds for them. Retention parameters were assigned values based on expert knowledge of the domain. Break and strength model parameters were the most uncertain. Their values were determined by qualitative expert judgement. Further discussion is given in Publication I.

		show as unrealistically long and frequent web breaks.	
	Initial conditions	Transients at the beginning of simulation, affecting the whole simulation.	Initial condition in all simulations was a steady state. This state was defined with domain expertise.
	Boundary conditions	Unrealistic or even non-physical evolution of model state.	Boundary conditions of the model were determined with domain experts to be representative of the process under study.
Verification model Publication I	Model equations inadequate for their purpose	Model state variables behave in unrealistic way. Numerical problems (error messages).	Underlying equations for conservation of mass and energy are based on solid physical background and have been utilized successfully in prior simulations in the same domain (papermaking).
	Parameter values especially filler retention model parameters	Numerical difficulties. Unrealistic simulation results. Unrealistic filler concentration around the process	At the time of model construction, numerical difficulties were corrected. Simulation model was tested during construction by running it in steady state and in transients. Filler retention model parameters were tuned to be realistic with expert judgement. All parameters were subjected perturbations in model construction and simulation results changed as expected.
	Initial conditions	Unrealistic transients at the beginning of simulation.	Same initial condition as in Optimization model, Publication I was used.

	Boundary conditions especially introduction of "bad TMP"	Unrealistic or even non-physical evolution of model state. Numerical difficulties.	Same boundary condition as in Optimization model, Publication I was used. Introduction of the concept and modelling of "bad TMP" was based on practical experiences of project partners.
Paper mill model Publication II	This model was the same as the Optimization model, Publication I. Thus, the same arguments as above apply.		
Control law Publication II	Pairing of controlled and manipulated variables	Controlled variables do not stay under control. Model state is not stable.	Pairing was designed to resemble the logic that operators of a real mill use to keep the controlled variables under control.
	Choice of control law parameters		The nominal values of the control law parameters were chosen with expert judgement. Publication explicitly conducted a sensitivity analysis of the control law parameters.
Two-stage separation model	Model equations inadequate for their purpose pressures and flows	Pressures and flows in the process are driven into unrealistic values.	Equations describing the pressure and flow evolution are based on solid physical background and have been utilized successfully in numerous cases before.

Publication III	membrane fouling model structure		Membrane fouling model was constructed with engineering expertise. It was noticed that the results heavily depend on this fouling model, and further work on it was implied.
	Model parameters sizing of pipelines and devices fouling model	Numerical difficulties. Unrealistic simulation results, e.g. flow velocities and pressures	Flow lines were sized so that realistic flow and pressures resulted. Fouling model parameters were determined to give realistic behaviour. During the simulation study, this model was noticed to be critical to the behaviour. Parameters were subjected to perturbations in model construction and simulation results changed as expected.
	Initial and boundary conditions	Unrealistic transients at the beginning of simulation. Unrealistic or even non-physical evolution of model state. Numerical difficulties.	Both initial and boundary condition were determined to have realistic values based on expertise of the modeller. Initial condition was subjected to perturbations in model construction and simulation results changed as expected.
Paper mill model Publication IV	Model equations	Model state variables behave in unrealistic way. Numerical problems (error messages).	Underlying equations for conservation of mass and energy are based on solid physical background and have been utilized successfully in prior simulations in the same domain (papermaking).
	Model parameters	Numerical difficulties. Unrealistic simulation results, e.g.	Model was parametrized by a subject matter expert to resemble a real paper mill process. In doing this, model parameters were subjected to perturbations in model construction and simulation results changed as expected. A set of 25 model parameters were chosen for sensitivity analysis.

	concentration, flow velocities and pressures	
Initial and boundary conditions	Unrealistic transients at the beginning of simulation. Unrealistic or even non-physical evolution of model state. Numerical difficulties.	Initial and boundary conditions were set to values representing a realistic paper mill.

Although it would be beneficial to give quantitative numerical evidence to support the model evaluation, it has been noted that also qualitative analysis is helpful (Parker, 2008a). Overall, the above analyses give support to the validity of the selected tools and models.

Generalizability

External validity of research is defined as the extent to which the results of a study can be generalized to other situations and to other people. We argue that the main result obtained from the case studies can be, in fact extended beyond the cases. Furthermore, we try to characterize such new cases.

The argumentation is that

1. The models and tools were appropriate for the task at hand (see previous chapter) and the tools are in fact applicable elsewhere also.
2. The cases represent realistic and not uncommon process industry situations.
3. The analyses were able to bring forth insights, which bring added value to a designer.

Thus, it stands to reason that applying such approach to other cases originating from the process industry while utilizing models with similar foundations, can provide extended added value. While this is not a fully inductive generalization of the results, it is in line with abductive reasoning (see for example Paavola, 2006). Abductive reasoning, originally proposed by Peirce in the early 1900s, is the third mode of scientific reasoning, in addition to induction and deduction. Abductive reasoning seeks for the simplest, most likely explanation (out of many possible ones) that accounts for the facts. It suggests that something may be true, but does not guarantee the conclusion, i.e. it closely resembles Occam's Razor where the simplest explanation is likely to be the correct one.

The abductive research process has been visualized by Kovács and Spens as an iterative loop, whereas inductive and deductive approaches are more linear. By this is meant that deduction starts from the theory and moves then towards empirical, while induction moves in the other direction. Abduction also has empirical observations as its starting point, but not solely them because it utilizes prior theoretical knowledge as a source inspiration and ideas. It incorporates the idea of a "guiding principle", which may be only an intuitive thought or even a well-formulated hypothesis. It is used to focus the empirical work on areas which are believed to bring new insights and ideas for theory development (Anttila, 2000). The following figure, which is adapted from (Kovács and Spens, 2005), depicts this.

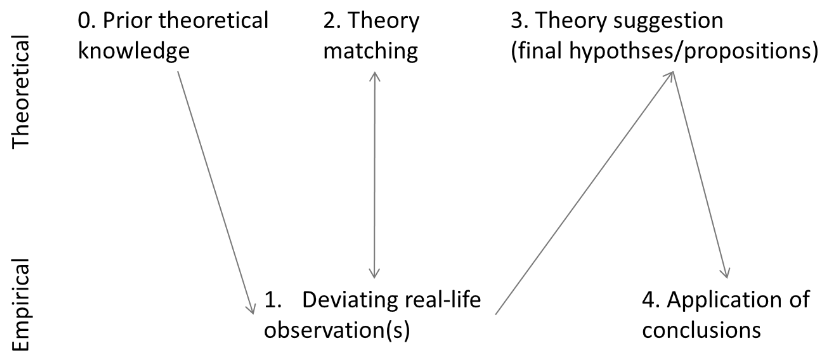

Figure 21 Abductive research process (Kovács and Spens, 2005)

To apply abductive reasoning here, we start with the prior that dynamic process simulation and methods such as optimization have been utilized in the process design field for a long time, as summarised in chapter 2. The real-life observation of step 1 was, that while dynamic process simulation is widely used, it "could be still put into better use". By this we mean that it was observed that many times extensive process models are constructed, simulated only a few times and then forgotten. Firstly, this seemed to be, on one hand, in conflict or at least not in line, with the lofty goals presented in the literature (see chapter 2). Secondly, this seemed like a terrible waste, in the sense that such models have required considerable expert effort. Furthermore, during several years such challenges as referred to in chapter 3 were starting to be seen. This led to the idea, that combining dynamic process simulation with other mathematical methods could be useful, especially over the life cycle of a process industry plant. This idea was iteratively tested and refined (step 2) in the case studies presented in chapter 3. Typically, case studies have been presented as linear processes following the standard research process of a number of planned subsequent phases. Dubois and Gadde point out that such approach is ill-suited for case research (Dubois and Gadde, 2002), since the researcher typically goes "back and forth" between different research activities and between empirical and theoretical work. In other words, practical cases bring new viewpoints, which then serve to re-orient the research and bring up new research questions. This was the situation also in this study. Inside each case study, a "lower-level" iterative approach was taken in definition of the simulation problem, the utilized methods and conduction of the computations. Step 3 of **Figure 21** is this thesis, where we propose that combining process simulation with other mathematical methods can be used to gain insights that help in overcoming practical challenges. Finally, the thesis work also started step 4 in the form of application of the combinations in cases not included in this thesis.

5.3 Limitations and future work

The presented work, like nearly all research, has its limitations and raises further issues to be tackled.

This thesis is **case-based** research and thus entails the limitations of all case research. The main question naturally is the generalizability of the results. In the previous chapter, I have attempted to alleviate concerns of this nature. Naturally, the final judgement on generalizability would come from further use of the approach, especially when used in real design work rather than academic research. To identify new cases in which the presented approach could be applied, we characterize the currently presented ones. Firstly, all the cases pertained to the process industry and more specifically continuous processes (as opposed to batch processes). This probably is not a rigid requirement and application to e.g. discrete manufacturing processes seems feasible: only the simulation models need to be changed. Thus, a natural avenue of future work would be to apply the approach to other domains as well. Secondly, in the cases there was present a lack of full input data, i.e. the models contained uncertainties. The status of this characterization is somewhat difficult. On one hand, if the problem at hand contains severe uncertainties, construction of the models may be impossible which prohibits entirely the application of the approach. On the other hand, if no uncertainties are present one may question whether such analyses are needed at all. Thus, it seems that in a process industry plant's life cycle, especially early phases are appropriate for the presented approaches. A third way to characterize potential cases of application is complexity. The studied cases were quite complex in the sense that they contained numerous parameters, inputs, state variables with several interactions, non-linearities and dynamics. This characterization seems quite rigid because if the processes were very simple, then many of the insights could most likely be obtained without resorting to computational methods. In relation to the second characterization, it should be noted that even with no uncertainties present, the complexity of the process alone can warrant the use of the approach. Thus, while being an interesting ingredient, uncertainties are not a requirement. With the above characterizations, we hope to help in guiding the future work.

The next avenue of future work is the **up-take** of the approaches presented above. At the very core, the presented approach relies on coupling computational tools, which presents a practical task of tools development. Firstly, the ease of use for the analyst is a requirement to reduce the time to perform the analyses. All of the cases presented in this thesis were implemented as a mixture of commercial tools and self-made pieces of code. A more systematic and user-friendly implementation would be beneficial in reducing manual work. In a similar vein, the computational speed is an issue that should be addressed. Naturally, new and more powerful hardware as well as readily available cloud computing resources alleviate this issue, but developments on the method or software side are probably also needed. Regarding the simulation tools, also comprehensiveness of the model libraries may require future work. It is desirable that the modelling tools chosen should already at the beginning of the analysis contain all or most of the needed unit operation models as otherwise time-consuming model development may prevent application of the presented approaches. Still, as no simulator is an all-encompassing package, it is also desirable for them to be adaptable, i.e. to provide the analyst a possibility to “tweak” them, both in fine-tuning of the models as well as in connecting the simulator to other tools. Furthermore, the time consumed in constructing the needed simulation models for each new case should be minimized. As it seems that the presented methods are most applicable in cases where an entirely new process is being designed, the rather straightforward idea of a large library of (sub-)process models from previous projects might not be feasible. Still, even the very early stages of the design nowadays produce plans, designs, etc., in a digital format which could be used, to some extent, in automatic generation of the simulation models. This would naturally entail appropriate transformations from the design software (e.g. COMOS and SmartPlant) to the simulation tool. Furthermore, advances in the field of automated process design (e.g. generative design) may prove useful.

The uptake of such approach, as well as other similar PSE methods, may lead to major changes in the way that **design work** is done, as was referred to in chapter 5.1. This change is especially interesting since the presented approach, while heavily computational in nature, does not exclude the role of the analyst’s expertise. In fact, it seems that the need for domain-specific expertise can become even more pronounced. This is because formulation of the problem at hand, as well as interpretation of the results, needs a person with adequate expertise. Thus, a future avenue for research would be to conduct studies on how practical design engineers would apply the presented approaches, thus putting more emphasis on the observation step of the action research cycle.

In this thesis, a selected set of mathematical methods were coupled with dynamic process simulation. This leads to two issues. First, the methods presented here are by no means complete, but rather an active research field. Thus, new developments in areas like global sensitivity analysis should be looked into. In addition, the natural question is whether other mathematical method integrations would be beneficial and how? For example, currently it seems that there is substantial hype around machine learning and big data methods. These both seem very interesting and their coupling could be a way forward.

6. Conclusion

This thesis presented research into extending the use of dynamic process simulation in order to gain added value, or in the terminology of DSR, utility to a process or control designer. The starting points for the work were certain challenges faced by a design engineer. First of the challenges was related to finding the right focus with limited resources. Secondly, doing design with limited knowledge. Finally, when planning the operation of the process, the designer faces often-conflicting objectives that need to be balanced and he/she needs to gain further insights into the process and its operation. The overriding theme was that the computational approach of combining dynamic simulation in the abovementioned other methods, help to alleviate these challenges.

In a bigger picture, the current trend of digitalization of the entire society, including the process industry, is progressing fast. This both enables and calls for this work. Clearly, the enabling aspect comes from the fact that this work relies on simulation models and is computational in nature. A key development here is abundant computing power. Traditionally, the power would be obtained from a dedicated high-performance computing cluster, but the trends are turning towards cloud computing. Azure, AWS and Google Cloud Platform are well-known examples. On the simulation side, the emerging trend is digital twins, digital representation of physical assets, which can incorporate simulation models. Conversely, these developments call for these kinds of approaches. In the current hype around digitalization, it seems that data is seen as a value of its own, but one could argue that only once something clever is done with, do we see added value. This thesis strives to help. It deals with one slice of this issue, by showing how simulator-generated data can bring utility.

The work was in four case studies. In them, dynamic process simulations were combined with a novel model comparison method, with global sensitivity analysis and with multiple objective optimization. The work involved construction of simulator models using various available tools, for example Apros® and Matlab™. An extensive search for mathematical methods was conducted. As mentioned previously, the ones presented here are only examples of such and it seems that much more could be done here in the future. A massive number of simulations were performed. The data generated in this way was then analysed, using process engineering know-how, conclusions were drawn and argumentation given to support the main result.

The cases were constructed in such a way that they pertain to a certain phase of a process industry plant's life cycle. This was done to highlight the approach's wider applicability and generalizability. Two cases were targeted to the early phases of the lifecycle. The first of them, Paper production, looked into gaining insight and confidence in the results of an optimal process design by utilizing more detailed dynamic models and the developed model comparison method. Details are in Publication I. The second case, Tower controls, then combined dynamic simulation with global sensitivity analysis, in order to focus the attention of a control designer to critical parts of the process and its control structure. The control structure was characterized with tens of parameters, which were the subject of the sensitivity analysis. A small subset arose as critical. Analysing the set of critical parameters focused attention towards certain process areas. The two latter cases were related to the operation phase of the plant. The Filtration case combined a dynamic process simulator and a multiple objective optimizer. This was done in order to derive an optimal running schedule. The process contained two filters, prone to fouling and a pumping system driving the filters. Interactive optimization was applied. The manner in which the optimization was conducted helped in gaining insight into the process' operation. Finally, the Bottleneck case combined dynamic process simulation again with global sensitivity analysis. This time bottlenecks were searched for. This separates the case from the Tower controls case as the control structure was not analysed. All the cases were computational studies, typically involving thousands of simulations and conducted with dedicated computational servers. Quite much work was involved in the technical setup of the simulations.

The main result, or claim, of this work was that added value or utility, beyond the traditional simulation results, could be extracted from simulation models when they are combined with other mathematical methods. This was supported by the case studies. The Paper production case showed that the proposed model comparison method works. This leads to the conclusion that it can be of help in gaining confidence in optimization results from simplified models, focusing the designer's attention as well as providing insights into the operation of the plant. In the Tower control case, the combination was able to highlight process areas where the control designer's attention should be focused. This was similar to the Bottleneck case. The Filtration case showed the feasibility of the combination as well as the ability of providing insight into the process operation. Combining these contributing results then gives support to the main result of this thesis.

The design of processes and their automation faces ever-growing demand for cost-effectiveness leading to challenges to the engineer over many phases of a process industry plant's life cycle. This thesis showed that extending dynamic simulation, as presented, seems promising in alleviating these challenges and thus adding value to the process or automation designers' work. The work presented is a starting point for new avenues of investigation and hopefully practical implementations.

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The process industry in Europe covers thousands of individual enterprises with millions of employees. This industry has a need for improved efficiency and competitiveness, which affects not only the company but also its subcontractors, for example process and automation designers. Their whose responsibilities often lie in the early phases of the plant's life cycle, leading to challenges such as limited available information and multiple objetives to fill. This work investigates how those challenges could be alleviated by extended use of dynamic process simulation via four case studies. Dynamic process simulation is extended by combining it with a novel model comparison method for optimization, with global sensitivity analysis and with multiple objective optimization.
Synthesizing the case studies' results, the thesis arrives to its main conclusion: Added value for the designer can be extracted from simulation models when they are combined with other mathematical methods.

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