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Design Optimization of Highly Uncertain Processes: Applications to Papermaking System

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Design Optimization of Highly Uncertain Processes: Applications to Papermaking System

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Abstract

In process design, the goal is to find a process structure that satisfies the desired targets and constraints. A typical task involves decision making related to the process flowsheet and equipment. This dissertation examines design optimization of papermaking process. The main emphasis is on the development of an optimal design procedure for highly uncertain processes with non-Gaussian uncertainties. The design problem is studied as a multiobjective task in which the most effective process structure is sought by maximizing the process long-term performance and minimizing the investment cost. As the assessment of the long-term performance requires that the process be operated optimally, the optimization of the process operation is studied as a subtask of the design problem.

Paper manufacturing is a complex process in which paper is produced from wood, water, and chemicals. The task is to manufacture uniform quality paper while minimizing the costs. If the paper web breaks, all the production is discarded. The unpredictable web breaks strongly disturb the paper production. As a result, the process has two separate operating points: normal operation and operation during web breaks. That poses challenges to the process operation as the transition between the operating points is somewhat random and the future evolution of the process is not completely predictable.

In model-based process optimization, the uncertainty related to the models affects the reliability of the results. The modelling uncertainty is associated with both the incomplete understanding of the process and the approximation due to computational reasons. In papermaking, the unpredictable web breaks are the largest source of uncertainty, but incomplete understanding is also related to e.g. the quality models of the paper. Besides modelling uncertainty, also the uncertainty about the available information, i.e. the measurement accuracy, affects the reliability of the optimization. In this thesis, scheduling of the measurement resources is studied as a part of the process optimization.

This dissertation proposes a procedure to systematically optimize the design and operation of a papermaking process. The procedure is presented at six stages, including problem formulation, modelling, operational optimization, design optimization,

robustness analysis, and validation. The main focus is at the operational and design optimization stages, but the purpose of all stages is discussed. The proposed procedure is demonstrated with case studies. The studied cases deal with two types of problems: discrete state systems with uncertain state information and continuous state systems with two operating points. In both groups, non-Gaussian uncertainty plays an important role.

Preface

The research presented in this thesis has been carried out at Department of Automation Science and Engineering at Tampere University of Technology in 2007–2012. I express my deepest gratitude to my supervisor, Professor Risto Ritala for his guidance and motivation during these years. I am grateful for the opportunity to work at the department and I appreciate the support he has given me. I am also grateful to Professor Sirkka-Liisa Jämsä-Jounela from Aalto University and Dr. Jussi Manninen from VTT for pre-examining the thesis.

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The atmosphere at our department has been inspiring and I have enjoyed the colourful discussions in our coffee room. I wish to thank my colleagues for the help and motivating working environment. My special thanks go to M.Sc. Heimo Ihalainen, Dr. Kimmo Konkarikoski, M.Sc. Pekka Kumpulainen, Dr. Mikko Laurikkala, Dr. Marja Mettänen, Dr. Miika Rajala, and M.Sc. Johanna Ylisaari.

My parents always said that I will be a researcher. They have told me that already as a kid I focused thoroughly on tasks I found interesting. I wish to thank my parents for their support and encouragement during the years.

Finally, I would like to thank my husband for love and proofreading. We have spent several evenings discussing control engineering and optimization, not to mention the great moments of solving MDP problems together. At the very end of the dissertation process, Elsa joined our family. I thank her for letting me sleep well enough to be able to finish this thesis.

Tampere, December 2012

Aino Ropponen

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List of symbols

b	break state
d	design candidate
F	system model
G	design objective function
g	objective function
H	investment cost
J	cost-to-go function
k	discrete time index
K	prediction horizon
M	measurement model
m	measurement control variable
$N(\mu,\sigma^2)$	Gaussian distribution
p	probability function
p_0	parameter of the accepted risk of broke tower flowing over
p_{br}	probability for break beginning
$p_i^{(up/down)}$	parameter of the accepted risk of storage tower flowing empty or over
p_{rec}	probability for recovering from a break
q	quality variable
Q	vector of the quality variables
q_0	set point of the quality variable
R	number of repetitions
T	simulation time
u	process control variable

V	amount of water/mass in the storage tower
V_{max}	storage tower capacity
w	system noise
W	weighting factor for objectives
x	system state
z	measurement value, i.e. observation
Z	distribution of the number of breaks
α	scalarization parameter or decision vector
β	scalarization parameter
ε	measurement noise
γ	discount factor
π	operational policy

List of publications

I Ropponen, A. and Ritala, R., 2008. Towards coherent quality management with Bayesian network quality model and stochastic dynamic optimization. In *Proceedings of Control Systems Pan-Pacific Conference*, Vancouver, Canada, June 16–18, 2008, pp. 177−181.

II Ropponen, A. and Ritala, R., 2010. Optimizing the design and operation of measurements for control: Dynamic optimization approach. *Measurement*, 43(1), pp. 9−20.

III Ropponen, A., Ritala, R. and Pistikopoulos, E.N., 2010. Broke management optimization in design of paper production systems. In S. Pierucci and G. Buzzi Ferraris, eds., *Proceedings of the 20th European Symposium on Computer Aided Process Engineering – ESCAPE 20*. Computer Aided Chemical Engineering, 28. Naples, Italy, June 6–9, 2010. Amsterdam: Elsevier, pp. 865−870.

IV Ropponen, A., Ritala, R. and Pistikopoulos, E.N., 2011. Optimization issues of the broke management system in papermaking. *Computers and Chemical Engineering*, 35, pp. 2510−2520.

V Ropponen, A., Ritala, R. and Pistikopoulos, E.N., 2010. Optimization issues of the broke management system - the value of the filler content measurement. In *Proceedings of Control Systems Conference*, Stockholm, Sweden, September 15–17, 2010, pp. 186−191.

VI Ropponen, A., Rajala, M. and Ritala, R., 2011. Multiobjective optimization of the pulp/water storage towers in design of paper production systems. In E.N. Pistikopoulos, M.C. Georgiadis and A.C. Kokossis, eds., *Proceedings of the 21st European Symposium on Computer Aided Process Engineering – ESCAPE 21*. Computer Aided Chemical Engineering, 29. Thessaloniki, Greece, May 29–June 1, 2011. Amsterdam: Elsevier, pp. 612−616.

1 Introduction

1.1 Status of the pulp and paper industry in Finland

Forest industry has been one of the pillars for the economics of Finland during the past decades. Thirty years ago, the share of the total value of the national export in the forest industry was over 40 % and the forest sector contributed over 10 % of Finland's gross domestic production (GDP) (FFIF, 2011; Metla, 2011; Diesen, 1998). Nowadays, the significance has decreased the total value of exports being 20 % (FFIF, 2011) and the share of GDP approximately 4 % (FFIF, 2011; Metla, 2011). In spite of the reduction in the economic significance, the annual production of paper and paperboard is now almost two times larger than in the 1980's, being 11.8 million tonnes in 2010 (FFIF, 2011), and Finland is the sixth largest producer of paper in the world (FFA, 2011). During the past ten years, the Finnish pulp and paper industry has faced severe challenges. High manufacturing costs and the remoteness from the global markets has caused paper machine closures and workforce reduction as manufacturing has been moved to countries of lower costs. During 2006−2011 over 30 manufacturing lines have been closed in Finland and over 4000 people have been discharged (Haukkasalo, 2011). However, 22 paper factories and 13 paperboard factories are still located in Finland and the pulp and paper industry employs directly almost 23000 people (FFIF, 2011). To overcome the challenges in the paper markets and maintain paper production in the country, innovations and new ways of producing paper are needed. This will require new products as well as new process structures. A key issue will be the reduction of the capital intensiveness of the mills.

Papermaking is a highly uncertain process moving randomly between roughly two operating points: normal run and operation within web breaks. The occurrence of the web breaks is unpredictable so the transition between the operating points is somewhat random. Web breaks disturb the production by causing all the production to be discarded. For economic reasons, the discarded production as well as the water squeezed from the process is reused in papermaking. As a result, the process operation becomes challenging. Traditionally, that has been dealt with in the process design by dividing the process into departments separated by large storage towers. The storage towers behave as buffers balancing the system during abnormal situations. The drawback of the large storage towers is not only the high investment cost but on a multigrade line also the slow draining of the towers. During a grade change large towers can cause problems as it takes longer time to use the stored discarded production.

Ideally, the design of a paper manufacturing line is a multiobjective optimization task of the capital costs and the process performance. In reality, this is not always the case as the process structure and the operation are not traditionally designed simultaneously. The structure has been designed based on the production requirements but dynamic optimization has not been utilized actively. Thus, the process operation has been forced to cope within the environment defined by the process structure.

1.2 Research problem

This dissertation considers a procedure to systematically optimize the design of a stochastic papermaking process. The focus is on highly uncertain processes in which the deviations are not Gaussian. In this thesis, process design is examined as a multiobjective optimization problem in which the aim is to find the most effective process structure by compromising between the capital costs and the process performance. As the assessment of the process performance requires optimal operational decisions, process operation is studied as a part of the design problem. The motivation lies in a **hypothesis** that by integrating the design of the process structure and the operation of it, the capital efficiency can be improved.

Process optimization problem can be divided into two levels based on whether the decision is associated with the process design or its operation. The goal at the upper/design level is to examine the decisions related to the process structure and equipment dimensions, whereas at the lower/operational level the decisions related to the actions taken during the process run are studied. The operational actions can be related to both process control or measurement decisions. At both levels, the objective can be expressed either by a single criterion or by a set of multiple criteria. If only one objective is considered, the optimal value of the objective function is unique if the problem is feasible. In case of multiple objectives, the optimal value of the objective function is seldom unique and either a decision maker or scalarization to a single objective problem is needed to end up with a conclusion.

In this thesis, an overall solution procedure of an optimal process design is presented in six stages: problem formulation, modelling, operational optimization, design optimization, robustness analysis, and validation. The target of each stage is described in Table 1 and discussed in more detail in Chapter 4. The stages are in a chronological order, but the procedure is iterative and steps backwards may be needed. The main emphases of this thesis are the operational and design optimization stages, but all stages are discussed in the application context.

Table 1. Proposed procedure for the optimal design of a paper manufacturing system.

Stage	Description
Problem formulation	The design candidates are defined and described verbally and/or using a process diagram. The criteria for the process structure and performance along with the constraints are determined verbally.
Modelling	The models needed for optimization and simulation are identified. In this thesis three types of process models are suggested: a prediction model for optimization, a nominal model for simulation, and a validation model for estimating the accuracy of the nominal model.
Operational optimization	The operational optimization problem including objectives, constraints, and degrees of freedom is formulated mathematically. The target is to optimize the operational decisions taking into account the process dynamics and the future evolution.
Design optimization	The design solution space is generated by simulating the process with varying design candidates. The most preferred candidate is selected from the design space. The goal is to optimize the expected lifetime performance of the design candidates with respect to the capital costs.
Robustness analysis	Robustness analysis of the chosen design candidate with respect to the most uncertain model parameters is analysed.
Validation	The chosen candidate is tested using the validation model.

The research problem in this thesis is to examine how these operational and design decisions can be optimized in the application context. The research questions can be addressed as follows.

- How should the papermaking process be designed optimally to acceptably compromise the capital costs and the process performance?
- How can the operational decisions of a highly uncertain process be optimized taking into account the future behaviour?
- How can the optimal measurement or control policy be calculated when information about the process state is not known exactly?
- How can the performance of a stochastic process be estimated if the probability distributions cannot be evaluated in advance?
- How can the process design options be compared?

1.3 Contributions

The main contributions of this thesis are:

- introduction of a systematic solution procedure for process design cases in papermaking,
- exploitation of multiobjective optimization in decision making at the paper mills,
- studying measurement system design and operation as a part of the process design and operation,
- utilization of probabilistic methods in operational optimization of highly uncertain processes,
- ideas for formulating and handling stochastic multiobjective optimization problems.

This thesis contains an introduction and six publications. The methodology and ideas presented in the papers have been developed together with the supervisor, prof. Ritala. The publications including the author's contribution are summarized below.

Publication I presents a dynamic optimization based method for scheduling controls and measurements of a finite-state stochastic system. The stochastic model was described as a Bayesian network. The method was tested using a case inspired by quality management in papermaking. The author was responsible for the case study and its calculations. The author has written the paper and analysed the results. Preliminary results of the problem were published in the article Ropponen and Ritala (2008a).

Publication II presents a method for scheduling the measurement resources and optimizing the design of a measurement system. The problem was described as a dynamic optimization task in which the state was partially observable and solved using a POMDP algorithm. Simple case studies of discrete state systems were presented to demonstrate the ideas. The author was responsible for the case studies and the analysis of the results, and wrote the main parts of the paper. Preliminary results of the method and the studied cases were published in the article Ropponen and Ritala (2008b).

Publication III presents a strategy for solving the operation of broke management in papermaking. The broke management task was addressed through a stochastic model and formulated as a multiobjective optimization problem. The optimization model was implemented by the author. The author was responsible for the writing the main parts of the manuscript.

Publication IV presents an optimization strategy for designing the broke management system presented in Publication III. The problem was addressed as a stochastic, bi-level optimization problem with multiple objectives at both levels. The process and optimization models used in the simulations were the same as those in Publication III. The author was responsible for the simulation results and their analysis. The author wrote the manuscript with the help by the co-authors.

Publication V extends the case presented in Publications III and IV by proposing a strategy for evaluating a value of a new measurement device in broke management system. The author was responsible for the simulations and the analysis of the results, and wrote the article.

Publication VI presents an operational optimization problem of a papermaking process. The methodology was similar to that in Publications III and IV, but the process studied was larger and the models more detailed. The model of the papermaking system was developed by Dr. Rajala. The optimization model was implemented by the author. The author was also responsible for the simulations and wrote the main parts of the manuscript.

1.4 Structure

This dissertation is organized as follows. Chapter 2 describes the paper manufacturing system and its design challenges. The operation of the main sections in papermaking is outlined, and the effect of web breaks on paper manufacturing is explained. Finally, the issues related to the paper quality are discussed. In Chapter 3, the process optimization including both the design and the operational tasks is discussed. The chapter reviews the basic structure of an optimization problem and presents ideas of multiobjective optimization. Systems models are discussed and algorithms for illustrating and solving process optimization problems are presented both for process operation and design. In Chapter 4, a procedure for systematically studying stochastic dynamic processes is presented at six stages. The purpose of each stage is described and the relation to paper manufacturing is outlined. In Chapter 5, the cases used in this thesis are introduced followed by the summary of analysis results presented in Chapter 6. Finally, Chapter 7 concludes the thesis by summarizing the main points and discussing the future challenges.

2 Paper manufacturing

Paper manufacturing is a large-scale process consisting of several subprocesses. In series of processes wood chips are pulped; the produced pulp together with water, filler, and chemicals are fed to the paper machine; the paper web is formed; water is removed, and finally the surface of the paper is finished. The detailed structure of the subprocesses depends on the desired characteristics of the paper. The paper products can be classified on the basis of their raw material composition, finishing actions, manufacturing technologies, and end use (Paulapuro, 2000), and typically the paper manufacturing line is built only for a specific end product (Paulapuro, 2008). The common end products of publication papers include e.g. newsprint, fine papers, and magazine papers such as super-calandered (SC) and light weighted coated (LWC) papers (Paulapuro, 2000). The paper products can be further classified based on their grammage i.e. basis weight. Typically, a paper machine can produce various basis weights of the same end product. This study focuses on printing papers, more precisely on SC paper that is high-gloss publication paper used for weekly magazines and commercial printings. The grammage of SC paper varies between 40 and 80 g/m^2, most typically being 40−60 g/m^2 (Jokio, 1999).

The paper web can be up to 10 meters wide and run in a speed up to 2000 m/min (Paulapuro, 2008), thus if the basis weight of the paper is 60 g/m^2, the overall production rate can be up to 60 tonnes/h. As the machine is operated round the clock, an average of 360 days a year, the annual production rate is of the order of $4{\cdot}10^5$ tonnes. Most of the paper grades are commodity products the efficiency of the production being the competitive asset in markets. Thus, the optimization of the production system is a relevant issue and even a small improvement can have a significant impact on the annual level.

The aim of this chapter is to give an overview of the papermaking process and outline the challenges related to it. The process is complex and consists of several subprocesses, which are not discussed in detail. The chapter is organized as follows. In Section 2.1, the papermaking process is described briefly, whereas in Section 2.2 the tower system and issues related the web breaks and flow management are discussed in more detail and in Section 2.3 the quality issues associated with papermaking are introduced.

2.1 Papermaking process

In general, the papermaking process consists of (i) pulp manufacturing, in which pulp is produced from wood fibres, chemicals and water, (ii) paper machine, in which pulp is fed to the wire and water is removed from the web, and (iii) finishing actions including e.g. reeling, coating, calendering, and cutting. Coating and calendering can be placed either before or after reeling depending whether those are situated online or offline with relation to the paper machine. Figure 1 presents the main sections of the papermaking process.

Pulp is the main ingredient of paper. It is produced from wood fibres by separating the fibres from wood either chemically or mechanically. In chemical pulping (CP), the wood chips are cooked in large digesters and by the action of heat and chemicals, lignin and other undesired ingredients are separated from the fibres (Gullichsen, 1999). In mechanical pulping (MP), wood is either ground or refined into small particles until they are reduced to fibres (Sundholm, 1999). Two common types of mechanical pulp are thermomechanical pulp (TMP) that is produced from wood chips by using heat/steam, and pressurized groundwood pulp (PGW) that is produced from logs using steam. The main difference between the chemical and mechanical pulps lies in lignin. Lignin is a compound that binds the fibres together. It affects negatively the paper strength, but on the other hand the utilization rate of wood is significantly lower if lignin is removed. In CP, lignin is separated and the yield of wood varies between 35 % and 60 %, by comparison the yield of mechanical pulp is 91−98% as the lignin remains (Stenius, 2000). Hence, the utilization rate of the raw material in mechanical pulp is approximately double compared with the chemical pulp.

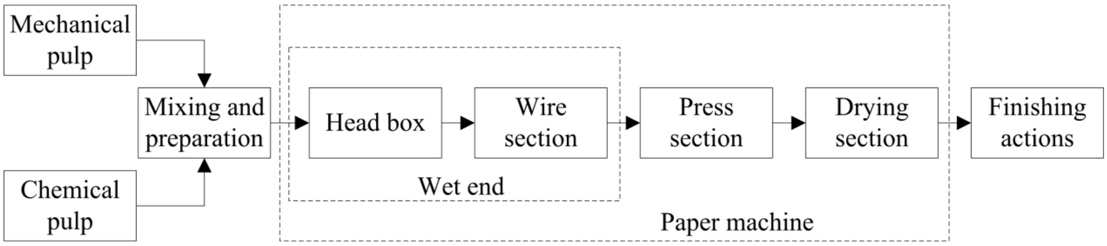

Figure 1. The main sections of the papermaking process.

The choice of the raw material depends mainly on the desired paper properties. As a consequence of the lack of lignin, chemical pulp improves the strength and brightness of the end product, but as more raw materials are needed, chemical pulp is more expensive than mechanical pulp. Mechanical pulp provides better opacity and printability, but suffers from the yellowing in process of time (Paulapuro, 2000). The production of mechanical pulp also requires large amount of electric energy (Sundholm, 1999); hence the cost-efficiency is dependent on the price of the electric energy. Typically, the printing papers consist of both pulp types, the ratio depending on the grade. Typical pulp ratios in SC paper are e.g. 70−90 % of mechanical pulp and 10−30 % of chemical pulp, the major part of the mechanical pulp being PGW (Paulapuro, 2000).

After the pulping section, the pulped material is pumped to the stock preparation where the pulp is diluted and fed to the mixing chest. At the mixing chest (blend chest) the diluted pulps are mixed with recycled fibres, water, chemicals, and fillers according to the desired recipe. The component fraction at the mixing chest affects directly the properties of the end product. See Table 2 for the fraction variation between the end products. Chemicals are added to the furnish both to improve the paper properties such as brightness or strength, and to improve the runnability of the process (Paulapuro, 2008; Neimo, 1999). Fillers, such as clay, talc, or titanium dioxide, are inexpensive ingredients that are used for improving printability, opacity, gloss, and brightness, but as a drawback the paper strength is deteriorated (Neimo, 1999). The main purpose of the mixing chest is to provide uniform material for the subsequent manufacturing sections.

From the mixing chest, the mixed pulp, i.e. furnish is lead to the paper machine. The main sections of the paper machine are head box, wire section, press section, and drying section. Before the head box, the consistency of the furnish is typically 0.2−1.0 % and it is transferred through pipe lines (Karlsson, 1999; Paulapuro, 2008). At the head box the paper web is formed. The main function of the head box is to feed the furnish evenly to wire (Paulapuro, 2008). After that, the main function of the rest of the sections is to decrease the water content of the web.

Table 2. The ratio of material components (MP, CP, and fillers) in SC, newsprint and fine papers (collected from Neimo, 1999; Paulapuro, 2000).

	MP (% of fibres)	CP (% of fibres)	filler
SC	70−90	10−30	4−35
newsprint	70−100 (if not recycled fibres)	0−30	0−15
fine papers	0−10	90−100	5−25 (20−25)

The dewatering starts from the wire section where the water is removed either through filtrating or thickening and can be further intensified by foils and vacuum (Paulapuro, 2008). The consistency increases to 15−25 % (Karlsson, 1999). From the wire section, the paper web is led to the press section, where the water content of the web is decreased to 33−55 % by compressing the water out (Karlsson, 1999). The web is pressed in 2−4 nips between rolls under a high pressure. That can be assisted by heating the web at the same time (Paulapuro, 2008). From the press section, the web is lead to the drying section where the water content is further decreased to attain the final moisture of 5−9 % (Karlsson, 1999). The dryer usually consists of series of hot metal cylinders through which the paper web passes and the water evaporates. Other methods for evaporating water include e.g. infrared, Condebelt and airborne drying (Karlsson, 1999).

After the drying section, the paper surface can be finished according to the desired paper type and characteristics. In coating, the paper surface is covered by a thin layer of a coating colour to improve the quality properties such as opacity, gloss, and printability (Lehtinen, 1999). The coating station can be placed either within the paper machine (online) or in a separate machine (offline) (Lehtinen, 1999). In calendering, the paper is led between rolls to make the surface glossy and smooth (Jokio, 1999). Also calendering can be placed either online or offline. SC paper is super-calandered between 10 or 12 rolls and the calendering process is always an offline machine (Jokio, 1999). Other finishing actions include reeling, winding, roll wrapping and handling, and sheet finishing (Jokio, 1999).

2.2 Tower system

The papermaking process is strongly affected by web breaks. Web breaks are unpredictable failures at any section of the papermaking line causing all the production to be discarded. As the occurrence of web breaks is random, breaks cause major disturbances to the system by delaying the process and upsetting the production (Roisum, 1990a; Orccotoma et al., 1997; Lama et al., 2003; Ahola, 2005; Dabros et al., 2005; Berton et al., 2006). The lost production caused by web breaks is 2−7 % (Ahola, 2005). As a result of the delays and lost production, the time spent in web breaks leads to financial penalties. The main source of web breaks are web defects such as holes, shives, and hairs (Roisum, 1990b). In addition, it is assumed that some correlation exists between the web strength and load, and web breaks (Roisum, 1990b; Orccotoma et al., 1997; Ahola, 2005).

To manage the stochastic disturbances caused by web breaks, the paper manufacturing process consists of storage towers for pulp and water. The storage towers act as buffers enabling to overcome the abnormal situation during the web breaks. Management of the flows between these storage towers is an important task in the operation of the paper production system. In this section, the function of the towers is described and the challenges of the tower management discussed.

2.2.1 Broke towers

In papermaking, the discarded production is called broke. Broke is generated in various parts of the process both at the paper machine and at the finishing processes (Paulapuro, 2008). The produced broke can be classified to wet and dry broke, the former meaning the wasted production from the manufacturing line and the latter the finished end product which does not satisfy the quality requirements. Dry broke is produced continuously e.g. from trimmings and cuttings, but the main reason of broke are web breaks.

As fresh pulp is expensive and broke contains fibres and other reusable materials, the produced broke is reused in papermaking by mixing it with fresh pulp. Before recycling, broke is diluted to the proper consistency and stored in a storage tower. Recycling is economically justified although the reuse impairs some properties of pulp and hence also the properties of the end product. The impairment may cause disturbances to the process and increase the risk for further breaks. The impairment results from the different material composition of the broke pulp as the several drying processes in the paper manufacturing line are likely to alter the pulp properties. In addition, broke contains chemicals and filler, thus the filler and chemical content of the mixed furnish is increased which can disturb the papermaking chemistry (Neimo, 1999; Paulapuro, 2008). The effect of the mixed furnish properties on the break probability is discussed e.g. by Orccotoma et al. (1997), Bonhivers et al. (2002), Lama et al. (2003), Dabros et al. (2004), Dabros et al. (2005), and Berton et al. (2006). On multi-production lines, grade changes can cause additional challenges, as the fibre and chemical compositions differ between the grades and after a grade change the stored broke pulp might not be usable (Paulapuro, 2008). To prevent the failures caused by the uneven broke, the towers for wet, dry, and coated broke can be separated. Typically, the capacity of the broke tower is designed to withstand the amount of paper produced in 2−4 hours (Paulapuro, 2008).

2.2.2 Water towers

The papermaking process requires a large amount of water. Water enables smooth transfer of pulp and dilution water is needed in several sections at the process. Water is also required for washing. The papermaking process can be described as circulation of water: at the beginning, water is added to the process, whereas at the latter parts the water is removed. To minimize the need of fresh water, the water removed from the drying processes is collected and recycled back to the process. The process water removed from the wire or web is called white water. It is not pure but includes fibre and chemical components. As some operations at the papermaking line require cleaner water, part of the water is filtrated. A common way is to feed the white water through a disc filter where the consistency is decreased. Filtrated waters can be classified as cloudy, clear, and super-clear filtrates based on their consistency (Paulapuro, 2008).

The demand of water increases during web breaks as dilution water is needed for the discarded production. To overcome the increased need of water, the process consists of water storage towers acting as buffer for abnormal situations. The water can be stored either as white water or as filtrated water, and separated storage towers exist also for specific filtrate consistencies (Paulapuro, 2008).

2.2.3 Flow management

An important task in paper manufacturing is to manage the flows between the storage towers. By dosing an appropriate amount of water, pulps, and broke, paper of uniform quality can be produced. Meanwhile, the tower volumes should be kept on acceptable levels to prevent the towers running empty or over. Figure 2 presents a simplified example of the tower system including storage towers for chemical and mechanical pulps, white water, clear filtrate, and wet and dry broke pulps.

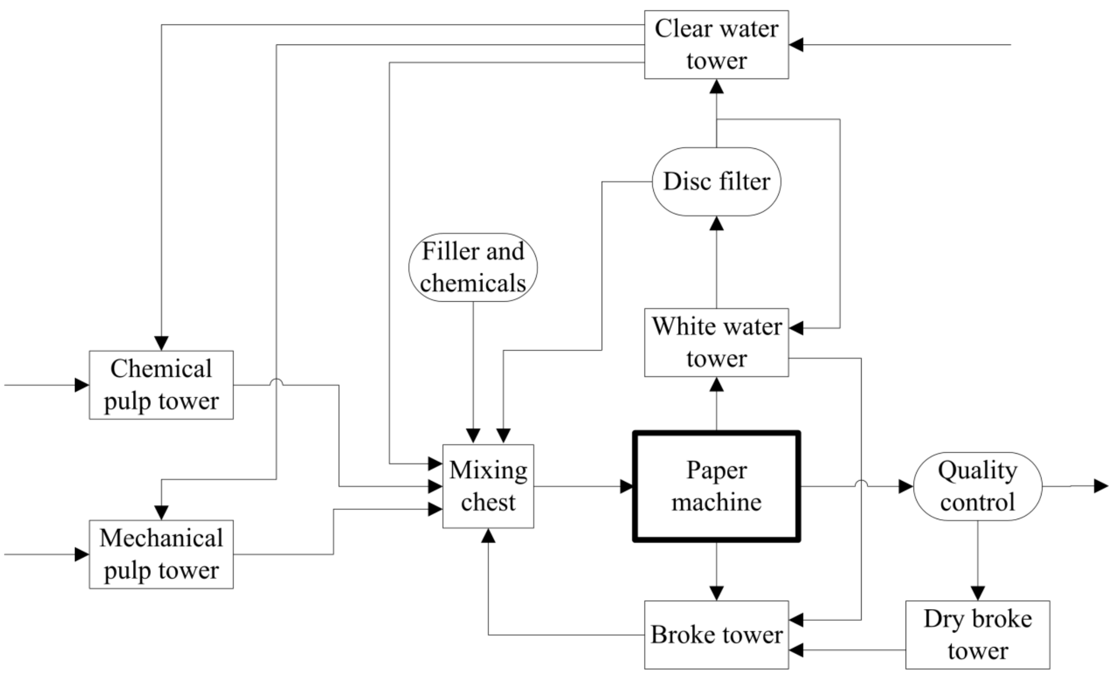

Figure 2. An example of a simplified process diagram.

Table 3. An example of typical process values in papermaking**.**

Variable	During normal operation	During a break
Inflow to the broke tower	0.65 t/min	15 t/min
Inflow to the white water tower	43 t/min	43 t/min
Outflow from the broke tower	1.2 t/min	3 t/min
Outflow from the white water tower	42 t/min	55 t/min

The management of the flows is not straightforward as the goals conflict and the tower levels correlate. During a web break, the discarded production is fed to a broke tower, thus the broke tower starts to fill up quickly. Meanwhile, the demand for white water increases as the produced broke requires dilution water, thus the white water tower starts to run empty. Table 3 presents how the typical flow volumes evolve both during the normal operation and during a break. A more detailed overview of the tower dynamics in paper manufacturing is presented e.g. by Orccotoma et al. (1997).

To keep the end product quality uniform, rapid changes of dosages should be avoided. For example, if the broke dosage is rapidly increased, e.g. to avoid overflow of the broke tower, the filler and chemical content of the mixed pulp grows, and thereby the quality of the paper alters. As the mixed furnish flows through several tanks and subprocesses, a quick change in the broke dosage causes transient disturbances to the end product as the control cannot be adjusted quickly enough to the new conditions. The management of the flows is typically the easier the larger the storage towers are, but simultaneously the investment cost increases. Thus, the design of the flow management system is basically a trade-off between the capital cost and the process performance.

2.3 Quality considerations

Printing and writing paper products can be classified firstly based on their main raw material, i.e. mechanical, chemical, or recycled fibre pulp, and secondly based on their end use (Paulapuro, 2000). Mechanical pulp dominating grades are typically used for newspapers (newsprint) and magazines (SC, LWC) (Paulapuro, 2000). Chemical pulp dominating paper grades are coated and uncoated fine papers that are used for e.g. magazines, catalogues, books, and copying paper (Paulapuro, 2000). In spite of the wide variety of the end products, paper grades are commodity products with standardized properties. Each grade has specific quality properties defined by the grade and the end use. Typical requirements include target values and tolerance limits e.g. for basis weight, moisture, filler content, thickness, density, bulk, formation, opacity, brightness, colour, rigidity, web strength, and printability (Leiviskä, 1999; Levlin, 1999). The operating task is to keep these properties as close to the target value as possible.

The quality properties can be managed by the actions taken throughout the production line. The fundamental control action is the selection of the raw materials i.e. the ratio of the mechanical, chemical, and recycled fibre pulps (Paulapuro, 2000). That is the main element affecting the end product properties. In addition, the wood species affects the end product quality as the fibre length and other properties differ. Other material components having impact on the paper quality are chemicals, fillers, and supplementary additives needed in paper production. In addition to these, the quality can be managed by the actions taken on the paper machine, e.g. coating, and by tuning the controllable parameters, such as temperature and pressure (Leiviskä, 1999).

The decisions about quality management are based on the measurement information about the paper web. Several quality properties, such as basis weight, filler content, and moisture can be measured continuously online by a scanning measurement device, and more accurate laboratory measurements can be executed regularly to support the decision making (Leiviskä, 1999; Levlin, 1999). Typically quality management is based on feedback control. If the quality is measured from the end product, there is a delay in such control. The challenge in the quality management lies in the conflicting targets as improvement of one property may deteriorate another (Leiviskä, 1999). As the models of how the actions affect the quality properties are not accurate, the decision making may be based on rather intuitive reasoning.

3 Process optimization

Process optimization refers to the strategy for finding the most effective decisions for utilizing the process. On the basis of the targets, process optimization can be divided into two tasks: design and operation. In process design, the decisions are related to the process and control structure, and dimensioning of the equipment. The target is to find a process structure that gives the highest value for the investment. In process operation, the decisions are related to the control actions that are taken during the process run. Thus, the operational task is to find the best achievable control actions for a given process structure. Between the design and operational tasks is the setting of the operational objectives, which is here treated as a part of the design task.

This chapter presents methods and algorithms to illustrate and solve process optimization problems. In Section 3.1 the structure of the optimization problem, including multiobjective formulation, is reviewed. In Section 3.2 system models are discussed, the main focus being in probabilistic models. Section 3.3 presents methods for optimal decision making in process operation and Section 3.4 methods for optimal decision making in process design.

3.1 Structure of the optimization problem

Optimization means selecting the most favourable decision amongst all available alternatives. It is usually formulated as a minimization of a cost function or maximization of a reward function, with respect to the actions. The problem may also have constraints, defining that the values of the actions must satisfy certain conditions. If the problem consists of several conflicting criteria, it is classified as a multiobjective optimization problem. In this section, the terminology of optimization is first introduced for the single-objective problem, and then the concept of multi-objective optimization is presented. For more detailed discussion on single-objective optimization see e.g. Himmelblau (1972), Nash and Sofer (1996), Edgar et al. (2001), Luenberger and Ye

(2008), and for more detailed discussion on multiple criteria optimization see e.g. Clark and Westerberg (1983), Steuer (1986), Miettinen (1999), Chinchuluun and Pardalos (2007), Branke et al. (2008).

3.1.1 Optimization in general

An optimization problem is formulated in general form as

$$\begin{aligned} &\min_u g(u) \\ &s.t. \quad h(u) = 0 \\ &\qquad\;\; e(u) \leq 0 \end{aligned} \tag{1}$$

where $g(u)$ is called an objective function, $h(u)$ an equality constraint, and $e(u)$ an inequality constraint. The aim is to find a solution vector u such that the value of the objective function $g(u)$ is minimized subject to ($s.t.$) the equality and inequality constraints. Equality and inequality constraints define the feasible region of the solution. A solution is feasible if it satisfies the constraints, i.e. the solution is inside the region defined by the constraints. If the feasible region is empty, the problem is called infeasible. Note that minimizing $g(u)$, equals to maximizing $-g(u)$, thus all maximization problems can be turned to minimization problems.

If the objective function and the constraints are linear, the optimization problem is classified as linear programming (LP); otherwise it is classified as nonlinear programming (NLP). Linear programming has been under research since 1940s and several methods, including e.g. simplex and interior-point methods, have been developed for solving LP problems (Edgar et al., 2001; Luenberger and Ye, 2008). Nonlinear programming problems are in general difficult to solve and a universal method providing a global solution for all types of problems does not exist. Approaches for solving NLP problems include e.g. Newton's method, Karush-Kuhn-Tucker conditions, penalty and barriers methods, and successive programming, the choice of the approach depending on the size and the type of the problem (Edgar et al., 2001). For a special class of convex NLP problems efficient algorithms providing a global solution exist. A problem is classified convex if both the objective function and the feasible region are convex (Edgar et al., 2001; Luenberger and Ye, 2008). A function is defined convex if the following holds for all $[u_1, u_2] \in \mathrm{R}$:

$$g(\omega \cdot u_1 + (1-\omega) \cdot u_2) \leq \omega \cdot g(u_1) + (1-\omega) \cdot g(u_2) \tag{2}$$

where $\omega \in [0,1]$ is a scalar factor. For a convex problem, a local solution is also a global solution.

Quadratic programming (QP) is a special case of convex NLP in which the objective function is quadratic and the constraints linear:

$$
\begin{aligned}
&\min_u \; g(u) = \frac{1}{2} u^T H u + c^T u \\
&s.t. \quad Au \le b \\
&\qquad\;\; Eu = d
\end{aligned}
\tag{3}
$$

where H is a matrix and c is a vector. There are several algorithms for solving QP problems efficiently and most optimization toolboxes include a QP solver.

An objective of an optimization problem can be turn to constraint by defining a limiting value for the criterion. The difference lies in if we are willing to e.g. minimize the energy usage or just define a bound that the usage should not exceed. As the solution cannot break the limiting values, the bounds can be classified as hard constraints, whereas the objective function expressing the preference of the solution can be classified as a soft constraint.

3.1.2 Multiobjective optimization

Traditionally, optimization refers to minimization or maximization of a single criterion. However, often in real-world problems there are several competitive criteria that should be considered simultaneously. For example, the task might be to maximize the process operational performance while minimizing the investment cost and the environmental detriment. If the optimization problem consists of more than one conflicting criterion, it is called multiobjective optimization. Multiobjective optimization problems are formulated as follows.

$$
\begin{aligned}
&\min_u \begin{cases} g_1(u) \\ g_2(u) \\ \vdots \\ g_n(u) \end{cases} \\
&s.t. \quad u \in U
\end{aligned}
\tag{4}
$$

where u is a vector of controls within feasible region U, and $g_1(u),\ldots,g_n(u)$ are the objective functions.

In single criterion problems, the optimal solution minimizes the objective function. There can be several solutions leading to this minimal value, but still the value of the objective function is unique. In multiple criteria problems there seldom exists a solution that is minimal for all objectives. Usually, there are several solutions which are optimal with respect to some of the objectives. If no other solution vector exists that improves one of the objective functions without deteriorating another objective function, the solution is Pareto optimal (Steuer, 1986; Miettinen, 1999; Chinchuluum, 2007). The following condition holds for Pareto optimality of the solution u^*:

$$g_i(u^*) \leq g_i(u) \quad \forall i \text{ and } \quad g_j(u^*) < g_j(u) \quad \text{for at least one } j. \tag{5}$$

Pareto optimal solutions are also called efficient or non-dominated. The collection of all non-dominated solutions is called Pareto optimal set or Pareto frontier. An example of a two-objective Pareto optimal frontier is presented in Figure 3.

Several methods exist for solving multiobjective optimization problems. Typically, the methods require a decision maker (DM) to express his or her preference at some stage of the problem solving (Miettinen, 1999). Based on the role of the DM, the problem is either scalarized into single-objective form according to the DM preference information, or a set of solutions from the Pareto frontier is obtained and presented to the DM who selects the most favourable solution. The drawback of the former is that the DM does not see the opportunities and may be conservative when expressing the preference information. On the other hand, the drawback of presenting the Pareto frontier lies in the computational challenges and in the visualization of problems with more than three objectives.

Probably the most common method for scalarizing multiple criteria problems is to use weighting factors to indicate the importance of the objectives. With weighting factors the problem can be scalarized by summing the weighted objectives together and solved as a single-objective problem. The problem takes the form

$$\begin{aligned} &\min \sum_{i=1}^{n} w_i g_i(u) \\ &s.t. \quad u \in U \end{aligned} \tag{6}$$

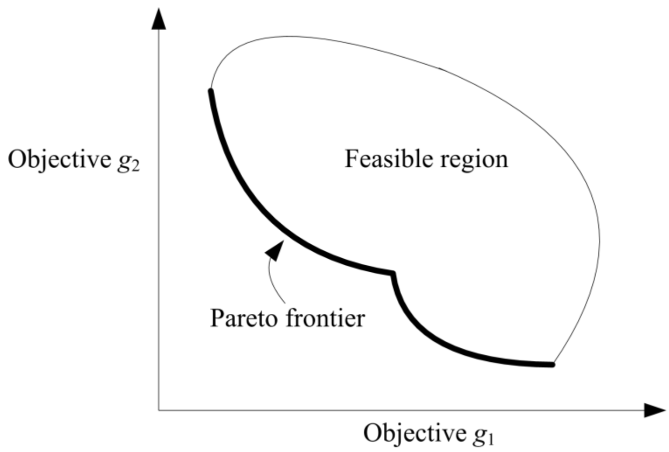

Figure 3. An example of feasible region and its Pareto optimal frontier.

where the weighting factors w_i are non-negative and typically chosen to sum to one (Miettinen, 1999). The weights can be defined beforehand and the problem solved as a single-objective optimization problem. Alternatively, if the problem is convex, a subset of the Pareto optimal frontier can be produced by varying the weights and solving several single-objective problems (Miettinen, 1999). Other well-known methods are e.g. ε-constraint method, lexicographic ordering, goal programming, and evolutionary algorithms (see e.g. Miettinen, 1999; Branke et al. 2008). In the ε-constraint method only one of the objectives is optimized while others are converted into constraints by introducing upper bounds for them and the different Pareto optimal solutions are obtained by varying the upper bounds. Lexicographic ordering and goal programming do not provide Pareto frontiers but only a single solution. Lexicographic ordering requires the DM to indicate the order of importance of the objectives which are then optimized in the same order whereas in the goal programming a desired aspiration level is defined for each objective and the deviation between the objective and the aspiration level is minimized. Evolutionary algorithms, such as genetic algorithms, are based on approximating the Pareto frontier by manipulating the population (Branke et al., 2008). Pareto optimality is not guaranteed (Hakanen, 2006), but evolutionary algorithms are claimed to have potential and their application is becoming exceedingly popular. In addition to these, several interactive methods have been presented in which the DM takes actively part in the optimization process by expressing his or her preferences about the direction of the solution (Miettinen, 1999; Branke et al., 2008).

The challenge in the multiobjective optimization lies in the presentation of the results to the DM. Pareto frontiers of two or three criteria can be easily visualized and it is rather straightforward for the DM to choose the most preferred solution. For dimensions higher than three, the visualization becomes challenging and it might be difficult to illustrate the trade-offs between the solutions. Several approaches have been introduced for visualizing multiobjective solutions with more than three objectives. One common approach is a spider web chart, also known as a radar chart, in which the results with respect to the objectives are presented on axes starting from the same point (Miettinen, 2003). Other methods include value path, bar chart, star coordinate system, petal diagram, and scatterplot (Miettinen, 1999; 2003). Engau and Wiecek (2007; 2008) introduced a subsystem approach in which the results are presented in several two-dimensional figures.

3.2 System models

Process optimization is based on a system model, i.e. a mathematical description of the real-world process. The system model describes the main elements and connections of the real world process, thus it illustrates how the state of the process changes as a function of the control actions. Let as denote the states of the system by x, the control variables affecting the system by u, and the model disturbance by w. Then the system dynamics of a discrete-time process can be described through a model F as

$$x(k+1) = F\big(x(k),...,x(0),u(k),...,u(0),w(k),...,w(0)\big) \tag{7}$$

where k denotes the discrete time index.

There are several ways to classify mathematical models. Typical classes are steady state or dynamic, linear or nonlinear, deterministic or probabilistic, and discrete or continuous. In this thesis, dynamic and stochastic systems are considered for both discrete and continuous system states. If the system state is known only through an uncertain measurement, the system is called partially observable, and the state information is expressed through a measurement model. Let us denote the measurement value, i.e. observation by z and the measurement disturbance by ε. Then the measurement can be described through a model M as

$$z(k) = M\big(x(k),\varepsilon(k)\big) \tag{8}$$

Figure 4 presents a block diagram of a model combining the system and measurement models. If only a limited number of measurements can be made simultaneously or the number of measurements is desired to be reduced due to the cost, also the measurements need to be controlled (Meier et al., 1967; Krishnamurthy, 2002). The measurement decision includes any combination of simultaneous measurements that the present measurement system allows. Let us denote the measurement choice by m. Then the measurement model takes a form.

$$z(k) = M\big(x(k),m(k),\varepsilon(k)\big) \tag{9}$$

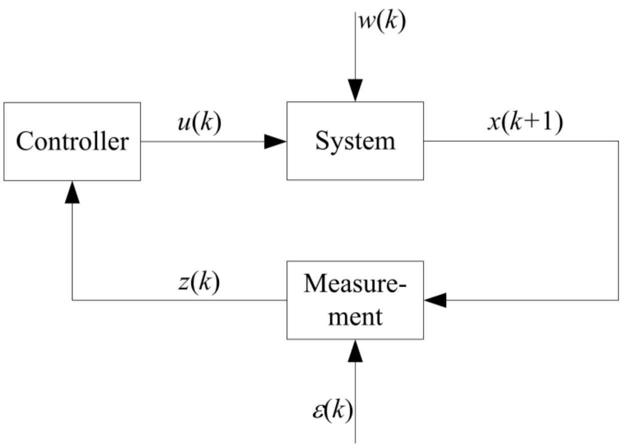

Figure 4. A block diagram of a system including measurement.

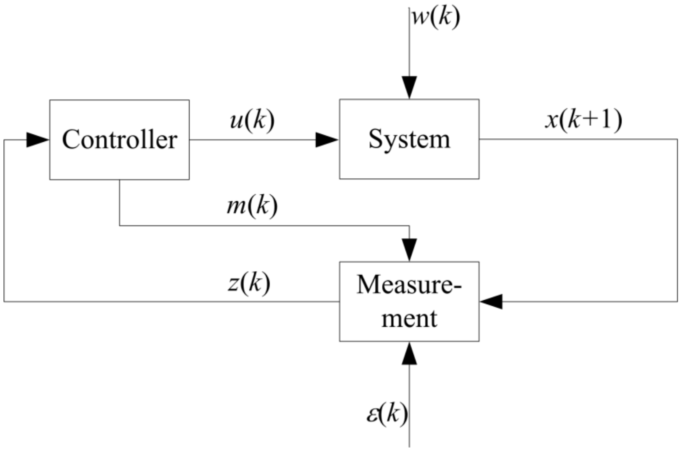

Figure 5. A block diagram of a system including the measurement selection (Meier et al., 1967).

A common example of combining measurement and system models is the linear dynamic state model with Gaussian system and measurement noises ($w(k)$ and $\varepsilon(k)$) expressed as

$$\begin{aligned} x(k+1) &= Ax(k) + Bu(k) + w(k) \qquad && w(k) \sim N(0, \Sigma_w) \\ z(k) &= C(m(k))x(k) + \varepsilon(k) && \varepsilon(k) \sim N(0, \Sigma_\varepsilon) \end{aligned} \tag{10}$$

where A is a state matrix, B an input matrix, $C(m(k))$ a measurement matrix depending on the measurement choice m, and $\sim N(\mu,\Sigma)$ denotes Gaussian distributed white noise with mean μ and covariance Σ. A block diagram of a model combining the system and measurement models including the measurement selection is presented in Figure 5.

3.2.1 Probabilistic system models

If the system is stochastic, i.e. there is randomness involved, the system dynamics in Eq. (7) can alternatively be described using a conditional probability function as $p_F(x(k+1)|x(k),\ldots,x(0);u(k),\ldots,u(0))$ which expresses the probability of the state $x(k+1)$ for known history of the state x and control u. Correspondingly, the measurement model can be described as conditional probability $p_M(z(k)|x(k),m(k))$, which describes the probability of the measurement value $z(k)$ with known state $x(k)$ and measurement selection $m(k)$.

The process variables can be either continuous or discrete valued. If the variables are continuous valued, p_F and p_M are probability density functions. Using this notation, the linear state model in Eq. (10) can be expressed as follows.

$$\begin{aligned} p_F(x(k+1) \mid x(k), u(k)) &= N(Ax(k) + Bu(k), \Sigma_w) \\ p_M(z(k) \mid x(k), m(k)) &= N(C(m(k))x(k), \Sigma_\varepsilon) \end{aligned} \tag{11}$$

If the variables can only have a finite number of values, probability mass functions are used and the conditional probabilities can be described using matrices (see e.g. Koller and Friedman, 2009). An example of a finite valued problem is a case of two states "acceptable" and "poor", denoted as "a" and "p", respectively, and control options u_1, u_2, u_3, and u_4. Then the conditional probabilities can be expressed by four [2×2]-sized matrices as follows.

$$
\begin{aligned}
& p_F\left(x(k+1) \mid x(k), u(k)=u_1\right) \\
&= \begin{bmatrix} p(x(k+1)=a \mid x(k)=a, u(k)=u_1) & p(x(k+1)=p \mid x(k)=a, u(k)=u_1) \\ p(x(k+1)=a \mid x(k)=p, u(k)=u_1) & p(x(k+1)=p \mid x(k)=p, u(k)=u_1) \end{bmatrix} \\
& \qquad\qquad \vdots \\
& p_F\left(x(k+1) \mid x(k), u(k)=u_4\right) \\
&= \begin{bmatrix} p(x(k+1)=a \mid x(k)=a, u(k)=u_4) & p(x(k+1)=p \mid x(k)=a, u(k)=u_4) \\ p(x(k+1)=a \mid x(k)=p, u(k)=u_4) & p(x(k+1)=p \mid x(k)=p, u(k)=u_4) \end{bmatrix}
\end{aligned}
\tag{12}
$$

Correspondingly, the measurement model of two measurement options m_1 and m_2, and three measurement values can be represented as

$$
\begin{aligned}
& p_M\left(z(k) \mid x(k), m(k)=m_1\right) \\
&= \begin{bmatrix} p\left(z(k)=1 \mid x(k)=a, m(k)=m_1\right) & p\left(z(k)=1 \mid x(k)=p, m(k)=m_1\right) \\ p\left(z(k)=2 \mid x(k)=a, m(k)=m_1\right) & p\left(z(k)=2 \mid x(k)=p, m(k)=m_1\right) \\ p\left(z(k)=3 \mid x(k)=a, m(k)=m_1\right) & p\left(z(k)=3 \mid x(k)=p, m(k)=m_1\right) \end{bmatrix}^T
\end{aligned}
\tag{13}
$$

and correspondingly for the measurement option m_2.

By using the Bayesian formula, the probability models for system dynamics and measurement can be combined, and the probability distribution of the state $x(k+1)$ after the observation $z(k+1)$ can be updated for given measurements and control history as

$$
\begin{aligned}
& p\left(x(k+1) \mid Z(k+1), U(k), M(k+1)\right) \\
&= \frac{p_M\left(z(k+1) \mid x(k+1), m(k+1)\right) p\left(x(k+1) \mid Z(k), U(k), M(k)\right)}{p\left(z(k+1) \mid Z(k), U(k), M(k+1)\right)} \\
&= C \cdot p_M\left(z(k+1) \mid x(k+1), m(k+1)\right) \\
& \qquad \cdot \int_{x(k)} p_F\left(x(k+1) \mid x(k), u(k)\right) \cdot p\left(x(k) \mid Z(k), U(k-1), M(k)\right) dx(k)
\end{aligned}
\tag{14}
$$

where $Z(k+1)=[z(k+1)\ \ Z(k)]T$ is a collection of the previous observation, $U(k)=[u(k)\ \ U(k-1)]T$ is a collection of the previous control actions, and $M(k+1)=[m(k+1)\ \ M(k)]^T$ is a collection of the previous measurement actions. C is a factor for normalization that is used instead of the denominator to ensure that the integral of the probability function equals to one.

3.2.2 Markov models

Markov model is a probabilistic model based on a Markov property, i.e. an assumption that the next state depends only on the current state and actions, not on the states and actions in the history (see e.g. Howard, 1960; Ross, 1970; Heyman and Sobel, 1982; Bishop, 2006). Markov models can be classified into several groups based on whether the system is autonomous or controlled, and whether the system state is fully observable or just partially observable. The simplest group of Markov models is called Markov chain. Markov chain is a model of an autonomous system whose state is fully observable, i.e. the probability function of the state x at time $k+1$ depends only on the distribution of the previous state $x(k)$. If the state is not fully observable, but the state is only known through uncertain measurement $z(k)$, the model is called hidden Markov model (HMM). The following holds for the HMM.

$$\begin{aligned} p_F\left(x(k+1) \mid x(k),..., x(0)\right) &= p_F\left(x(k+1) \mid x(k)\right) \\ p_M\left(z(k) \mid x(k),..., x(0)\right) &= p_M\left(z(k) \mid x(k)\right) \end{aligned} \tag{15}$$

Markov model that can be controlled with actions u is called Markov decision process (MDP) or partially observable Markov decision process (POMDP) depending on the observation of the state (Pineau et al., 2006; Powell, 2007). If the state of the process is fully observable, the process is called Markov decision process. The following holds for MDP.

$$p_F\left(x(k+1) \mid x(k),..., x(0); u(k),..., u(0)\right) = p_F\left(x(k+1) \mid x(k), u(k)\right) \tag{16}$$

MDP assumes that even if the process is stochastic, still after the decision is made, the state is fully known. That does not hold if the state is only known through uncertain measurement. Then the system is called partially observable Markov decision process (e.g. Åström, 1965; Smallwood and Sondik, 1971; Pineau et al., 2006) and the following holds.

$$\begin{aligned} p_F\left(x(k+1) \mid x(k),..., x(0); u(k),..., u(0)\right) &= p_F\left(x(k+1) \mid x(k), u(k)\right) \\ p_M\left(z(k) \mid x(k),..., x(0); m(k),..., m(0)\right) &= p_M\left(z(k) \mid x(k), m(k)\right) \end{aligned} \tag{17}$$

An example of the analysis of the POMDP is a Kalman filter (e.g. Åström and Wittenmark, 1997; Bar-Shalom et al., 2001) of a linear system with Gaussian noise (linear-quadratic estimator). Typically MDPs and POMDPs are used for optimizing of the future control sequences $u(k+1),\ldots,u(k+K)$. MDPs can be solved exactly using dynamic programming or reinforcement learning, but for POMDPs the exact solution is more difficult to calculate, though approximate solutions exist.

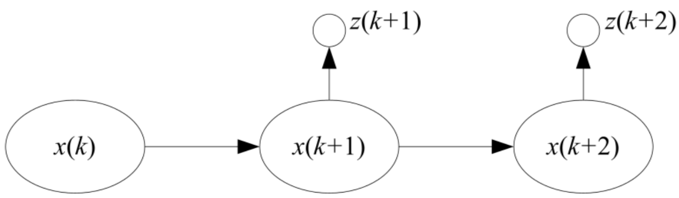

Figure 6. An example of a hidden Markov model (HMM) described as dynamic BN (Koller and Friedman, 2009).

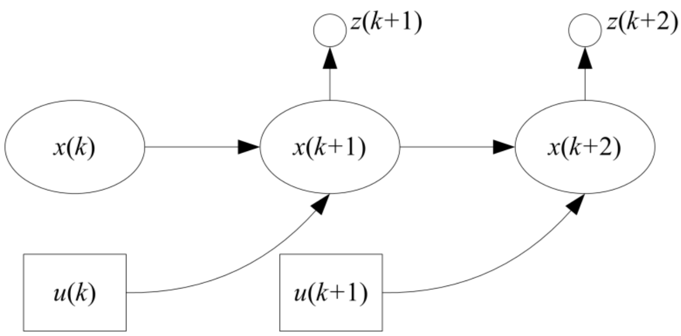

Figure 7. An example of a partially observable nonlinear stochastic process (POMDP) described as dynamic BN.

3.2.3 Dynamic Bayesian network

Bayesian network (BN) is a graphical model representing relationships between random variables (Jensen, 2001; Bishop, 2006; Koller and Friedman, 2009). The relationships are described as conditional probability densities and the inference is based on Bayesian reasoning. The network consists of nodes and edges representing the random variables and their conditional dependences. Dynamic Bayesian network is a BN describing dynamic sequences (Koller and Friedman, 2009; Russell and Norvig, 2010). An example of a HMM described as dynamic BN is presented in Figure 6, and an example of a POMDP described as dynamic BN in Figure 7.

3.3 Process operation

In process operation, the goal is to optimize the decisions related to the process control, such as the selection of the flow rates or consistencies. The objectives can include e.g. quality targets and minimization of the operational costs caused by the states and actions. A typical target is to minimize the squared error of the observed variable from its set point with a scalar penalty term for the control variable (Camacho and Bordons, 1999; Maciejowski, 2002). As the process is operated based on information about the process state, the operational problem may also contain decisions related to scheduling of the measurement resources. That is basically a compromise between the utility of the expected measurement information and the measuring costs.

The system and measurement models can be seen as equality constraints of the optimization problem (Goodwin et al., 2005) and the process optimization problem including the measurement selection can be formulated in general terms as follows.

$$\begin{aligned} &\min_{u,m} E\{g_1(x,u,m)\},\ldots,E\{g_n(x,u,m)\} \\ &s.t.\quad x(k+1) = F\left(x(k),\ldots,x(0),u(k),\ldots,u(0),w(k),\ldots,w(0)\right) \\ &\qquad\;\; z(k) = M\left(x(k),m(k),\varepsilon\right) \\ &\qquad\;\; u \in U \end{aligned} \tag{18}$$

where $g_1,\ldots,g_n$ are the performance objectives of the operational problem and F is the stochastic system model. The expected values are calculated with respect to the current state information. When studying dynamic systems, the actions made in the past affect the current state of the system. Hence, to take the future evolution of the process into account it is not enough to optimize the preferred next action, but the decisions should be optimized several time-steps ahead. The operational optimization problem of such case can be formulated as a cumulative sum of the expected future performance over a time horizon as follows.

$$\begin{aligned} &\min_{\substack{u(0),\ldots u(K-1)\\ m(1),\ldots,m(K)}} \sum_{k=0}^{K-1} \gamma^k E\{g_1(u(k),x(k+1),m(k+1)),\ldots,g_n(u(k),x(k+1),m(k+1))\} \\ &s.t.\quad x(k+1) = F\left(x(k),\ldots,x(0),u(k),\ldots,u(0),w(k),\ldots,w(0)\right) \\ &\qquad\;\; z(k) = M\left(x(k),m(k),\varepsilon(k)\right) \\ &\qquad\;\; u \in U \end{aligned} \tag{19}$$

where γ is a time-discounting factor, weighting the short time horizon more the long time horizon ($0<\gamma<1$) and K is the time horizon for operational optimization. Optimization of the these kinds of process operation problems have been under research since 1950s when Bellman discovered the first concept of dynamic programming, and later on plenty of studies have been done in the fields of model predictive control (MPC), Markov decision process (MDP), and partially observable Markov decision process (POMDP), see e.g. Bellman (1957), Åström (1965), Smallwood and Sondik (1973), Monahan (1982), Bertsekas (1995), Camacho and Bordons (1999), Goodwin et al. (2005), Thrun et al. (2005), and Pineau et al. (2006). The measurement scheduling problems are studied e.g. by Meier et al. (1967), Mehra (1976), and Krishnamurthy (2002). The following subsections present these methods. Often in practical process operation, the DM is not present, and hence the conflicting objectives need to be scalarized in single-objective form. Therefore, in the following subsections, the analysis is presented for single-objective problems only.

3.3.1 Bellman equation

Let us simplify the equation presented in Eq. (19) and assume a dynamic deterministic control problem formulated as follows.

$$
\begin{aligned}
& J\big(x(0)\big) = \min_{u(0),\ldots,u(K-1)} \sum_{k=0}^{K-1} \gamma^k g\big(x(k+1), u(k)\big) \\
& s.t. \quad x(k+1) = F\big(x(k), u(k)\big) \\
& \qquad\; u \in U
\end{aligned}
\tag{20}
$$

Thus, the target is to find the optimal actions $u_0,\ldots,u_{K-1}$ that minimize the overall cost during the time horizon K. $J(x(0))$ presents the smallest sum of the costs as a function of the initial state $x(0)$. By separating the current costs from the future costs, the optimization problem can be presented in a recursive form as follows.

$$
\begin{aligned}
& J\big(x(K)\big) = g\big(x(K)\big) \\
& J\big(x(k)\big) = \min_{u(0),\ldots,u(K-1)} \Big[g\big(x(k+1), u(k)\big) + \gamma^k J\big(x(k+1)\big)\Big], \qquad k = 0,1,\ldots,K-1 \\
& s.t. \quad x(k+1) = F\big(x(k), u(k)\big) \\
& \qquad\; u \in U
\end{aligned}
\tag{21}
$$

This separated formulation in Eq. (21) is called Bellman equation and it is the base for dynamic programming. The same formulation can be used also for stochastic processes, e.g. MDPs or POMDPs. The problem formulation is similar to the deterministic problem, except that the state is represented as a probability density function $p_F(x(k+1)|x(k),u(k))$ and the objective function as an expected performance. The Bellman equation of MDP problem is formulated as follows.

$$
\begin{aligned}
& J\big(x(0)\big) = \min_{u(0),\ldots,u(K-1)} \sum_{k=0}^{K-1} \gamma^k E_x\big\{g\big(x(k+1), u(k)\big)\big\} \\
& s.t. \quad x(k+1) \sim p_F\big(x(k+1) \mid x(k), u(k)\big) \\
& \qquad\; u \in U
\end{aligned}
\tag{22}
$$

where E_x denotes the expected value with respect to the stochastic state model $p_F(x(k+1)|x(k),u(k))$. It can be presented in the recursive form as follows.

$$
\begin{aligned}
& J\big(x(k)\big) = \min_{u(k)} E_x\big\{g\big(x(k+1), u(k)\big)\big\} + \gamma^k J\big(x(k+1)\big) \\
& s.t. \quad x(k+1) \sim p_F\big(x(k+1) \mid x(k), u(k)\big) \\
& \qquad\; u \in U
\end{aligned}
\tag{23}
$$

Correspondingly, the recursive Bellman equation for POMDP problem including measurement scheduling can be formulated as follows.

$$J\left(p\left(x(k)\right)\right)=\min_{u(k),m(k+1)} E_{x(k)}\left\{g\left(x(k+1),u(k),m(k+1)\right)\right\} \\ +\gamma^{k} E_{z^{m}(k+1)}\left\{J\left(p\left(x(k+1)\mid u(k),m(k+1),z^{m}(k+1),p\left(x(k)\right)\right)\right)\right\} \tag{24}$$

$$\begin{aligned} s.t.\quad & x(k+1)\sim p_{F}\left(x(k+1)\mid x(k),u(k)\right) \\ & z^{m}(k)\sim p_{M}\left(z^{m}(k)\mid x(k),m(k)\right) \\ & u\in U \end{aligned}$$

where z^m is the measurement value obtained using the measurement choice m. E_x and E_z are the expected values with respect to the stochastic state model $p_F(x(k+1)|x(k),u(k))$ and the measurement model $p_M(z^m(k)|x(k),m(k))$, respectively, and $p(x(k))$ denotes the state information after the measurement $m(k)$. The objective function is calculated as a function of the controls $u(k)$ and $m(k+1)$ and the state $x(k+1)$. For a finite-state system, the objective function in Eq. (24) can be formulated as follows.

$$\begin{aligned} & J\left(p\left(x(k)\right)\right) \\ & =\min_{u(k),m(k+1)}\sum_{j} g\left(x(k+1),u(k),m(k+1)\right)p\left(x(k+1)=j\mid u(k),m(k+1),z^{m}(k+1),p\left(x(k)=i\right)\right) \\ & \qquad +\gamma^{k}\sum_{j} J\left(p\left(x(k+1)\mid u(k),z^{m}(k+1),p\left(x(k)\right)\right)\right)p\left(z^{m}(k+1)\right) \end{aligned} \tag{25}$$

where the probabilities can be obtained by applying Bayesian inference, thus

$$\begin{aligned} & p\left(x(k+1)=j\mid u(k),m(k+1),z^{m}(k+1),p\left(x(k)\right)\right) \\ & =\sum_{i}\frac{p_{M}\left(z^{m}(k+1)\mid x(k+1)=j,m(k+1)\right)p_{F}\left(x(k+1)=j\mid x(k)=i,u(k)\right)p\left(x(k)=i\right)}{P\left(z^{m}(k+1)\right)} \end{aligned} \tag{26}$$

where

$$\begin{aligned} & P\left(z^{m}(k+1)\right) \\ & =\sum_{i,j} p_{M}\left(z^{m}(k+1)\mid x(k+1)=j,m(k+1)\right)p_{F}\left(x(k+1)=j\mid x(k)=i,u(k)\right)p\left(x(k)=i\right) \end{aligned}$$

It is worthwhile to point out that a linear quadratic Gaussian (LQG) problem of the form

$$\begin{aligned} J(x_k) &= \min_{u_k, m_k} E\left\{\sum_{k=0}^{K-1} x(k)^T Qx(k) + u(k)^T Ru(k)\right\} \\ s.t. \quad & x(k+1) = Ax(k) + Bu(k) + w(k) \quad w(k) \sim N(0, \Sigma_w) \\ & z(k) = Cx(k) + \varepsilon(k) \qquad\qquad\quad\; \varepsilon(k) \sim N(0, \Sigma_\varepsilon) \end{aligned} \tag{27}$$

where Q and R are cost matrices with respect to the state and control, is an example of the POMDP problem. It is probably the most fundamental optimal control problems, and it was elegantly solved by Rudolf Kalman (1960a; 1960b). The problem is well-studied e.g. by Åström (1970), Åström and Wittenmark (1997), and Franklin et al. (1998).

3.3.2 Dynamic programming

Dynamic programming is a recursive algorithm for solving sequential decision problems described in the previous subsections. The target in dynamic programming is to solve the optimal actions for the entire time horizon $k = 0,\ldots,K$ while minimizing the objective function (Bertsekas, 1995; Powell, 2007). The result for a fully observable problems is a decision rule, also called a policy or a control law, that indicates the optimal actions u^* for all possible states $x(0),\ldots,x(K)$ (Bellman, 1957). Thus, the policy maps the states into actions. Let us denote the policy as π. The optimal actions at time k can be then derived from the policy as a function of the current state, thus $u^*=\pi(x(k))$. The advantage of the dynamic programming algorithm lies in that there is no need for online calculation during the operation, but the problem can be solved offline beforehand and the optimal actions can be executed according to the current state. The idea is best known from Richard Bellman's studies in 1950s and he was the first one who used the term dynamic programming (Bellman, 1957).

In the literature, several formulations can be found under the term dynamic programming. The traditional algorithm, presented by Bellman, solves the problem as backwards recursion and it is often referred as backward dynamic programming or backwards induction (Bellman, 1957; Powell, 2007). Let us examine the deterministic problem described in Eq. (21). The calculation of the backward dynamic programming is started from the final state at time $k=K$. First $J(x(K))$ is calculated as a function of the possible states $x(K)$. Then the time stage is shifted backwards to $k = K-1$, and $J(x(K-1))$ is solved for known $J(x(K))$. The optimal actions $u^*(K-1)$ can be now obtained as a function of the state $x(K-1)$, thus

$$\pi(x(K-1)) = \arg\min_{u(K-1)} g(x(K-1), u(K-1)) + \gamma^{K-1} J(x(K)) \tag{28}$$

The time stage is shifted again backwards to $k = K-2$ and $J(x(K-2))$ is solved for known $J(x(K-1))$. The same procedure is repeated until $k = 0$. Finally, the optimal policy can be determined as a function of the initial state $x(0)$. The same algorithm can be used both for continuous and discrete state problems, although often in practical studies, analytical solution for continuous state problem is not possible and discretization to finite-state is needed to solve dynamic programming problem (Bertsekas, 1995).

Similar backward algorithm holds also for stochastic problems where expected values are used instead of the exact ones. A finite-state MDP problem can be solved as follows.

$$\begin{aligned}\pi\big(x(K-1)\big) &= \arg\min_{u(K-1)} E\{g\big(x(K),u(K-1)\big)\} + \gamma^{K-1}J\big(x(K)\big) \\ &= \arg\min_{u(K-1)} \sum_{x_{K-2}} g\big(x(K),u(K-1)\big)p\big(x(K)\,|\,x(K-1),u(K-2)\big) + \gamma^{K-1}J\big(x(K)\big)\end{aligned} \tag{29}$$

The result of Eq. (29) is a look-up table where the optimal action for each possible state is tabulated.

The backward dynamic programming only holds for finite horizon problems. For infinite horizon problems, popular algorithms include value iteration and policy iteration (see e.g. Howard, 1960; Bertsekas, 2001; Powell, 2007). It is notable that for finite horizon, backward dynamic programming and value iteration are identical and often value iteration is used as a synonym for backward dynamic programming. Infinite horizon problems are interesting as often the planning horizon cannot be specified beforehand and on the other hand infinite horizon problem of a stationary system leads to a stationary policy that does not vary in time. Hence, the policy remains the same for each time instant.

3.3.3 Solution methods for finite-state POMDP problems

Apart from certain special cases like LQG, POMDP problems are often solved in finite-state form (see e.g. Åström, 1970; Smallwood and Sondik, 1973; Monahan, 1982; Lovejoy, 1991; Cassandra et al., 1994; Kaebling et al., 1998; Pineau et al., 2006). That is due to the complexity of analytical solution of POMDP. As in POMDP problems the state information is only known through uncertain measurement, the optimal policy should be calculated as a function of the state probability, rather than as a function of the exact state like in MDP, hence $u^*=\pi(p(x(k)))$. The solution of a finite-state POMDPs should be calculated over a state probability $p(x(k)=i)$, thus although the state is discretized, the solution is a function of a continuous probability vector. Hence the problem turns to continuous-state MDP problem (Smallwood and Sondik, 1973; Bertsekas, 1995).

A significant basis for the POMDP research was presented by Edward Sondik in his PhD dissertation in 1971 as he proved that the optimal cost function of a finite-state and finite-horizon POMDP is always piecewise-linear and concave on the probabilistic space (Smallwood and Sondik, 1973; Monahan, 1982). Based on the Sondik's work, the optimal cost function at time k can be presented as a collection of vectors, each vector defining the optimal actions for a certain region of the state probability $p(x(k)=i)$. Figure 8 shows an example of that for a two-state case.

Let us denote the optimal action vectors by α, and the collection of α-vectors by $\Gamma(k)$. Thus, $\Gamma(k)$ is collection of all possible actions (control and measurement) that can be performed at time k. The problem in Eq. (24) can be reformulated as follows.

$$J\big(p\big(x(k)=i\big)\big) = \min_{\alpha \in \Gamma(k)} \alpha^T p\big(x(k)=i\big) \tag{30}$$

where

$$\sum_i p\big(x(k)=i\big) = 1 .$$

The optimal policies can be then calculated by multiple iterations of dynamic programming. More detailed solution algorithm for the problem is presented e.g. in Thrun et al. (2005) and Pineau et al. (2006). It is proved that the method provides exact solution to a POMDP problem of finite planning horizon and finite set of states and actions. The drawback of the method is the increasing number of α-vectors as the optimization horizon increases. The problem becomes harder as the number of discrete states and/or planning horizon increases and the time required to solve the problem can be doubly exponential in the time horizon (Kaebling et al., 1998; Pineau et al., 2006). Several

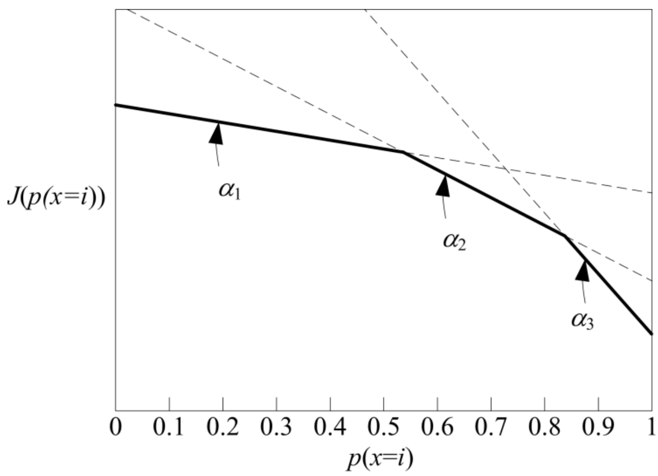

Figure 8. An example of a piecewise-linear and concave POMDP solution of a two-state problem.

approximate algorithms have been introduced to overcome the increasing complexity of the exact solution as the number of states or planning horizon increases (see e.g. Lovejoy, 1991; Pineau et al., 2003; Spaan and Vlassis, 2005). Typically the approximated algorithms calculate the solution in a limited set of probability points.

3.3.4 Model predictive control

Model predictive control (MPC) is a control strategy based on online optimization (see e.g. Camacho and Bordons, 1999; Mayne et al., 2000; Maciejowski, 2002, Rawlings and Mayne, 2009; Findeisen et al., 2007). In MPC, a finite horizon optimization problem is solved online at each time step based on the current state information. The first control value of the optimized sequence is applied while the others are rejected. At the next time step the prediction horizon is shifted forward and the optimization problem is solved again based on the new measurement data obtained (see Figure 9). The strategy is also called receding horizon control. The main difference between MPC and dynamic programming is that in MPC optimization is repeated on each time instant, whereas dynamic programming (and its extensions) provides an offline control law i.e. the optimal decisions are computed beforehand as a function of the possible states. If the planning horizon is predetermined, the dynamic programming and MPC formulations are identical. Dynamic programming based methods often suffer from the

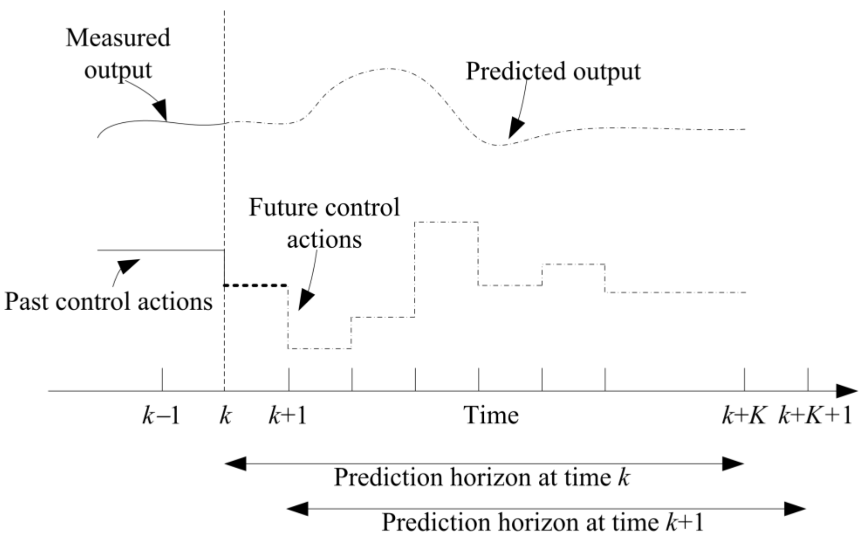

Figure 9. MPC procedure: the optimization problem is solved at time k over a prediction horizon $k+K$. The first control value (bold dotted line) is applied and at time $k+1$ the prediction horizon is shifted forward and the optimization problem is solved again over a prediction horizon $k+K+1$ (see e.g. Camacho and Bordons, 1999; Maciejowski, 2002).

increasing complexity as the planning horizon expands, thus the offline computation of the control law becomes difficult or impossible. As in MPC the optimization problem is calculated over a shorter time horizon during the operation, the problem remains solvable. MPC controllers are widely used in industry, especially in the field of chemical engineering.

In control engineering, MPC problems are most typically formulated as minimization of the squared error variable:

$$\begin{aligned}
&\min_u \sum_{k=1}^{K} \gamma^k \big(x_s(k) - x(k)\big)^T W_1 \big(x_s(k) - x(k)\big) + \sum_{k=1}^{K} \beta^k \Delta u(k)^T W_2 \Delta u(k) \\
&s.t. \quad x(k+1) = F\big(x(k),...,x(0),u(k),...,u(0),w(k),...,w(0)\big) \\
&\qquad\; z(k) = M\big(x(k),m(k),\varepsilon(k)\big) \\
&\qquad\; u \in U
\end{aligned} \tag{31}$$

where $x_s(k)$ is a set point of the controlled variable $x(k)$, W_1 and W_2 are weighting matrices, and γ and β time-discounting factors. The problem in Eq. (31) can be reformulated to the quadratic programming (QP) form if the process dynamics and the measurement model are linear, and solved using QP techniques. However, if MPC is understood as a procedure rather than as a classical control engineering, the problem does not necessarily have to be similar to Eq. (31).

3.3.5 Multiobjective process control

Most of the control problems consist of multiple criteria. Typically there are several properties whose squared deviation from the set point is required to be minimized. The target in process control is to find a balance between these, often competing objectives. The balance can be found either by utilizing the expert knowledge of the DM or by scalarizing the problem mathematically. In the former, the DM could ideally choose between several Pareto optimal control options, whereas in the latter, the Pareto optimal solutions are scalarized based on some a priori information.

Although the control problems often consist of several conflicting criteria, multiobjective optimization is not very widely discussed field in control engineering. Traditionally the control problems are treated as single-objective ones by using weighting factors, often referred as tuning parameters, that are adjusted based on manual tuning i.e. expert knowledge, or methods like Ziegler-Nichols (Åström and Wittenmark, 1997). However, a few studies exist about multiobjective process control, see e.g. Kerrigan and Maciejowski (2002), Aggelogiannaki and Sarimveis (2006), De Vito and Scattolini (2007), Wojsznis et al. (2007), Gambier (2008), Bemporad and Mũnoz de la Peña (2009). Most of the existing studies apply weighting method, compromise programming, lexicographic optimization, or evolutionary algorithms.

3.4 Process design

In process design, the goal is to find an optimal process structure that satisfies the desired targets and constraints. In the previous section, strategies for optimizing the process operation were discussed. The target was to obtain a control law or to manage the process based on the online optimization. In process design, the task is to optimize the environment for the operation, thus the equipment and their connections needed in the process operation. Process design problems have been discussed in the literature for decades especially in the area of chemical engineering (see e.g. Nishida et al., 1976; Schweiger and Floudas, 1997; Seferlis and Georgiadis, 2004; Westerberg, 2004; Ricardez-Sandoval et al., 2009). Traditionally process design has been studied on a steady-state mode based on the mass and energy balances, independently from the dynamic process operation problem (Schweiger and Floudas, 1997; Ricardez-Sandoval et al., 2009).

3.4.1 Design task and degrees of freedom

In process design, a typical task involves decisions related to the process flow-sheet and the dimensioning of the equipment with specific targets for the process performance and the investment cost. The task is to find a trade-off between these objectives. A key question in the decision making is how much the process can cost to cover the investment and turn a profit. The task can also be formulated opposite way by asking what the process performance should be to cover the costs. As the assessment of the process performance requires optimal operational decisions, the design task includes optimization of the operational control policy. An important part of the process design is also the optimization of the measurement system. That means selecting the measurement devices needed to provide the most valuable information for the process operation. The value of the measurement devices must be analysed with respect to their cost and expected utility.

In general, the design problem consists of two classes of objectives. In one class are the fixed objectives whose cost or utility does not change over time. A typical example of these is the investment cost i.e. the cost associated with the process structure and its building. In the other class are the objectives cumulating or averaged over the life span. These are typically process performance metrics such as targets for the production rate and quality, material and energy usage, and process availability. Often the performance objectives are discounted versions of the operational objectives indicating the lifetime behaviour. In addition, environmental and safety issues, and the failure rate can be part of the optimization problem. The optimal structure should be obtained by taking into account the long-term future profit, thus by estimating the product life-cycle (e.g.

Biegler et al., 1997). The analysis can be based e.g. on the net present value (e.g. Biegler et al., 1997).

The decision variables i.e. the degrees of freedom in the process design problem can be both continuous and discrete. Typical tasks in the process design are to choose a proper number of devices or to find an optimal flow-sheet amongst a few options. Thus, the variables are integer. If the task is to find proper parameter values or optimal dimensions for the devices, the variables can be either continuous or discrete, but typically the values are bounded. An optimization problem consisting of both continuous and integer variables is referred to mixed-integer programming (Floudas, 1995; Biegler et al., 1997; Nowak, 2005; Lee and Leyffer, 2012). Any option that fulfils the constraints of the degrees of freedom is a design candidate. When assessing the optimal process performance, each design candidate must be operated optimally. Hence, the control policy is solved for each candidate. As the design analysis must be faced without the DM, the multiobjective operational problems must be scalarized to the single-objective form. Thus, even if the multiple objectives in the operation are assessed by the DM, in the design analysis only scalarized forms of the operational problem are applicable. The scalarization parameters of the operational problem are degrees of freedom in the design optimization. Hence, the degrees of freedom in the design optimization are

- process structure
- control and measurement structure
- dimensions and other parameters
- control and measurement policy including the scalarization parameters

The degrees of freedom can be further divided into two groups based on whether the variables affect the process structure, or only the process performance. The process performance variables can be changed afterwards whereas the variables affecting the process structure are fixed as the structure cannot be easily changed without rebuilding.

3.4.2 Optimization problem

An optimization problem of N design objectives ($G_1,\ldots,G_N$), and $d \in D$ candidates can be formulated as follows.

$$
\begin{aligned}
& d^* = \arg\min_{d} \begin{cases} G_1(d,\pi) \\ \vdots \\ G_N(d,\pi) \end{cases} \\
& s.t. \quad d \in D \\
& \qquad \pi = \pi^{d_o} \\
& \qquad d = \begin{bmatrix} d_s & d_o \end{bmatrix}
\end{aligned}
\tag{32}
$$

where d_o refers to the degrees of freedom affecting only the process performance, d_s to the degrees of freedom affecting the process structure, and π^{d_o} is the result of the operational optimization solved using methods described in the previous section.

As the optimization of the control strategy is part of the process design optimization, the design problem consists of two levels. Ideally both levels should be optimized simultaneously and hence, the design stage fixes the strategy of process operation. That is referred as integrated process design and operation (Ricardez-Sandoval et al., 2009; Seferlis and Georgiadis, 2004). Several approached have been proposed for solving design and operation problems simultaneously, but no generalized method has been presented. The proposed methods can be roughly classified into two categories based on whether the integrated problem is solved in a steady state or dynamic mode (Bansal, 2000; Sakizlis, 2003; Ricardez-Sandoval et al., 2009). Majority of the recent studies have been examined in the dynamic framework (see e.g. Mohideen et al., 1996; Schweiger and Floudas, 1997; Bansal et al., 2000; Kookos and Perkins, 2001; Sakizlis et al., 2004; Flores-Tlacuahuac and Biegler, 2007).

3.4.3 Uncertainty in process design

As the real world processes are seldom deterministic, the presence of uncertainty should be taken account in the process design. Pistikopoulos (1995) categorized the sources of uncertainties in process engineering as: model-inherent, process-inherent, external, and discrete uncertainty. The first one is related to the physical properties and transfer coefficient, the second one to the flowrate and temperature variations, the third one to product demands, prices, and environmental conditions, and the fourth one e.g. to equipment availability. In the majority of the existing process design studies, uncertainty is assumed to be bounded, or the probability density function of the uncertain parameter known a priori (e.g. Pistikopoulos and Ierapetritou, 1995). In the former case, the controller is typically designed based on the worst case scenario (e.g. Perkins and Walsh, 1996), or multi-period decomposition approach (e.g. Mohideen et al., 1996). If the probability density function of the uncertain parameter is known, the problem can be solved by calculating the expected profit related to the design

$$E\{g(d,x)\} = \int_x f(x)g(d,x)dx \tag{33}$$

where $f(x)$ is the probability density function of the uncertain parameter and g is the operational objective function. If the probability density function is not exactly known, several scenarios can be used and a weighted sum calculated based on the assumed probabilities of each scenario (Sundqvist et al., 2003). That is reasonable when estimating e.g. future energy prices. Brengel and Seider (1992) presented a coordinated design and control optimization strategy of nonlinear processes by simulating MPC with disturbance scenarios.

When studying dynamic, stochastic processes, the future evolution of the process states is not predictable and the probability distributions are not always possible to be evaluated in advance. Hence, even though the short-term actions can be optimized (operational optimization), the expected long-term performance is not known (design optimization). In these cases, the expected performance of a chosen design candidate can be obtained through simulations by utilizing a mathematical model that behaves like the real process. The expected performance can be calculated as an integral over a time horizon T which is in the ideal case the entire life span of the process. This can be formulated as follows.

$$G(d,\pi) = \frac{1}{T}\int_0^T g(x(t),\pi(x(t)))dt \underset{T\to\infty}{\to} E\{g(x,\pi(x))\} \tag{34}$$

where g is the operational objective function as a function of the process state and the control policy. That is a brute force method, but if the probability distributions cannot be evaluated in advance, that seems to be the only way to obtain the expected values.

3.4.4 Multiobjective design analysis

As the design task typically consists of multiple objectives, the most preferred candidate must be chosen from the Pareto optimal set of the design options. The decision can be based on the DM’s assessment from the Pareto optimal frontier or the problem can be scalarized to a single-objective form. An advantage in presenting the results in multi-objective form is the potentiality of finding alternative solution approaches. The DM can compare different approaches and see the trade-offs between the solution options. However, the difficulty lies in the illustration of the results to the DM. Pareto frontiers of two or three criteria can be easily visualized, but for higher dimensions, the visualization becomes challenging. Several approaches have been introduced to illustrate multiobjective solutions with more than three objectives as discussed in Section 3.1.

Although most of the studies in process design deal with single-objective problems, various studies on multiobjective process design exist. Typically the multiobjective design problems contain two objectives and are solved using ε-constraint method (e.g. Palazoglu and Arkun, 1986; Luyben and Floudas, 1994; Schweiger and Floudas, 1997) or weighted sum method (e.g. Lim et al., 1999; Ko and Moon, 2002). Hakanen (2006) applied interactive method for multiobjective design problems with more than two objectives.

4 Process design in paper manufacturing – a systematic solution procedure

This chapter present a design procedure for finding an optimal process structure in papermaking applications. The proposed procedure is formulated at six stages: problem formulation, modelling, operational optimization, design optimization, robustness analysis and validation. These stages are described and discussed in Sections 4.1–4.6.

4.1 Problem formulation

The first stage in the design procedure is to define the process under consideration and set the goals for the process performance. That includes

(i) process description
(ii) metrics for the process performance, including constraints and other limitations
(iii) degrees of freedom
(iv) reference process information
(v) long-term scenarios

The process description (i) means detailed information about the process and its motivation. That can be formulated verbally and/or using a process diagram. Process description includes also specification of the process environment and the disturbances, i.e. the situations the process should manage. The desired process performance (ii) means the criteria for the process behaviour, for example the required production rate and time, the targets and tolerances for the product quality, and the usage of materials and energy. It is also important to define how the optimization problem will be defined, i.e. is the quality defined as an absolute target value or as a square deviation from the target, and are the criteria formulated as constraints or objectives. In addition to the performance constraints, the process may also consist of other limitations such as maximum and minimum flow rates or consistencies. The process model is also an equality constraint, but it will be set up at the second stage of the design procedure. The degrees of freedom (iii) define the set of variables amongst which the optimal solution is sought. At the design level, the degrees of freedom define the set of the possible design candidates. At the operational level the degrees of freedom are the controllable variables, but as the models are not fixed, those may be rather difficult to define at this stage. Reference process information (iv) states the benefits compared to the current best available technology (BAT). Finally, in order to make an investment decision, the time horizon for the repayment or the discounting interest should be stated and the long-term scenarios (v) for e.g. product demand, electricity price, and state subsidy defined.

In papermaking the stages includes e.g. (i) description of the process together with the process diagram, and information about the unit processes, typical flows and consistencies at each section, and production schedules, (ii) quality set points and tolerances, desired energy and material usage, production per time unit, average time spent in grade changes, quality variations, and maximum break rate, (iii) controllable flows and consistencies (operational), and equipment, components, and structure alternatives (design), (iv) the BAT process production, break rate, and material usage, (v) long-term predictions for the product demand and price, electricity and material (wood) price, environmental regulations, and availability of educated workforce.

4.2 Modelling

The second stage in the process design is modelling. For systematic process design of papermaking process, three types of process models are suggested in this thesis: one for optimization of the operational actions, one for simulation of the process, and one for estimating the accuracy of the other models and sensitivity of the solutions. All of the models are in a way superstructures (see e.g. Biegler et al., 1997) consisting of all possible design alternatives.

The model for the optimization is called prediction model. It is used as a constraint in the operational optimization problem. Prediction model is the most simplified of these three, as in order to run the optimization algorithms, the model cannot be too complicated. Prediction model contains simplified assumptions how the process will evolve in a short time horizon. For simulation of the process long-term behaviour, nominal model is used. It can be used for experimental purposes to simulate the process performance in varying situations or different control strategies can be tried. Long-term performance, i.e. the value of the objective functions in design optimization, can be evaluated by

Table 4. Description of the three types of models used for process design.

Model type	Description	Program
Validation model	Most accurate, used for validation.	e.g. Apros
Nominal model	For design optimization.	e.g. Matlab
Prediction model (operational optimizer)	Simplified, for operational optimization. Used within the nominal model.	e.g. Matlab

running the simulator together with the prediction model nested in it. Nominal model illustrates the main features of the process and is more realistic than the prediction model, but in order to run process simulation online, the model still includes approximations. The third model is called validation model. It is the most accurate one including more realistic features than the other two models. The validation model is typically computationally heavy, thus it is used for estimating the accuracy and sensitivity of the results obtained using the nominal model. The description of these three models is collected in Table 4. The mathematical models are implemented as computer programs.

In papermaking, the prediction model can for example contain assumptions for certain consistencies being constant over the prediction horizon, or the quality is modelled assuming linearity. The nominal model can contain certain simplification related to the unit processes e.g. mixing dynamics.

4.3 Operational optimization

Based on the first two stages, the optimization problem both for the design and operational levels can be formulated. The goal at the operational level is to optimize the operational process decisions for a given process structure by taking into account the process dynamics and future evolution. The first step at the operational level is to formulate the problem mathematically in a solvable optimization form. The formulation contains the objectives, constraints, and degrees of freedom defined at the first stage (Section 4.1), and the prediction model defined at the second stage (Section 4.2). If the problem is multiobjective, scalarization to the single-objective form might be required. The second step at the operational level is to solve the problem. Possible methods for optimizing the controls several time-steps ahead were discussed in Section 3.3. Depending on the problem and the chosen optimization method, the solution is either a set of numbers indicating the optimal actions to be executed, or a control law which indicates the optimal actions as a function of the current state information. The operation optimization also requires selection of the model parameters such as scalarization parameters and time-discounting factor. These are degrees of freedom at the design level, but an acceptable range for the parameters needs to be defined. That is often a trial and error problem based on dynamic optimization simulation.

In papermaking, operational optimization includes decisions about e.g. the flow rates, consistencies, and chemical dosages. Uncertain measurements, interactions between the variables, and process delays can cause difficulties to the process operation. The main challenge, however, lies in the web breaks. The unpredictable web breaks change the process operating point and are likely to disturb the process operation.

4.4 Design optimization

The target at the design stage is to optimize the expected lifetime performance of the process with respect to the capital costs, thus to find a trade-off between the investment costs and the process performance. The design optimization stage consists of (i) selection of the design strategy and (ii) selection of the most preferred solution from the design space of the Pareto optimal set.

4.4.1 Design strategy

Optimization of the process performance is a key task both at the operational and design levels. At the operational level the control decisions affecting the performance are optimized over a short time horizon based on the prediction model. At the design level, the task is to obtain a process structure that enables good performance in long-term. As in this thesis, dynamic and highly stochastic processes are examined, the future evolution of the process states is not predictable. The objective functions of the process performance can be evaluated based on long-term simulations by running the nominal model together with the prediction model. In an ideal case, the process is simulated over the entire life span (see Eq. (34)). As in this thesis the studied cases are stochastic, the performance is actually a random variable. Hence, the long-term performance is calculated as a mean of a sequence of similar simulations.

Depending on the process properties, the initial conditions of the simulator (nominal model) can be either fixed or chosen randomly before each run. Also, the process can be simulated either for a pre-specified time or until some finishing criterion fulfils e.g. until a machine failure. If the finishing criterion fulfils, the simulation is started again. To obtain reliable estimates, the simulation should cover at least days to months of real time. The expected performance $G(d, \pi)$ per time unit can be calculated as

$$E\{G(d,\pi)\} = \frac{\sum_{r=1}^{R}\sum_{t=0}^{T(r)-1} g\big(x(t+1,r), u^*(t,r), m^*(t+1,r)\big)}{\sum_{r=1}^{R} T(r)} \tag{35}$$

where T is the simulation time, R is the number of similar repetitions, and g is the value of the operational objective function when operating according to the optimized actions u^* and m^*. A diagram of the simulation based algorithm is presented in Figure 10.

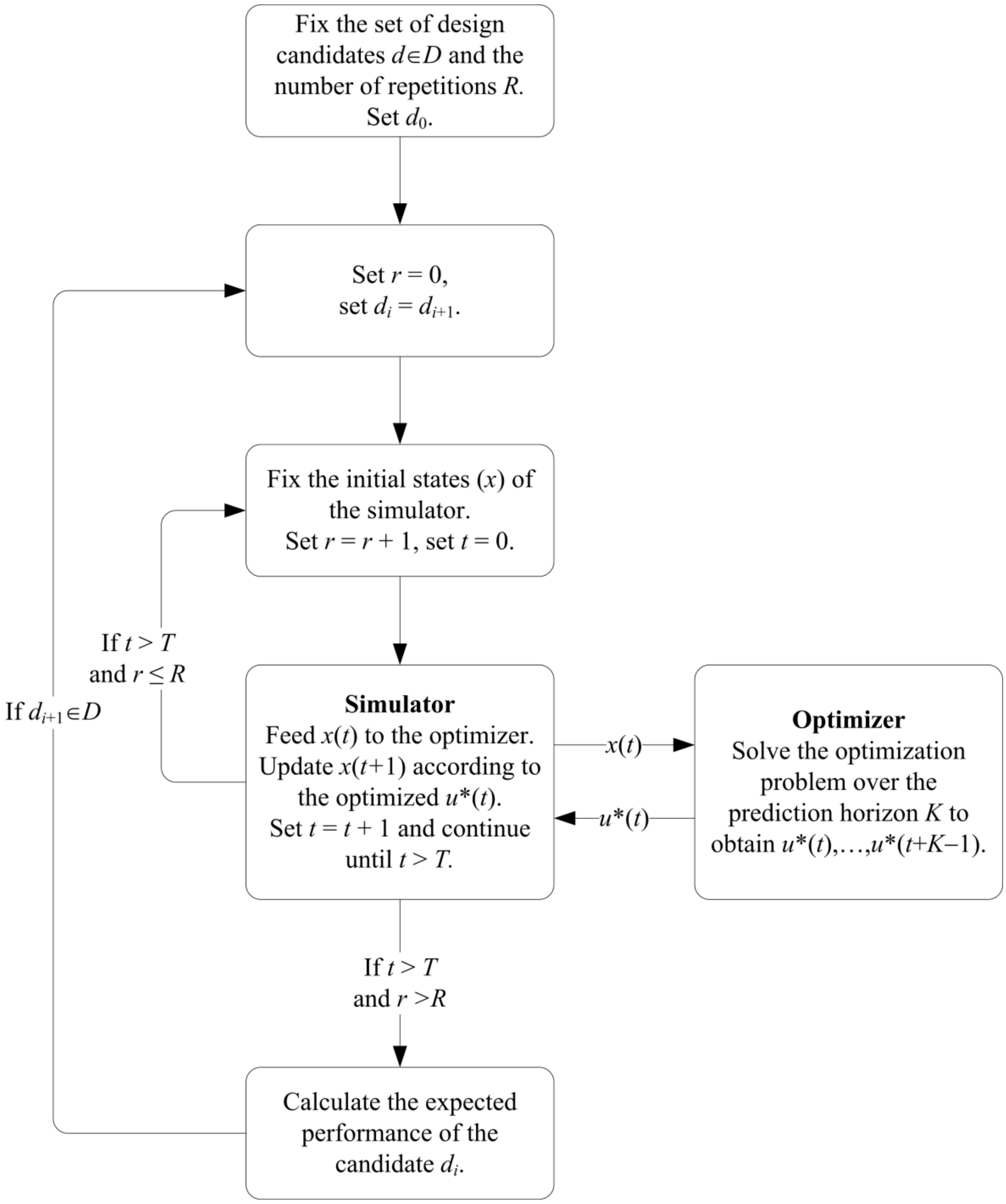

Figure 10. The procedure for estimating the performance of the selected set of design candidates. Here, the set of design candidates is fixed in advance without any sophisticated analysis method during the procedure.

The same procedure must be repeated for each design candidate to obtain the design space and the Pareto optimal set.

4.4.2 Design analysis

Once the expected performance is calculated for each design candidate, the most preferred candidate can be chosen from the Pareto optimal set of the design candidates. The selection can be made based on the DM's assessment or by scalarizing the design space using some other method. As mentioned in Sections 3.1 and 3.4, the difficulty in presenting the Pareto optimal candidates to the DM lies in the illustration of multiple objectives. One approach for illustrating the candidates is to present the results in several two-dimensional figures based on their preference of the objectives. The method is inspired by the work presented by Engau and Wiecek (2007; 2008). Let us assume a problem of four objectives. At the first phase, a simulated set of the design solutions is first presented to the DM with respect to the two most important objectives. The DM selects a set of most preferable candidates amongst these primary objectives. At the second phase, the chosen set of candidates is presented to the DM with respect to the secondary objectives. The DM either chooses the most preferable final solution from the Pareto set of the secondary objectives or a new set of design candidates is generated in a neighbourhood of the initial candidates and the phases one and two are repeated. An example of the method is shown in Figure 11.

A practical scalarization approach for comparing the Pareto optimal candidates is to convert all objectives to monetary units. Then the expected operational costs and profits can be summed together with the investment cost, and the optimal design assessed with

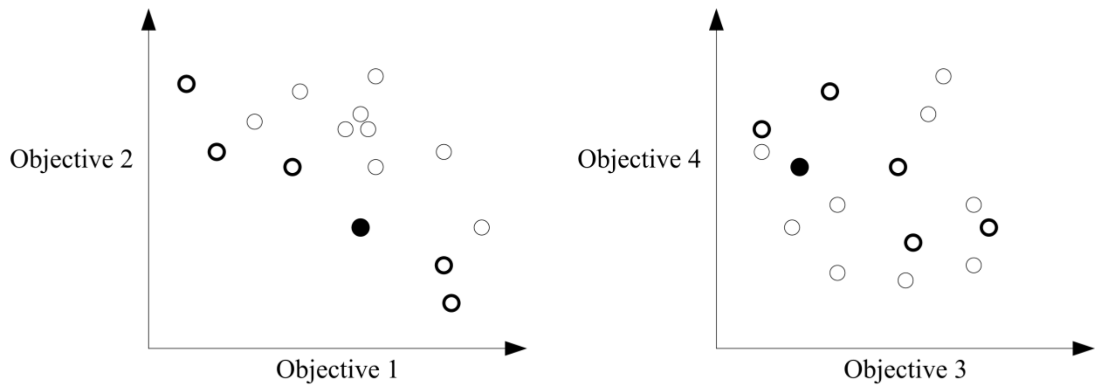

Figure 11. An example of the subsystem approach in which the design candidates are first presented with respect to the primary objectives and then with respect to the secondary objectives. The darker circles are the Pareto optimal candidates with respect to the primary objectives. The black circle indicates the chosen design candidate.

respect to the minimum overall costs or repayment period. The optimization problem is formulated as

$$\min_{d}\left[T_d \cdot E\{G(d,\pi)\} + H(d)\right] \tag{36}$$

where $H(d)$ is the investment cost of the design candidate d, T_d is process life span, and $G(d,\pi)$ is the operational cost per time unit. The weighted sum approach can be seen as a net present value problem (Biegler et al., 1997). A drawback in expressing all the objectives in monetary form lies in the difficulty of defining cost for everything. It is not always reasonable to define a monetary value for the quality deviations, and it can be even harder for environmental or social issues. Other difficulty lies in the uncertainty about the scenarios, e.g. how to predict the evolution of the product demand or energy price. Despite of these drawbacks, monetary units are still the basis for the investment decisions.

4.5 Robustness analysis

After selecting the design candidate, the robustness of the chosen candidate must be analysed. The process model and its parameters are based on certain assumptions of the real process behaviour. If these assumptions of are not correct or the conditions change over time, the chosen model or its parameters might not be applicable. Robustness describes the model's ability to operate in different conditions where the chosen model parameters are not valid. The better the model performs in varying parameter conditions, the more robust it is. Robust model is insensitive towards changes and disturbances.

In robustness analysis the model's sensitivity towards the most uncertain parameter is studied. The robustness of the chosen design can be examined by simulating the process using different parameter values in the simulator (nominal model) than in the optimizer (prediction model). The procedure is similar to the one presented in Figure 10, but this time the parameters under the robustness analysis are varied and the simulation is operated only for the chosen design candidate. The parameter values are cross-studied in the simulator and optimizer, thus each parameter value is simulated against all others and the expected performance is calculated for each parameter pair. Based on this, the robustness of each parameter can be analysed and if necessary, the chosen design solution can be reconsidered.

In the paper production system, parameters of the break probability model are based on rather vague assumptions. Thus, the robustness with respect to the break model parameters needs to be studied.

4.6 Validation

The nominal model used in the design optimization is based on approximations of the real system, thus it might contain certain inaccuracies. Validation model is more realistic including more features of the real process. The accuracy of the nominal model can be tested by running the both models from the same initial conditions and using the same actions through the simulation. In an ideal case, the behaviour of the models would coincide exactly, though usually it is enough if the performance is close to each other. If the behaviour of the nominal model does not correlate with the validation model, it might be necessary to reconsider the nominal model before implementation.

5 Case formulations and their motivation

This chapter introduces the five case studies analysed in this thesis. The cases can be classified to two groups based on the state being discrete or continuous. Publications I−II present examples of discrete state problems and Publications III−VI present examples of continuous state problems. The motivation for all cases lies in paper production.

The main focus in Cases 1−3 (Publications I−II) is the integration of measurement and control scheduling. In these cases, the system state is not known exactly, but through uncertain measurements, thus the system is partially observable. As there is a price for measuring, the measurement resources are limited, and the measurement information is not exact, the challenge is to determinate whether it is worthwhile to measure or not. In some cases, the challenge lies in which measurement device to use. For dynamic processes, the optimization of the actions should be done taking into account the future evolution of the process. To clarify the field of the problem, Case 1 provides a simple example. Its motivation lies in the simplicity for illustrating the basic concepts relevant in more complex cases. The motivation of Cases 2 and 3 is rather idealized maintenance, and quality management, respectively. The problems are formulated in discrete state form, as in maintenance and quality management cases, it is often reasonable to categorize the system states into classes. The uncertainty appears both in the system dynamics and the measurement description. For Cases 1 and 3 only the operational optimization of the integrated measurement and control scheduling is studied, whereas for Case 2 also the measurement system design is examined. Cases 1−3 are discussed in Sections 5.1−5.3.

Cases 4−5 (Publications III−VI) deal with design and management of the storage tower system in paper manufacturing. The design task in these cases is to determine the optimal storage tower capacities by maximizing the process performance and minimizing the investment cost associated with the towers capacities. The operational task is to produce good quality paper by maximizing the effective production time while preventing storage towers running empty or over. In Case 4, the broke management part of the process is considered, with one storage tower and one controllable flow, filler content variation being an indicator of quality. Case 5 is an extended version of Case 4, including additional storage towers, control flows, and quality indicators. The uncertainty in both cases appears from the unpredictable web breaks, causing the system highly stochastic. To prevent the towers running over or empty during a sudden web break, the control variables must be changed quickly which typically deteriorates the end product quality. The challenge lies in the optimization of the control variables over a long time horizon, without knowing when a new break occurs and how long it last. Cases 4−5 are discussed in Sections 5.4−5.5.

5.1 Case 1: Two-state system

Publication II presents a two-state system. It is the simplest case, and the basic idea of the discrete-state system management can be easily illustrated by this example. The problem consists of two states (x), with two alternative control options (u), and two measurement options (m). Let us call the states as "good" and "poor", and the control options (u) as "run as usual" and "make a correction". The additional cost of the state "poor" is 0.9 units, and the additional cost of the corrective action is 0.5 units. The task is to optimize the control and measurement actions by taking into account the future behaviour of the system. By minimizing the expected costs over a time horizon, the actions can be scheduled. The transition probabilities from time k to $k+1$ are defined as Markov chain as follows.

$$
\begin{aligned}
&p_F\,(x(k+1)\,|\,x(k),u(k) = \text{"run as usual"}) = \begin{bmatrix} 0.7 & 0.3 \\ 0.2 & 0.8 \end{bmatrix} \\
&p_F\,(x(k+1)\,|\,x(k),u(k) = \text{"make a correction"}) = \begin{bmatrix} 0.9 & 0.1 \\ 0.8 & 0.2 \end{bmatrix}
\end{aligned}
\tag{37}
$$

which can be read as: if the state at time k was "good" and the action taken was "run as usual", the probability of state "good" at $k+1$ is 0.7, and the probability of the state "poor" is 0.3”. The state can be measured with the following probability matrices:

$$
\begin{aligned}
&p_M\left(z^m(k)\,|\,x(k),m(k)=1\right) = \begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix} \\
&p_M\left(z^m(k)\,|\,x(k),m(k)=2\right) = \begin{bmatrix} 0.95 & 0.05 \\ 0.05 & 0.95 \end{bmatrix}
\end{aligned}
\tag{38}
$$

The upper matrix for $m = 1$ indicates that no measurement is made, as the probabilities are independent on the state for the both observations. With the measurement option $m = 2$, the states can be distinguished but there is 0.05 probability of an error. The cost of the measurement option $m = 2$ is 0.03 units.

5.2 Case 2: Three-state maintenance problem

Publications II presents an example of a maintenance problem of three states. It is an extended version of the two-state system presented in the previous section and it is inspired by the case studied by Smallwood and Sondik (1973). At the operational level, the task is to optimize the controls and measurements over a time horizon to support the decision making whereas at the design level the task is to analyse the value of the measurement accuracy.

Let us call the three states as: "good", "acceptable", and "poor", each state having its own cost: 0, 0.5, and 1 unit, respectively. The system can be controlled with three actions with costs 0, 1, and 2 units. The transition probabilities are defined as follows.

$$
\begin{aligned}
p_F(x(k+1) \mid x(k), u(k)=1) &= \begin{bmatrix} 0.81 & 0.18 & 0.01 \\ 0 & 0.9 & 0.1 \\ 0 & 0 & 1 \end{bmatrix} \\
p_F(x(k+1) \mid x(k), u(k)=2) &= \begin{bmatrix} 1 & 0 & 0 \\ 0.7 & 0.2 & 0.1 \\ 0.2 & 0.7 & 0.1 \end{bmatrix} \\
p_F(x(k+1) \mid x(k), u(k)=3) &= \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}
\end{aligned}
\tag{39}
$$

which can be read as: if the state at time k was "acceptable", and the control action taken was $u(k) = 1$, then the probability of the state "acceptable" is 0.9 and the probability of the state "poor" is 0.1. Note that the third action turns the process certainly to the state "good". To support the decision making, a two-valued measurement with a cost of 0.2 units can be made. The measurement options are to not measure ($m = 1$) and to measure ($m = 2$) with the probabilities.

$$p_M\left(z^m(k) \mid x(k), m(k)=1\right)=\begin{bmatrix}1 & 0\\ 1 & 0\\ 1 & 0\end{bmatrix}$$
$$p_M\left(z^m(k) \mid x(k), m(k)=2\right)=\begin{bmatrix}1 & 0\\ 0.5 & 0.5\\ 0.25 & 0.75\end{bmatrix} \tag{40}$$

At the design level, the system is studied by introducing a parameter d as an indicator for the measurement accuracy:

$$p_M\left(z^m(k) \mid x(k), m(k)=1\right)=\begin{bmatrix}1 & 0\\ 1 & 0\\ 1 & 0\end{bmatrix}$$
$$p_M\left(z^m(k) \mid x(k), m(k)=2\right)=\begin{bmatrix}1-d & d\\ 0.5 & 0.5\\ d & 1-d\end{bmatrix} \tag{41}$$

The smaller the parameter d is, the easier it is to distinguish the states 1 and 3, but both states can be still confused with the state 2. The design task is to calculate the operational costs as a function of the design parameter d when the operational policy has been optimized for each d.

5.3 Case 3: Bayesian network based quality management

Publication I presents an example of a Bayesian network -based quality management in papermaking. The operational task is to manage paper strength (x_s) and brightness (x_b) by controlling the dosage of the bleaching chemicals (u_b) and the fibre fraction ratio (u_f). Brightness is mainly manipulated by the dosage of the bleaching chemicals, and strength by the fibre fraction ratio, but both control actions have also impact on the other quality variable by increasing the outcome uncertainty. The effect of the fibre fraction ratio control is assumed to take place in one time step, and the effect of the bleaching chemical in two time steps, the time step resolution corresponding approximately with the manufacturing time of one machine reel. Hence, the transition probability of the quality variable brightness is described as $p_F(x_b(k+1)|x_b(k),u_b(k-2),u_f(k-1))$ and the transition probability of the quality variable strength as $p_F(x_s(k+1)|x_s(k),u_b(k-2),u_f(k-1))$. The current states of the quality variables can be estimated through uncertain offline measurements, but only one measurement can be made at time. Figure 12 presents a dynamic Bayesian network of the studied case.

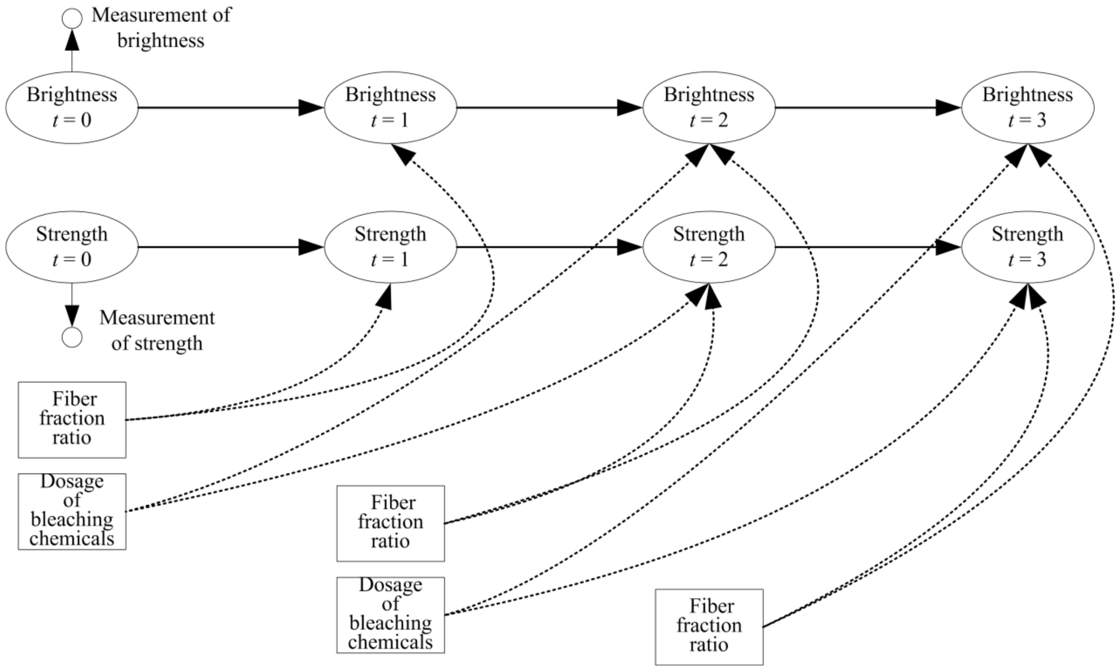

Figure 12. Case 3 presented as a Bayesian network.

The quality variables, controls, and measurement values are all discretized. The discrete values of the quality variable brightness are defined as "critical" ($x_b = 1$), "low" ($x_b = 2$), "ok" ($x_b = 3$), and "too high" ($x_b = 4$), and the discrete values of the quality variable strength as "critical" ($x_s = 1$), "low"($x_s = 2$), and "ok" ($x_s = 3$). Both controls actions (u_b and u_f) have three values. The measurement of brightness is discretized to eight values, and the measurement of strength to seven values. Such categorization is justified as it is often more interesting to know the group the variable belongs to, rather than the exact numerical value. An example of the transition probability matrix for brightness is:

$$
\begin{aligned}
p_F(x_b(k+1) \mid x_b(k), u_b(k-2) = 1, u_f(k-1) = 2) &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0.8 & 0.2 & 0 & 0 \\ 0.45 & 0.45 & 0.1 & 0 \\ 0.2 & 0.6 & 0.2 & 0 \end{bmatrix} \\
p_F(x_b(k+1) \mid x_b(k), u_b(k-2) = 2, u_f(k-1) = 2) &= \begin{bmatrix} 0.6 & 0.2 & 0.2 & 0 \\ 0.2 & 0.7 & 0.1 & 0 \\ 0 & 0.15 & 0.7 & 0.15 \\ 0 & 0.05 & 0.15 & 0.8 \end{bmatrix} \\
p_F(x_b(k+1) \mid x_b(k), u_b(k-2) = 3, u_f(k-1) = 2) &= \begin{bmatrix} 0.5 & 0.4 & 0.1 & 0 \\ 0.05 & 0.25 & 0.6 & 0.1 \\ 0 & 0.05 & 0.25 & 0.7 \\ 0 & 0 & 0.05 & 0.95 \end{bmatrix}
\end{aligned}
\tag{42}
$$

Overall, the size of the transition probability matrix for quality variable brightness is [4×4×3×3], and for quality variable strength [3×3×3×3].

5.4 Case 4: Broke management

Publications III−V examine broke management in paper manufacturing. In Case 4, the task at the operational level is to control the broke system by manipulating the dosage of the recycled broke pulp while producing good quality paper and preventing the storage tower overflow. At the design level the task is to determine the optimal capacity of the broke tower. Figure 13 presents the key process areas of the case.

In this study, filler content variation of the end product is used as an indicator of the paper quality and the target is to minimize the squared deviation of the filler content from its set point. As the discarded production fed to the broke tower is diluted using white water that contains filler, the reuse of broke increases the filler content of the mixed pulp. Filler content can be measured at the paper machine, but the feedback control is slow and a change of the broke dosage causes transient disturbance to the end product taking approximately 1–2 hours.

The objectives of the operational optimization problem are to prevent the broke tower running empty (i), to minimize the time within breaks (ii), and to manage the filler variation of the paper (iii) by manipulating the dosage of the discarded production. The optimization problem also consists of an objective to assure smoothness of the broke dosage (iv). The optimization should take into account the future evolution of the process, thus the control actions should be optimized several hours ahead. The operational optimization problem can be formulated as follows.

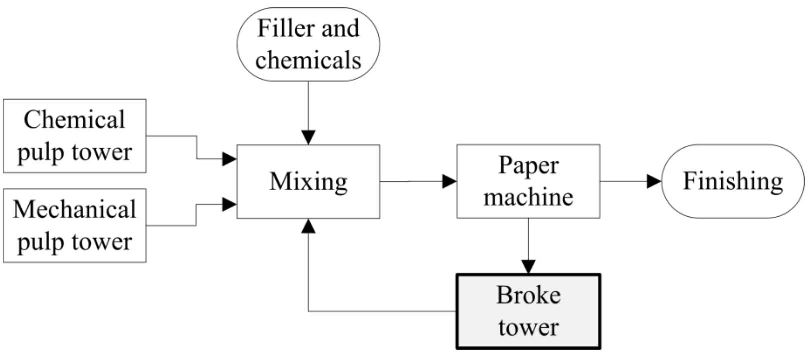

Figure 13. A diagram of the broke management case. The wasted production from the paper machine is fed to the broke tower and recycled back to process.

$$
\min_{\{u(n+k)\}_{k=0}^{K-1}} \left\{ \begin{array}{ll} \max\limits_{k=0,..,K-1} \left[\dfrac{p(V(n+k) \geq V_{max})}{p_{of}(k)} \right] & \text{(i)} \\ \sum\limits_{k=0}^{K-1} \gamma^k p_{br}(u_{eff}(n+k)) & \text{(ii)} \\ \sum\limits_{k=0}^{K-1} \gamma^k q_{filler}(n+k)^2 & \text{(iii)} \\ \sum\limits_{k=0}^{K-1} \gamma^k \left(u(n+k-1) - u(n+k) \right)^2 & \text{(iv)} \end{array} \right. \tag{43}
$$

$$
\begin{aligned} s.t. \quad & P(V(n+k) < 0) = 0 \\ & 0 \leq u(n+k) \leq u_{\max} \end{aligned}
$$

where V_{max} is the capacity of the broke tower, i.e. the maximum amount of broke in the tower, $V(n)$ is the amount of broke in the tower at time n, q_{filler} is the filler content deviation, p_{br} is the probability of breaks, $u(n)$ is the broke dosage from the storage tower to the process, γ is a time-discounting factor for the objectives, $p_{of}(k)$ is a function of accepted risk of an overflow k time steps from the present time n, and u_{eff} is an effective dosage defining the dynamics between the broke dosage and the break probability with s as a vector of coefficients:

$$
u_{eff}(n) = \sum_{i=1}^{\infty} s(i)u(n-i) \qquad \sum_{i=1}^{\infty} s(i) = 1 \tag{44}
$$

The filler content deviation is defined as a transient/impulse with coefficients that sum up to zero as

$$
q_{filler}(n) = \sum_{i=1}^{\infty} h(i)u(n-i) \qquad \sum_{i=1}^{\infty} h(i) = 0 \tag{45}
$$

where $h(n)$ is the vector of the filler response coefficients chosen to correspond to typical closed loop filler dynamics on paper machines. The discrete-time dynamics of the broke tower are described as

$$
V(n+1) = V(n) - u(n) + (1 - b(n))v_0 + b(n)v_1 \tag{46}
$$

where v_0 is the amount of broke generated per time step when there is no break and v_1 is the amount of broke generated during a break ($v_1 >> v_0$). Table 5 provides an example of the values used in this study.

The challenge in this case lies in the random occurrence of breaks. The level of broke in the storage tower depends on the number of breaks. As the controls should be optimized several hours ahead, the time within breaks during the optimization horizon should be known. As the actual number of breaks is not known in advance, the problem must be

Table 5. An example of typical process values of the nominal values used in Case 4. VU refers to volume unit.

Variable	Nominal value	Process (e.g.)
Time step	1	5 min
Broke generated during normal run (v_0)	0.1 VU/time step	0.14 m^3/min
Broke generated during a break (v_1)	10 VU/time step	14.4 m^3/min
Typical broke dosage (u)	2 VU/time step	2.88 m^3/min
Tower capacity (V_{max})	400 VU	2880 m^3

solved based on the probability of breaks. In this study, the break state is described as a binary variable (b), 0 denoting the normal run and 1 that the break is on. The probabilities of the break is on $p(b(n)=0)$ and off $p(b(n)=1)$ at time instant n are modelled as a two-state Markov chain

$$\begin{bmatrix} p(b(n)=0) \\ p(b(n)=1) \end{bmatrix} = \begin{bmatrix} 1-p_{br}(n) & p_{rec}(n) \\ p_{br}(n) & 1-p_{rec}(n) \end{bmatrix} \begin{bmatrix} p(b(n-1)=0) \\ p(b(n-1)=1) \end{bmatrix} \tag{47}$$

where $p_{br}(n)$ and $p_{rec}(n)$ are the transition probabilities for a break beginning and recovering from the break, respectively. Here, it is assumed that the use of broke pulp weakens the paper web which increases the probability of further breaks. The break probability is defined as a function of the effective broke dosage (u_{eff}) as follows.

$$p_{br}(u_{eff}(n)) = p_{min} + \frac{p_{max} - p_{min}}{1 + \exp\left(-\dfrac{u_{eff}(n) - u_{th}}{\sigma_w}\right)} \tag{48}$$

where p_{min} is the break probability at low broke dosage, p_{max} is the upper limit at high broke dosage, u_{th} defines the threshold which the dosage considerably increases the break risk, σ_w describes how rapidly the transition from regular break risk to increased break risk occurs as a function of dosage. In this study the parameter values used are u_{th}= 2, σ_w = 0.2, p_{min}= 0.03, and p_{max}= 0.1. The recovery probability $p_{rec}(n)$ is assumed constant. Based on these, the probabilities of the number of breaks for each time instant on the horizon can be calculated (Figure 14). A vicious circle arises easily as during a break the storage tower fills up quickly and it is necessary to dose higher amount of broke to the process, but at the same time the risk of further breaks increases. Furthermore, rapid changes of broke dosage are likely to deteriorate the end product quality as the feedback control of filler and chemicals cannot be adjusted quickly enough to meet the new conditions. Optimization of the broke dosage has been also studied e.g. by Bonhivers et al. (2002), Lama et al. (2003), Dabros et al. (2004), Dabros et al. (2005),

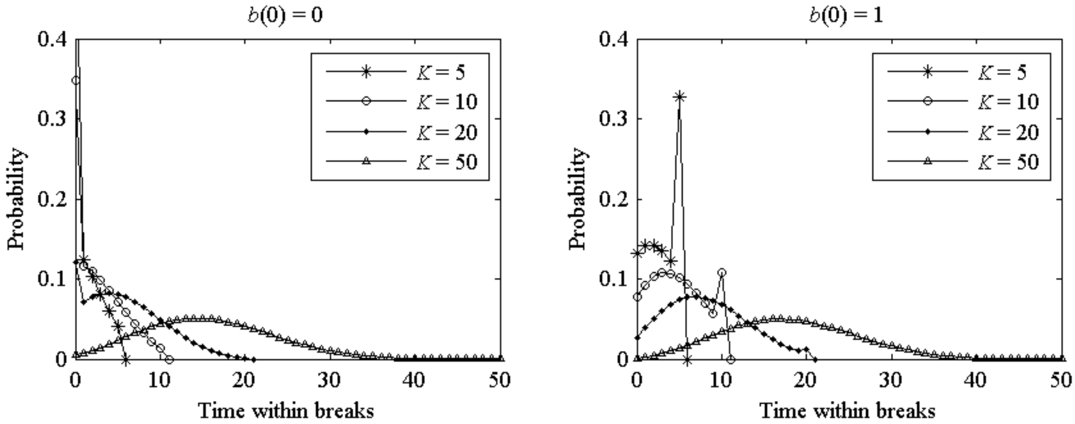

Figure 14. The probabilities of the time within breaks for four prediction horizons (5, 10, 20, 50). Left, the probabilities are calculated for the initial state *b* = 0, i.e. break is on. Right: the probabilities are calculated for the initial state *b* = 1. Note that for long horizon (*K* = 50) the initial state does not have impact on the probabilities, whereas for short horizon (*K* = 5) the initial state has a strong impact.

and Berton et al. (2006), but in these studies broke dosage has not been considered affecting the break risk.

The design objectives in Case 4 are to minimize the investment cost associated with the storage tower capacity, and to maximize the process performance. The process performance is defined as expected values of the operational objectives. The problem takes a form

$$\min_{d} \begin{cases} H(V_{max}) \\ -E_{\Psi}\{T_{of}\} \\ E_{\Psi}\{p_{br}\} \\ E_{\Psi}\{q_{filler}^{2}\} \\ E_{\Psi}\{(u(n+1)-u(n))^{2}\} \end{cases} \tag{49}$$
$$s.t.\ V_{max} \geq 0$$

where $E_{\Psi}\{\}$ denotes the expectation value of the system performance as Ψ is the stochastic process with applied dosage policy, $H(V_{max})$ is the investment cost of the tower capacity V_{max}, and T_{of} is the time until the broke tower overflows. The degrees of freedom are the capacity of the broke tower and the parameters from the operational level.

5.5 Case 5: Flow management at SC production line

Publication VI studies an extended version of the broke management case presented in Section 5.4. The case consists of four storage towers whose levels are manipulated by five control flows. At the design level the target is to determine the capacity of the towers and the related scalarization parameters of the operational management whereas the target at the operational level is to determine the flow operation during the run. The towers are clear water, white water, broke, and dry broke towers. The control flows to be optimized are broke dosage, dry broke pulping rate, white water dosage, recycled water flow from disc filter to white water, and clean water intake, denoted in Figure 15 by $u_1,\ldots,u_5$, respectively.

The number of quality properties is in this study increased to three: filler content (q_{filler}), amount of material per web area i.e. basis weight (q_{bw}) and web strength ($q_{strength}$). The target is to minimize the squared deviation of each quality variable from its set point while preventing any of the towers running empty or overflowing. The control flows $u_1,\ldots,u_5$ should be optimized several hours ahead. The challenges are similar as in the broke management case: breaks affect the process by disturbing the balance between the towers and by deteriorating the quality of the end product. In this case the balance between the four towers becomes even more critical as during a break

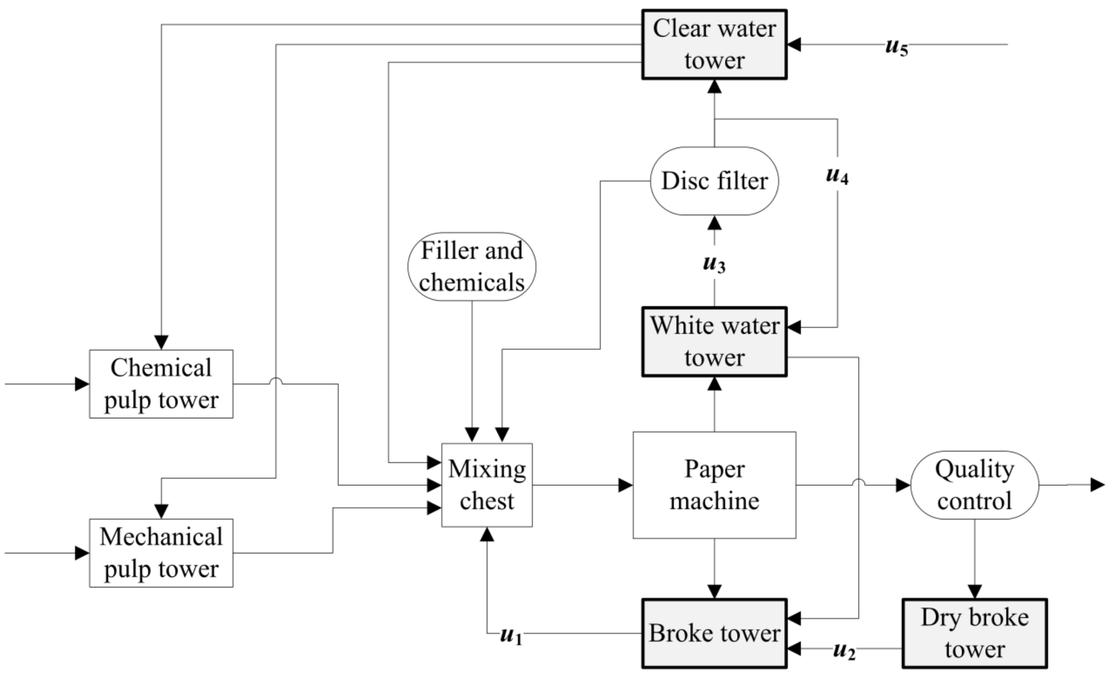

Figure 15. A diagram of Case 5. The towers considered are: clear water, white water, broke and dry broke towers. The flows to be optimized are denoted by $u_1,\ldots,u_5$.

broke tower starts to fill up, while the white water tower runs empty. The operational optimization is formulated as follows.

$$\min_{\{u(n+k)\}_{k=0}^{K-1}} \begin{cases} \sum_{k=0}^{K-1} \gamma^k \left(q_{filler}(n+k+1) - q_{0,filler}\right)^2 \\ \sum_{k=0}^{K-1} \gamma^k \left(q_{bw}(n+k+1) - q_{0,bw}\right)^2 \\ \sum_{k=0}^{K-1} \gamma^k \left(q_{strength}(n+k+1) - q_{0,strength}\right)^2 \\ \sum_{k=0}^{K-1} \gamma^k \left(u(n+k) - u(n+k-1)\right)^2 \end{cases} \tag{50}$$

$$s.t. \quad V_{min,i} \le V_i(n) \le V_{max,i}$$
$$u_{min,j} \le u_j(n) \le u_{max,j}$$

where $i = 1, \ldots, 4$ stands for the clean water, white water, broke, and dry broke towers, respectively, $V_i(n)$ is the volume of water/pulp in the tower i at time n, $V_{max,i}$ and $V_{min,i}$ are the maximum and minimum volumes of material in the towers, and $u(n)$ is a vector of controls $u_1, \ldots, u_5$, with $u_{min,j}$ and $u_{max,j}$ as the lower and upper bounds. The paper quality for the prediction model is defined as

$$Q(n+k) = Q(n) + \sum_{k'=1}^{K_m} D(k')\left(u(n+k-k') - u(n-k')\right) \tag{51}$$

where $Q(n) = \begin{bmatrix} q_{filler}(n) \\ q_{bw}(n) \\ q_{strength}(n) \end{bmatrix}$

and $D(k')$ is a matrix of coefficients obtained through step response tests by changing one control variable at a time and K_m is the model order. Thus, the current quality is assumed to depend only on the actions taken within the previous K_m time steps. Similarly to Eq. (46), the tower dynamics of Case 5 are presented as

$$V(n+1) = V(n) + Au + Bb(n) + C \tag{52}$$

where A, B, and C are modelling matrices obtained through expert knowledge. The break state probabilities are modelled as a two-state Markov chain (see Eq. (47)). The transition probabilities $p_{br}(n)$ and $p_{rec}(n)$ are assumed to be in the following relationship to the paper strength:

$$\begin{aligned} p_{br}(n) &= \min\left\{a_A \exp\left[a_B / \left(s(n) - s_{0,br}\right)\right], 1\right\} \\ p_{rec}(n) &= \max\left\{1 - a_C \exp\left[a_D / \left(s(n) - s_{0,rec}\right)\right], 0\right\} \end{aligned} \tag{53}$$

where $s_{0,br}$ and $s_{0,rec}$ are the nominal strength indices for a break and a recovery from a break, respectively, a_A, a_B, a_C, and a_D are parameters, and $s(n)$ is the current strength of the paper. The current strength is in the nominal model calculated with respect to the composition of the paper web.

6 Summary of the analysis results

This chapter summarizes the analysis of the cases presented in Chapter 5. The analysis is based on the methodology presented in Chapter 4. The models used in the cases are assumed to be known, thus modelling issues are not covered. The experiments are based on computer simulations. Section 6.1 presents results of operational problems, including optimal measurement scheduling. Section 6.2 presents results of process design problems, including measurement design tasks. The main focus in the analysis is to show how the methodology can be applied to practical cases. The cases are somewhat idealized compared to practical conceptual process design because the emphasis in this work is on the development of the methodology.

6.1 Operational management

Process operation is discussed in Publications I−IV and VI. The task in Cases 1−3 (Publications I−II) is to optimize the control and measurement actions over a time horizon by minimizing the operational costs caused by the future states and actions. In these cases the states and actions are discrete valued and the state information is uncertain. The problems include optimization of both the controls and measurements. Cases 4−5 (Publications III−IV) are continuous state studies. The state information is expected to be known, thus there is no measurement uncertainty, but the process is highly unpredictable and stochastic due to the sudden changes of the operating point.

6.1.1 Cases 1−2

Cases 1−2 are simple Markov processes. They are studied using POMDP techniques. The task in Case 1 is to optimize measurements and controls of a two-state system. The problem is solved using the exact POMDP algorithm. The use of exact algorithm is possible as the problem is small. Figure 16 presents the decision vectors of Case 1 for the infinite horizon. The decision plane consists of three alternatives depending on the

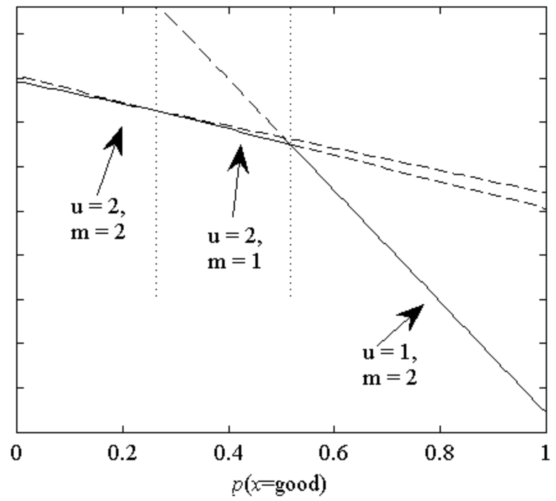

Figure 16. Optimal action vectors for Case 1.

information about the current state of the system. If the probability of the state "good" is larger than 0.52, the optimal action is to run as usual (u = 1) and measure at the next time step (m = 2). If the probability of the state "good" is between 0.26 and 0.52, the optimal action is to make a correction (u = 2), but not measure (m = 1). If the probability of the state "good" is rather unlikely, smaller than 0.26, the optimal action is to make a correction (u = 2) and measure afterwards (m = 2). As the problem is solved for all information about the current state, there is no need to recalculate the actions. Thus, the same actions are optimal also in the future.

The task in Case 2 is similar to Case 1, but this time the number of states and controls is increased to three. The problem is solved using a point-based algorithm (Pineau et al., 2003; Spaan and Vlassis, 2005), in which the planes of the optimal actions are calculated based on predefined points in the state information space. Here, a regular grid of points is chosen. Figures 17−20 present the decision planes of Case 2. As the system consists of three states, the decision planes can be illustrated using two dimensional triangles where the horizontal and vertical axes present probabilities of two of the states and the probability of the third state is $1-p(x=\text{"good"})-p(x=\text{"acceptable"})$. Thus, at the end of the horizontal axis the probability of the state "good" is 1, at the end of the vertical axis the probability of the state "acceptable" is 1, and in the origin the system is certainly in the poor state. In Figures 17−19, the optimal actions planes are presented for the prediction horizons K = 2, K = 5, and K = 8. The grid points are shown as dots, whereas the lines illustrate the decision borders. Thus, the areas illustrated in colours present the decision planes where the optimal actions are same. The legends refer to the optimal actions, first number indicating the optimal control and the latter the optimal measurement option. From the figures it can be seen that for shortest horizon only the controls u = 1 and u = 2 are used. For longer horizon it becomes more important to ensure that the process turns to state "good", and the plane of the control u = 3 becomes larger. Also with longer time horizon, the importance of measuring grows.

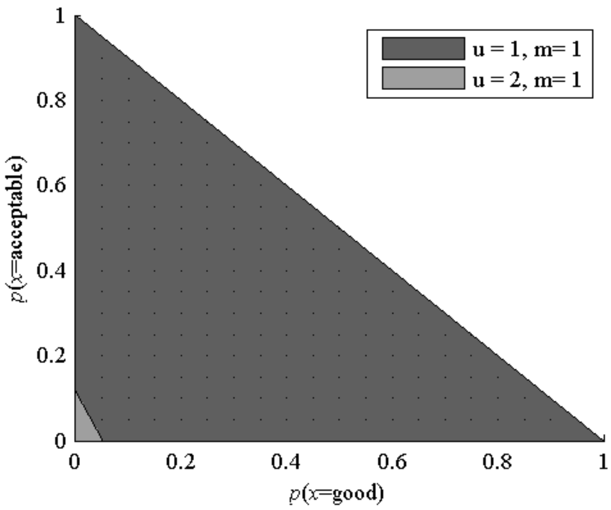

Figure 17. Decision planes of Case 2 for the prediction horizon K = 2. For majority of the state probabilities the optimal actions are to control u = 1 and to measure m = 1. Only close to the origin, thus when the state is most certainly "poor", the optimal action is to control 2.

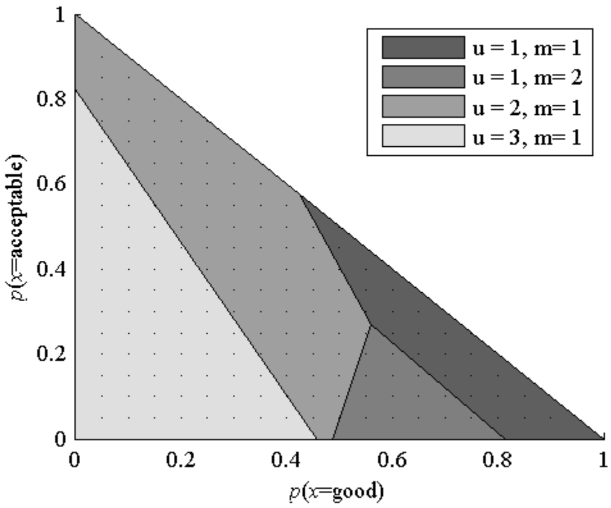

Figure 18. Decision planes of Case 2 for the prediction horizon K = 5. The number of decision planes is increased to four. For example, if the probabilities of the state are [0.2 0.7 0.1], the optimal actions are to control u = 2 and not to measure (m = 1).

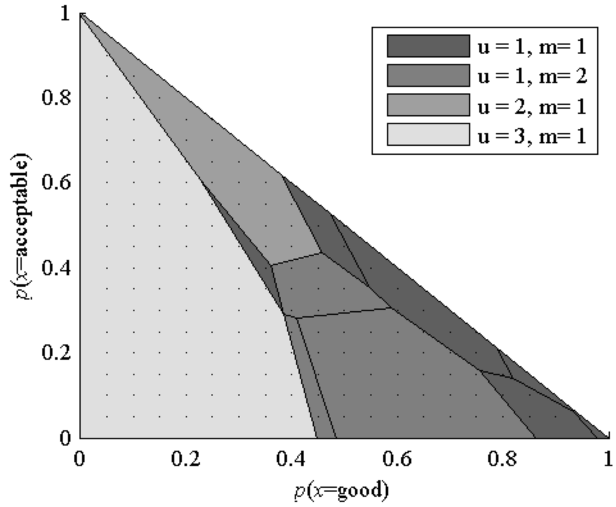

Figure 19. Decision planes of Case 2 for the prediction horizon K = 8. The number of the optimal α-vectors is increased to 11, but the number of optimal action alternatives is still four. The area of the measurement option 2 is larger than in the case of the prediction horizon K = 5.

The above results are calculated using the point-based approximate algorithm. As a comparison, the same problems are also solved using the exact algorithm for POMDP problem. In Figure 20, solution for the prediction horizon K = 8 is showed. The result differs slightly from the result obtained using point-based algorithm as the number of α-vectors is 11 in the approximated case and 13 in the exact case. However, as it can be seen from Figures 19 and 20, the difference in the decision planes is quite minor. The calculation time is about 400-fold using the exact solution algorithm.

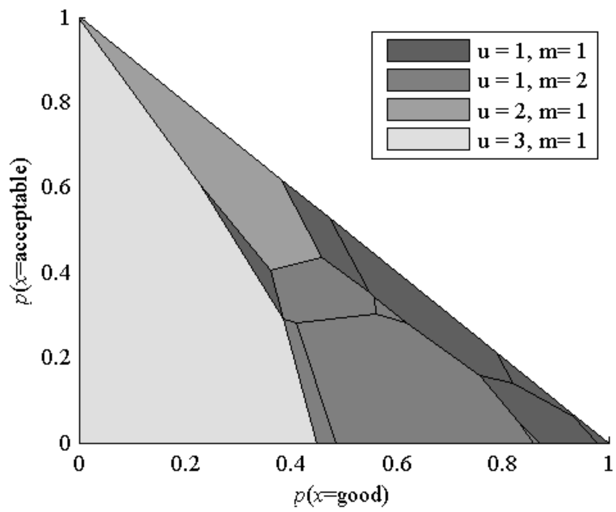

Figure 20. Case 2 of prediction horizon K = 8 solved using the exact POMDP algorithm.

6.1.2 Case 3

The task in Case 3 is to manage paper brightness and strength by manipulating the fibre fraction ratio and the dosage of the bleaching chemicals. The case is an extended version of Cases 1 and 2, but as it consists of correlated variables with different delays, it is far more complicated as the previous problems, and it cannot be solved using the tools for POMDP. The problem is solved using a rather brute force method, i.e. by propagating the prior probabilities forward in the horizon and calculating the costs backwards. The method provides an exact solution but is computationally demanding. For each time instant, 18 combinations of actions (control and measurement) exist, hence with prediction horizon $K = 3$, over 5800 action options are available. Taking into account the observation alternatives, almost 37000 cost values need to be calculated to obtain the optimal action sequence for a single time instant.

Table 6 summarizes an example of the results where the simulated process is managed according to the optimized actions. The simulation starts from a situation where both quality variables are at the state ‘low’ ($x_b = 2$, $x_s = 2$). At the first time instant $t = 0$, the optimal control of bleaching chemical is $u_b = 2$, the optimal control of the fibre fraction ratio $u_f = 3$, and the optimal measurement choice is to observe strength. The measurement value obtained is 4. The optimal measurement choices for the following time instants are to measure brightness (k=2) and strength (k=3). The cost for poor strength has been defined higher than the cost for poor brightness, and hence it is reasonable to control strength prior to brightness. At time instants $t = 1,\ldots,4$, the simulation is in a balance and the measurements follow the schedule from previous time steps. At $t = 4$, measurement value of the strength is unexpectedly low ($z_s = 1$), and the measurement

Table 6. Summary of the case study results with optimization horizon $K = 3$. In all pairs in the table, the first value refers to the brightness (b) and the second to the strength (s). The first line presents the values of the measurements chosen to be made, '–' denoting that measurement is not made. The second line gives the optimal and implemented actions based on the measurement value. The third line gives the true (non-observable) process states (note the different scale of measurements and states). For the future time instants $k = 2$ and 3, only the optimal measurements are given.

		$t = 0$		$t = 1$		$t = 2$		$t = 3$		$t = 4$		$t = 5$		$t = 6$		$t = 7$		$t = 8$	
k	variable	b	s	b	s	b	s	b	s	b	s	b	s	b	s	b	s	b	s
1	Meas. value (z)	–	4	4	–	–	4	4	–	–	1	–	6	–	4	4	–	–	6
	Opt. control (u)	2	3	2	2	2	3	2	3	2	3	2	2	2	3	2	2	2	2
	True state (x)	2	2	2	2	2	3	2	2	2	1	2	3	2	2	2	3	2	3
2	Opt. meas. (m)	m	–	–	m	m	–	–	m	m	–	m	–	m	–	–	m	m	–
3	Opt. meas. (m)	–	m	m	–	–	m	m	–	–	m	m	–	–	m	m	–	–	m

schedule is updated. The next measurement value is however surprisingly high (z_s = 6), and the schedule is again changed. After this sudden disturbance, the process returns to normal and measurement scheduling is again balanced.

6.1.3 Cases 4−5

The task in Case 4 is to manipulate the dosage of the discarded production while preventing the broke tower running empty (i), minimizing the time within breaks (ii), managing the filler variation of the paper (iii), and assuring the smoothness of the broke dosage (iv). The task in Case 5 is similar to Case 4, only that the problem is increased to cover four towers and the number of quality properties is increased to three.

The problems are solved using similar strategies. The objectives of preventing the towers running empty or over are formulated as constraints. The rest of the objectives are summed together by introducing scalar factors behaving as weights. Thus, the multiobjective problems are reformulated as a single-objective optimization problem. In both cases the scalarization leads to a quadratic objective function. The challenge lies in the unpredictable occurrence of breaks as the level of the towers depends on the number of breaks (see Eq. (46) and Eq. (52)). In order to solve the optimization problem, the user must define an acceptable risk for the towers running empty or over. If no risk is accepted, the problem must be solved with an assumption that break is on at each time instant, which is unlikely and hence restricts the problem solving (see Ropponen and Ritala, 2012). By utilizing the user-defined risk, the number of breaks to be prepared of can be calculated and the problem can be solved using quadratic programming tools. The optimization problem of Case 4, takes a form

$$\begin{aligned}
&\min_{\{u(n+k)\}_{k=0}^{K-1}} \sum_{k=0}^{K-1} \gamma^k \left(c_f(n+k)^2 + \alpha\big(u(n+k)-u(n+k-1)\big)^2 + \beta u(n+k-1)^2 \right) \\
&s.t. \quad P(V(n+k) > V_{\max}) \le 1-(1-p_0)^k \equiv p_{of}(k) \\
&\qquad\;\; P(V(n+k) < 0) = 0 \quad k = 1,\dots,K \\
&\qquad\;\; 0 \le u(n+k) \le u_{\max} \quad k = 1,\dots,K
\end{aligned} \tag{54}$$

where α and β are the scalarization parameters required to transform the multiobjective problem into a single objective problem, and p_0 is a parameter for the accepted overflow risk. Thus, the control design needs to specify the parameters γ, β, p_0, K, and γ. By utilizing Eq. (46), the constraint of the broke tower overflow can be rewritten as

$$-\sum_{k=0}^{K-1} u(n+k) \le V_{\max} - V(n) - kv_0 - (v_1 - v_0) F^{-1}_{Z_{b(n)}(k)}(1 - p_{of}(k)) \tag{55}$$

where $Z_{b(n)}(k)$ is the number of breaks between time instants $n+1$ and $n+k$ and F_Z denotes its cumulative distribution. Correspondingly, the optimization problem of Case 5 takes a form

$$\begin{aligned}
&\min_{\{u(n+k)\}_{k=0}^{K-1}} \sum_{k=0}^{K-1} \gamma^k \left(\left(Q(n+k+1)-Q_0\right)^T W \left(Q(n+k+1)-Q_0\right) + \left(\alpha^T \left(u(n+k)-u(n+k-1)\right)\right)^2 \right) \\
&s.t. \quad A_i \sum_{k'=0}^{K-1} u(n+k') \le V_{\max,i} - V_i(n) - kC_i - B_i F^{-1}_{Z_{b(n)}(k)}\left(p_i^{(up)}(k)\right) \\
&\qquad -A_i \sum_{k'=0}^{K-1} u(n+k') \le V_i(n) + kCi + B_i F^{-1}_{Z_{b(n)}(k)}\left(p_i^{(down)}(k)\right) - V_{\min,i} \\
&\qquad u_{\min,j} \le u_j(n) \le u_{\max,j}
\end{aligned} \tag{56}$$

where $\alpha = [\alpha_1 \quad \alpha_2 \quad \alpha_3 \quad \alpha_4 \quad \alpha_5]$ is a scalarization vector for the controls, A, B, and C are modelling matrices obtained through expert knowledge, Q is a vector of the quality variables (Eq. (51)), Q_0 includes the set points for the quality variables, and W is a matrix for the scalarization weights:

$$W = \begin{bmatrix} w_1 & 0 & 0 \\ 0 & w_2 & 0 \\ 0 & 0 & w_3 \end{bmatrix}.$$

Here $p_i^{(up/down)}(k)$ is a function of the accepted risk that the tower runs over or empty, for exact expression, see Table 7. As web breaks do not cause major disturbances to the clean water and dry broke towers, no risk for tower flowing over or running empty is accepted, and B_i is chosen to be 0 for them. The control design needs to specify the parameters K, $p_2^{(up)}$, $p_2^{(down)}$, $p_3^{(up)}$, $p_3^{(down)}$, $\gamma(k)$, w_1, w_2, w_3, α_1, α_2, α_3, α_4, α_5.

With the almost linear constraints, both of the problems (Cases 4 and 5) turn out to be close to the quadratic programming (QP) form. As the break probability depends on the web strength which in turn depends on the optimized control actions, iteration steps may be required before the final solution as described in Publications III and IV. The above problems are studied in the model predictive control (MPC) scheme by simulating the process together with the operational optimization. Figure 21 presents an

Table 7. Function of the accepted risk that the white-water and broke towers run empty or over.

	$p_i^{(up)}(k)$	$p_i^{(down)}(k)$
White water tower	$1-\left(1-p_2^{(up)}\right)^k$	$\left(1-p_2^{(down)}\right)^k$
Broke tower	$\left(1-p_3^{(up)}\right)^k$	$1-\left(1-p_3^{(down)}\right)^k$

example of such simulation for Case 4. The simulation begins from the initial states $b(0) = 0$ and $V(0) = 0$, i.e. no break and the broke tower is empty, and it is continued until the broke tower flows over. At the beginning the broke dosage is low and the level of the broke tower rises. At $t = 290$ the broke dosage is increased quickly due to the break state and high level of broke in the storage tower. That causes transient peak to the filler content variation. The quick increase of broke ratio recurs also at $t = 356$ and $t = 425$, but after the last rise, the dosage decreases slowly to value close to zero. It is noteworthy that as the smoothness of the broke dosage was chosen to be one of the objectives, the recovery from the high dosages is slow. However, the rising of the dosage is very rapid due to the importance of preventing the storage tower running over. At $t = 925$ the dosage is again increased rapidly, and 100 time steps later, the broke tower overflows due to the frequent breaks. It is worthwhile to point out that for illustrating purposes the break probability is chosen rather high in this study.

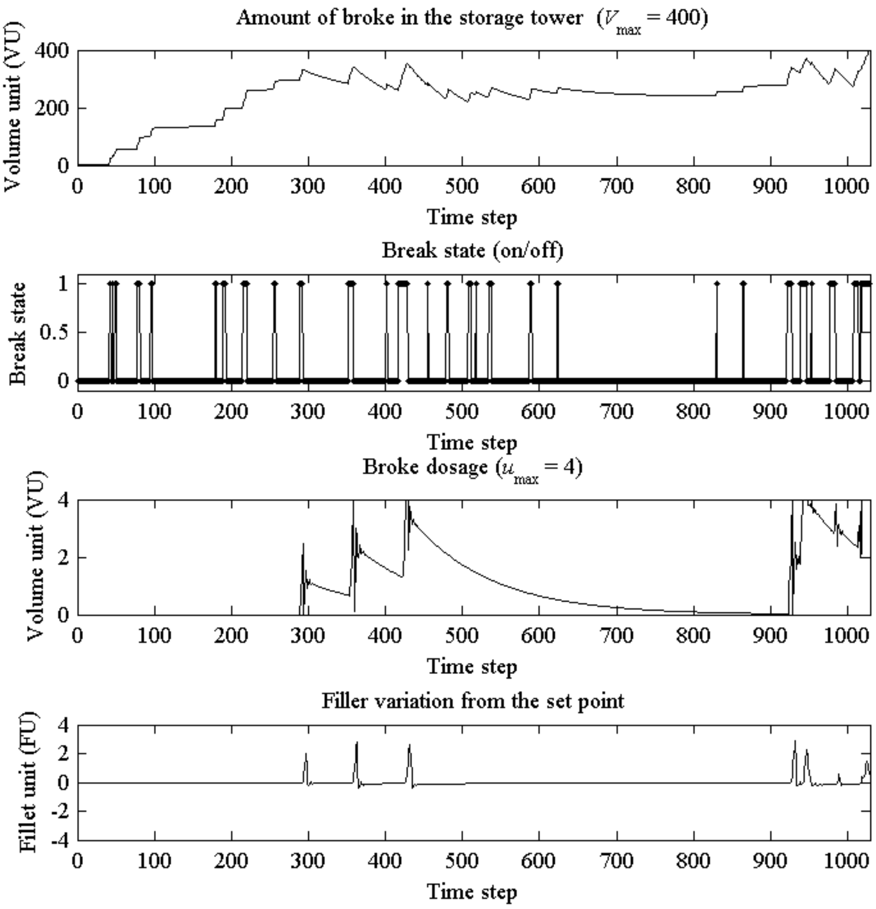

Figure 21. Example of the process simulation in Case 4. Broke dosage is obtained from the operational optimization. The parameter values used are α = 0.1, β = 0.01, p_0 = 0.01, K = 30, and γ = 0.99^k. Time step corresponds to 10 min.

Figure 22 presents an example of similar simulation for Case 5 where the process is simulated for 5000 minutes. In this case, the features of the process are not as clear as in Figure 21 for Case 4, but still the effects of the break instants can be seen e.g. in broke and white water towers whose levels correlate with the breaks but in reversed ways.

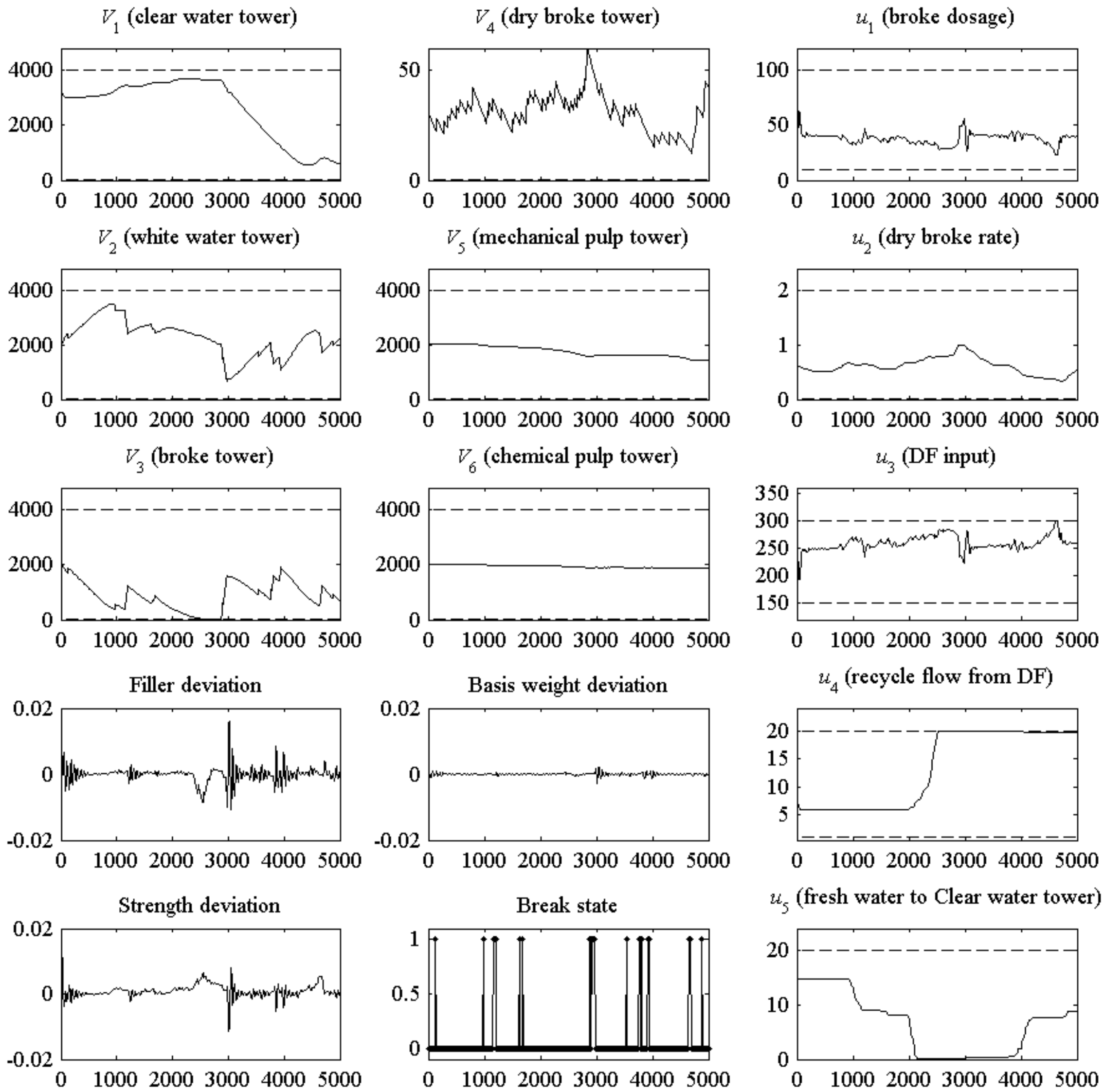

Figure 22. Example of the process simulation in Case 5. Flows $u_1,\ldots,u_5$ are obtained from the operational optimization. In each plot the vertical axis is time in minutes, time step being 10 min. Dash lines are the minimum and maximum values of each variable. For filler, basis weight and strength, relative deviation from their set point is presented. The parameter values used are: $K = 50$, $K_m = 30$, $p_2^{(up)} = p_3^{(down)} = 0$, $p_2^{(down)} = p_3^{(up)} = 0.05$, $\gamma(k) = 0.99^k$, $w_1 = 1/0.01^2$, $w_2 = 1/0.1^2$, $w_3 = 1/0.05^2$, $\alpha_1 = \alpha_3 = \alpha_5 = 0.05/u_j^{(nom)}$, $\alpha_2 = \alpha_4 = 0.5/u_j^{(nom)}$, where $u_j^{(nom)}$ is the nominal value of each control flow.

6.2 Process design

Process design problem for Cases 2, 4, and 5 are discussed in Publications II, IV, V, and VI. The design task in Case 2 (Publication II) is to examine the value of a measurement device with respect to the measurement accuracy. The design task in Cases 4 and 5 is to determine the optimal capacity of the storage towers by minimizing the investment cost associated with the tower capacity while maximizing the performance (Publications IV and VI) and to estimate a value of new measurement device (Publication V). Robustness is analysed only for Case 4 (see Section 6.3). The maintenance problem in Case 2 is formulated by presenting the objectives in monetary values, whereas the tower volume problems are formulated as multiobjective optimization problems with conflicting criteria. The problems are solved according to the methodology presented in Section 4.4, i.e. by simulating the processes over a time horizon for each design candidate and calculating the means.

6.2.1 Case 2

The design task in Case 2 is examined with test cases where the measurement accuracy is the degree of freedom. Thus, the operational problem is solved and the triangle-shaped decision plane obtained for a set of design parameter values *d*. The optimization horizon is K = 8. As the system is stochastic and the initial state affects the operation, simulations for each design option are repeated 100 times. The expected operational costs $G(d,\pi)$ during the simulation time are calculated as a mean of these 100 simulations:

$$E\{G(d,\pi)\} = \frac{1}{100}\sum_{r=1}^{100}\sum_{t=1}^{1000} g\left(x_{t,r}, m_{t,r}, u_{t-1,r}\right) \tag{57}$$

where g is the operational cost as a function of the state and actions. The value of a more accurate measurement device can be analysed by comparing the mean operational costs between the studied design options. Figures 23 and 24 present the decision planes for d = 0.1 and d = 0.2. The system is simulated according to the optimized actions and the operational costs are calculated. Each simulation run is started from a randomly chosen initial state and the simulation is carried on till 1000 time steps. The true state is simulated in parallel to sample measurement data. The probability states attained in the simulations are expressed by black crosses (×) in Figures 23 and 24. It can be seen that during the simulation (1000 time steps) only a limited set of probability points are visited.

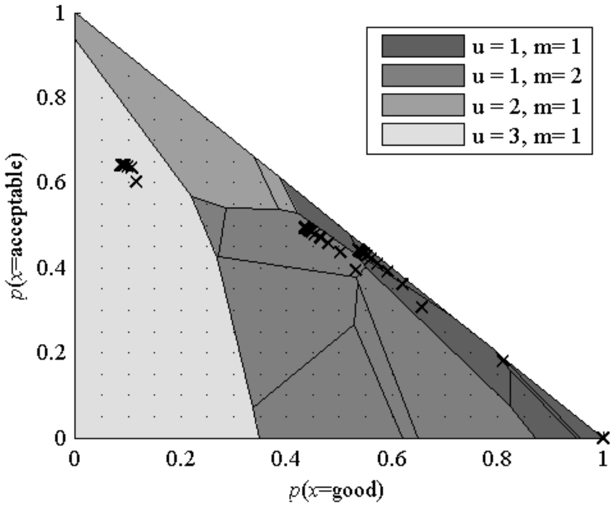

Figure 23. Decision planes 1 for *d* = 0.1 in Case 2. The expected operational costs over 1000 time steps were 514 units.

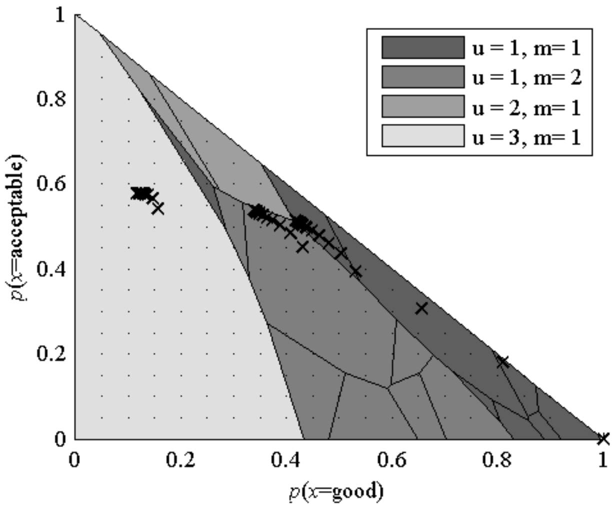

Figure 24. Decision planes for *d* = 0.2 in Case 2. The expected operational costs over 1000 time steps were 530 units.

Figure 25 presents the growth of the operational cost as a function of the design parameter *d*. The diagram shows the expected operational cost in 1000 time steps. It can be seen that when comparing the design parameter values 0 and 0.2, the expected operational costs are about 40 units higher in the latter case. On the other hand, the operational costs do not increase for values larger than 0.2. An obvious reason for that can be seen in Figure 26, which presents the number of measurement made during the 1000 time instants. For large values of *d*, the measurement device is so inaccurate that measuring does not provide useful information compared to its cost, and measurements are not made.

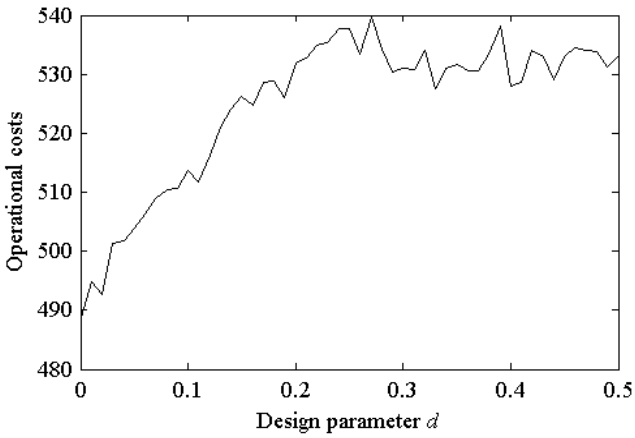

Figure 25. The growth of the operational costs as a function of the design parameter *d*.

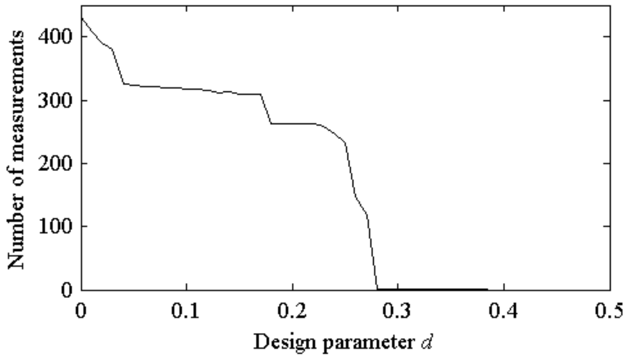

Figure 26. The number of measurements made during 1000 step simulation as a function of the design parameter *d*.

The results in Figure 25 can be used as a base for the analysis of the value of a more accurate measurement device. Of course for proper analysis, the operational costs should be calculated with respect to the real life time of the device by taking into account the discount factors as discussed in Chapter 4. In Publication II, also the effect of the controller performance on the measurement design is analysed by studying cases where the uncertainty in the system dynamics matrix is both impaired and improved. The results are also compared with an ideal case without measurement uncertainty.

It is important to notice, that after the design problem is solved i.e. the design parameter *d* is selected, the operational policy π is fixed. That means that once the decision planes, i.e. the areas in the triangle, are calculated for the selected design parameter, there is no need for recalculation of the controls. During the run, the operation just follows the policy defined by the design decision. Only if the process or the measurement system drifts in time (e.g. due to dirtiness), the decision planes need to be recalculated.

6.2.2 Cases 4−5

The design task in Cases 4 and 5 is to determine optimal capacities of the storage towers. In Case 4, only the broke tower volume is addressed whereas in Case 5 also white water, clear water and dry broke tower volumes are involved. In addition to the tower capacities, the scalarization parameters are degrees of freedom of the design problem. That is because the scalarization parameters define weights for the objectives and hence impact on the long-term performance. Thus, even though the operational policy cannot be solved offline as in Case 2, the design optimization still addresses the process operation.

For the design simulations, a set of design candidates is first selected. As the operational simulations are computationally heavy, the selected design space must be rather sparse. The expected values for each candidate are obtained through the operational process model simulations with the online optimization running in parallel. The simulations are executed until the broke tower in Case 4 or one of the four towers in Case 5 runs empty or over and repeated 20 times for calculating the means of the process performance objective function. For proper analysis the number of repetitions should be increased significantly, but for our purposes 20 repetitions is enough to present the methodological point of view. It has been studied that approximately 80 repetitions are needed for reliable estimates (Steponavice and Ruuska). In Case 4, the simulations are started using a design space of 126 options including 7 values for V_{max}, 6 values for β, three values for p_0, and one value for α, K, and γ. Figure 27 shows the design candidates with respect to the four objectives presented using the subsystem approach explained in Section 4.4. The circled candidate is chosen to be the most interesting in the decision maker's point of view.

The design analysis can be further carried out by introducing a new set of design candidates in the neighbourhood of the chosen design. These are presented in Figure 28. Now the decision maker can select a group of candidates from the set of the primary objectives (on the left). The final design can be selected from the Pareto optimal set of these candidates with respect to the secondary objectives (on the right). The selection of the design candidate not only fixes the tower capacity, but also the operational policy is decided as the scalarization parameters are degrees of freedom. However, the parameters can be modified later on if the process alters or the decision maker's opinion changes.

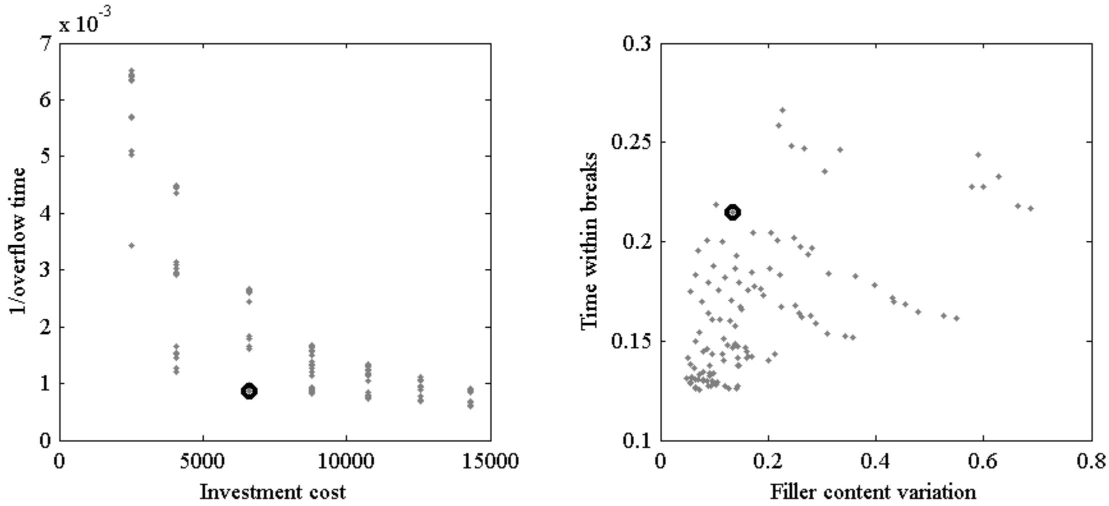

Figure 27. An example of the design plane obtained through simulations of 126 design candidates in Case 4 ($V_{\max}$ = [100 200 400 600 800 1000 1200], β = [0.01 0.02 0.03 0.05 0.08 0.1], p_0 = [0.1 0.01 0.001], α = 0.1, K = 30, $\gamma(k) = 0.99^k$). Left: Design solutions with respect to the investment cost and time until a production stop. Right: Same candidates at the filler-breaks plane. The decision maker's choice is marked by a circle. It is worthwhile to point out that for illustrating the properties of the system, break probability was chosen to be relatively high, and thus the time within breaks is high.

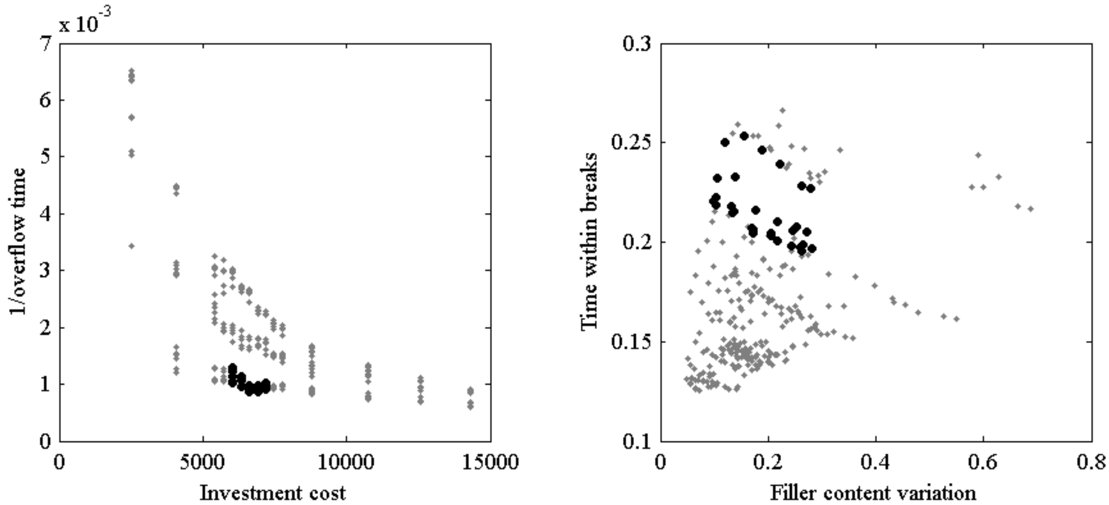

Figure 28. A new set of 144 design solutions is generated in the neighbourhood of the chosen design (V_{max} = [300 325 350 375 425 450 475 500], β, p_0, and α as before). The DM's choices from the set of the primary objectives are marked with black dots. The final decision can be selected from the Pareto optimal set of these candidates amongst the secondary objectives.

A similar study is also carried out for Case 5, although without the extended analysis of the design candidates. Figure 29 presents the set of design candidates with respect to the primary and secondary objectives. The Pareto optimal candidates with respect to the

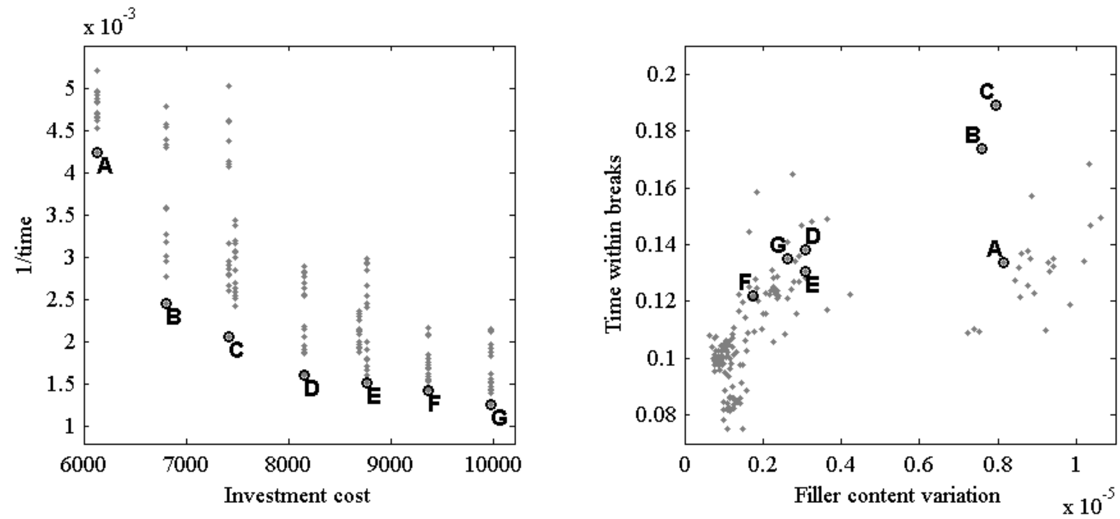

Figure 29. Example of the design plane obtained through simulations in Case 5 ($V_{max,1}$ = [2000 3000 4000], $V_{max,2} = V_{max,3}$ = [2000 3000 4000], $K = 50$, $K_m = 30$, $\gamma(k) = 0.99^k$, $p_2^{(down)} = p_3^{(up)}$ = [0.01 0.05], $p_2^{(up)} = p_3^{(down)} = 0$, w_1 = [0.5 1 2]/0.01^2, w_2 = [0.5 1 2]/0.1^2, $w_3 = 1/0.05^2$, $\alpha_1 = \alpha_3 = \alpha_5 = 0.05/u_j^{(nom)}$, $\alpha_2 = \alpha_4 = 0.5/u_j^{(nom)}$. Left: Design solutions with respect to the investment cost and time until production stop, Pareto-optimal designs circled. Right: Same designs and Pareto-optimal set at the filler-breaks plane.

investment cost and the time until one of the towers runs empty or over (primary objectives) are circled, and presented also with respect to the filler content variation and time within breaks (secondary objectives).

The analysis of the process design can be further extended by analysing the value of a measurement device. For example, if the filler content of the recycled broke would be measured, the amount of fresh filler dosed to the mixing chest could be adjusted by feed-forward control. The task at the design level is to evaluate whether there is a financial benefit in the utilization of such information. The utility analysis is not straightforward but can be estimated by measuring the improvement with respect to the other objectives. For example, the value of the filler content measurement could be analysed by calculating the difference in the time within breaks. Here, the analysis is presented for Case 4. Figure 30 shows an example of the Pareto optimal design candidates with respect to the filler content variation and the time within breaks. If the filler content measurement were available, all the candidates would be shifted to the vertical axis as in the ideal case the filler content variation of the end product would turn to zero. Then, the optimal design would be the candidate denoted by (c) as it minimizes the time within breaks. If the filler content measurement is not available, the optimal solution depends on the DM's personal assessment, i.e. the DM decides the level of the acceptable filler content variation. In Figure 30, the filler variation limits 0.12 and 0.2 are marked by dotted lines and the optimal designs denoted by (a) and (b).

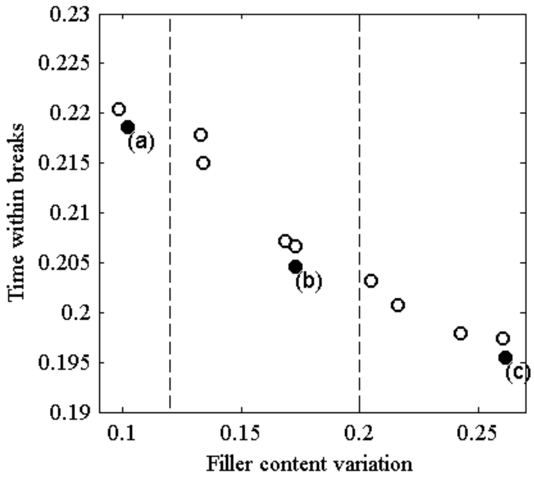

Figure 30. The Pareto curve amongst which the final design should be chosen. Dotted lines indicate the filler variation limit 0.12 and 0.2. Black dots (a), (b), and (c) are the optimal solutions for the chosen limits.

The value of the filler content measurement can be analysed by comparing the improvement in the time within breaks. The values of the cases (a), (b), and (c) are collected to Table 8 and it can be seen that the time within breaks is decreased more than two percentage points from the solution (a) to the solution (c). The final decision about the utility of the filler content measurement should be analysed based on the price and the maintenance costs of the device and the operational costs caused by the higher time within breaks.

6.3 Robustness

The above results of Cases 4–5 rely heavily on the assumption that the break probability model is known (see Eq. (48) for Case 4). In reality it is not known precisely and there is significant uncertainty about the model. To examine the robustness towards the

Table 8. The time within breaks in % at the selected filler variation level. Note that for illustrating purposes the break probabilities was chosen to be rather high.

	Filler content variation	Time within breaks
Filler limit 0.12	0.1021	0.2186
Filler limit 0.2	0.1729	0.2046
With filler measurement	0	0.1974

Table 9. Additional break probability parameters used for the robustness simulations in Case 4 (see Eq. 48). In the original simulations, medium (Med) probabilities were used.

Break probability level	$p_{\min}$	$p_{\max}$
High	0.05	0.12
Med	0.03	0.1
Low	0.01	0.08

break probability, the design simulations of the chosen design candidate in Case 4 are rerun using different break probability parameters in the simulator than in the optimizer. The parameter options for the break probability model are shown in Table 9. The parameter values are cross-studied, thus nine simulation runs are carried out.

Results of the cross-studied robustness simulations for one design candidate are collected in Table 10. For example "High/Low" means that the parameter values of the real process i.e. simulator are "High", but in the optimizer values "Low" are used. It can be seen that in this case, the mean overflow time is more than 50 units lower and the mean filler variation more than 0.04 units higher compared to the case where the probability model ‘High’ is used also in the optimizer. On the other hand, the time within breaks is a bit higher in the case "High/High" than in the case "High/Low". That is result of a tighter broke dosage policy in the case "High/High". If the break probability is high it is reasonable to keep the dosage higher to prevent the tower overflow. Meanwhile the risk of further breaks increases. The same occurrence can be seen in the other cases. Based on these, it seems reasonable to overestimate the break probability,

Table 10. Robustness analysis of the selected design for three break probability functions.

Break probability (real process /optimizer)	Overflow time	Filler variation	Time in breaks
High/ High	491.64	0.1335	0.2981
High/ Med	467.78	0.1547	0.2931
High/ Low	427.94	0.1800	0.2866
Med/ High	895.44	0.1175	0.2323
Med/ Med	900.94	0.1359	0.2250
Med/ Low	896.40	0.1518	0.2199
Low/ High	3327.9	0.0737	0.1056
Low/ Med	3225.1	0.0840	0.0997
Low/ Low	2650.2	0.0962	0.0989

rather than underestimate. If a too low break probability model is chosen, the performance can be remarkably lower, as the overflow time decreases and filler content variation increases. On the other hand, if a too high break probability model is chosen, the time within breaks increases.

7 Conclusion

This dissertation presented a procedure for optimal design of paper manufacturing systems. The main emphasis was on the development of the optimal design methodology for highly uncertain processes with non-Gaussian uncertainties. The proposed procedure consists of six stages: problem formulation, modelling, operational optimization, design optimization, robustness analysis, and validation. The purpose of each stage was described, but the main focus was at the operational and design optimization stages.

In model-based process optimization, the uncertainty about the models and the available process information affects the reliability of the operation and design. The modelling uncertainty is related to both the incomplete understanding about the process and the approximation due to computational reasons. The uncertainty about the available information is associated with the measurement inaccuracy. Like the majority of real-world processes, also the papermaking process is stochastic, meaning that all the causalities are not understood and hence the future evolution of the process is not completely predictable. In the paper manufacturing process, there is an exceptional source of disturbance – web breaks. The more or less unpredictable web breaks change the operation point abruptly, posing extra challenge to the process operation. Understanding the sources of uncertainty in process optimization enables more efficient utilization of the process.

In process design, the task is to find an optimal process structure which compromises the process performance and the investment costs. As the assessment of the process performance requires optimal operational decisions, operational optimization needs to be studied as a part of the design optimization. At the operational level, decisions made during the process operation are optimized. This includes decisions about flows and consistencies as well as about the utilization of measuring resources. Typically, the decisions must be optimized over a certain prediction horizon, the proper solution method for operational optimization depending on the properties of the problem. Small finite-state cases can be solved using the POMDP solution framework, but for larger problems with delays, approximate methods must be utilized. If the problem is not solvable offline for the entire prediction horizon, it can be solved online with the MPC procedure in which the problem is solved over a shorter horizon and the optimization is repeated at each time instant. At the design level, the process performance over the entire life span is optimized. The probability distributions of stochastic systems are not always possible to be evaluated in advance. In this thesis, the expected long-term performance of highly uncertain processes was calculated from a sequence of shorter simulations.

Both the operational and design problems can contain of several conflicting criteria. In such cases, a single, unambiguous solution may not exist and the problem must be analysed using methods from the field of multiobjective optimization. In this thesis, the multiobjective operational problems were scalarized to a single-objective form. For design problems, the Pareto optimal set has been obtained through a large set of simulations. The final decision has been attained either by scalarizing the alternatives to monetary values or by presenting the non-dominated options to the decision maker in two-dimensional figures.

The proposed methodology has been tested with five case examples. The studied cases can be divided into two groups, one focusing on the simultaneous optimization of the control decisions and measurement resources, and the other on the optimization of highly stochastic processes. The cases in the first group consist of a finite number of states, the uncertainty about the measurement information being the main challenge. The solution methods were based on the POMDP framework combined with the MPC procedure. The examples showed that small problems of only a few states, such as maintenance and quality management, can be operated and designed on the basis of the proposed procedure, although the problems easily suffer from the curse of dimensionality as the number of states or the prediction horizon increases. Sometimes brute force optimization as in Case 3 is needed. The case studies also illustrated the purpose of scheduling the measurements in situations where the measuring resources are limited. The cases in the second group presented large, continuous-state problems which were solved within the MPC procedure using quadratic programming tools. The cases had two distinct operation points, which brought major challenges to the operation of the processes. In these cases, the uncertainty about the measurement information was not taken into account, but the value of a new measurement device was studied for one of the cases. The cases illustrated the challenges of optimization of large, highly stochastic systems and showed the need for process simulations as a chance to design such processes.

Based on the case studies, the proposed procedure for optimizing the design and operation of highly uncertain processes seems promising. However, the studied cases were rather idealized, and further work is needed to solve more realistic cases. Simulation based design optimization requires lots of simulations, and the selection of the design candidate set is not trivial. In this thesis, the selection was based on rather intuitive reasoning, but for further studies more sophisticated approaches are needed. Another challenge for the future research is the curse of dimensionality, especially in the case of finite-state systems.

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