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Mikko Linnala

SIMULATION AND OPTIMIZATION TOOLS IN PAPER MACHINE CONCEPT DESIGN

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Supervisors	Professor Jari Hämäläinen Department of Mathematics and Physics Lappeenranta University of Technology Finland
	Professor Kaj Backfolk Department of Chemical Technology Lappeenranta University of Technology Finland
Reviewers	Professor Efstratios Pistikopoulos Department of Chemical Engineering Imperial College London United Kingdom
	Professor Kauko Leiviskä Department of Process and Environmental Engineering University of Oulu Finland
Opponent	Professor Kauko Leiviskä Department of Process and Environmental Engineering University of Oulu Finland
Custos	Professor Jari Hämäläinen Department of Mathematics and Physics Lappeenranta University of Technology Finland

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ABSTRACT

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Simulation and optimization tools in paper machine concept design

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The last decade has shown that the global paper industry needs new processes and products in order to reassert its position in the industry. As the paper markets in Western Europe and North America have stabilized, the competition has tightened. Along with the development of more cost-effective processes and products, new process design methods are also required to break the old molds and create new ideas.

This thesis discusses the development of a process design methodology based on simulation and optimization methods. A bi-level optimization problem and a solution procedure for it are formulated and illustrated. Computational models and simulation are used to illustrate the phenomena inside a real process and mathematical optimization is exploited to find out the best process structures and control principles for the process. Dynamic process models are used inside the bi-level optimization problem, which is assumed to be dynamic and multiobjective due to the nature of papermaking processes.

The numerical experiments show that the bi-level optimization approach is useful for different kinds of problems related to process design and optimization. Here, the design methodology is applied to a constrained process area of a papermaking line. However, the same methodology is applicable to all types of industrial processes, e.g., the design of biorefiners, because the methodology is totally generalized and can be easily modified.

Keywords: Modeling, simulation, optimization, papermaking, process design
UDC: 676, 519.85, 004.94

To my family,

Jenni and Milka

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Kuopio, 1st of October, 2012

Mikko Linnala

LIST OF PUBLICATIONS

This thesis is based on the following papers, which are referred to in the text by the Roman numerals I-IV.

I Linnala, M., Ruotsalainen, H., Madetoja, E., Savolainen, J. and Hämäläinen, J., Dynamic simulation and optimization of an SC papermaking line - illustrated with case studies, *Nordic Pulp and Paper Research Journal* 25(2), 213–220, 2010.

II Linnala, M., Madetoja, E., Ruotsalainen, H. and Hämäläinen, J., Bi-level optimization for a dynamic multiobjective problem, *Engineering Optimization* 44(2), 195–207, 2012.

III Linnala, M. and Hämäläinen, J., Improvement of the cost efficiency in papermaking with optimization tools, *The Journal of Science and Technology for Forest Products and Processes* 1(2), 71–76, 2011.

IV Linnala, M. and Hämäläinen, J., Bi-level optimization in papermaking process design, *Nordic Pulp and Paper Research Journal*, accepted for publication, 2012.

In addition to the scientific journal articles listed above, this thesis is based on the research published in the following peer-reviewed scientific conference papers.

Linnala, M., Ruotsalainen, H., Madetoja, E. and Savolainen, J., Dynamic multiobjective optimization in papermaking process simulation, *CD-proceedings of Papermaking Research Symposium*, PRS2009, Madetoja, E., Niskanen, H. and Hämäläinen, J. (Eds.), Kuopio, Finland, June 1–4, 2009.

Linnala, M. and Hämäläinen, J., Model-based optimization in papermaking process design, *Proceedings of Progress in Paper Physics Seminar*, PPPS2011, Hirn, U. (Ed.), Graz, Austria, September 5–8, 2011.

The author of this thesis is the principal author of both the papers, which are not included here.

Author's contribution

All publications are a result of joint work with the supervisors, co-authors and other research partners in the EffTech and EffNet programs of Finnish Bioeconomy Cluster FIBIC Oy. The author is the principal and corresponding writer in all Publications I-IV.

In Publication I, the author was responsible for the modeling work of the paper machine area. The other parts of the model were built by Jouni Savolainen from VTT Technical Research Centre of Finland. The development of the two-way interaction between the software as well as the optimization problem definition was made in cooperation with the co-writers. However, the author was responsible for the practical implementation and conducting the numerical experiments.

In Publication II, the author was responsible for the numerical experiments and practical implementation of the bi-level optimization problem. The bi-level optimization problem and the solution algorithm were developed in cooperation with Elina Madetoja and Henri Ruotsalainen. The co-writers Elina Madetoja, Henri Ruotsalainen and Jari Hämäläinen participated in the overall development of the optimization problems in both Publications I and II.

In Publications III and IV, the author was responsible for the optimization problem formulations, practical implementations as well as conducting the numerical experiments. However, the optimization problems presented in the numerical experiments were developed together with the co-writer Jari Hämäläinen.

CONTENTS

ABBREVIATIONS AND NOMENCLATURE

CFD	computational fluid dynamics
CU	currency unit
PI	proportional-integral
$\boldsymbol{a}$	vector of upper-level optimization variables
$\tilde{\boldsymbol{a}}$	current values of upper-level optimization variables
$\boldsymbol{a}^*$	optimal values of upper-level optimization variables
f_i	i^{th} lower-level objective function
$\boldsymbol{f}$	vector of lower-level objective functions
F_j	j^{th} upper-level objective function
h	systems of differential and algebraic equation constraints
$\boldsymbol{p}$	vector of steady/constant parameters
S_a	feasible set of upper-level optimization variables
S_u	feasible set of lower-level optimization variables
S_x	feasible set of process state parameters
t_f	length of time horizon
T_{sim}	length of simulation horizon
T_{pred}	length of prediction horizon
$\boldsymbol{u}$	vector of lower-level optimization variables
$\tilde{\boldsymbol{u}}$	current values of lower-level optimization variables
$\boldsymbol{u}^*$	optimal values of lower-level optimization variables
$\boldsymbol{x}$	vector of process state variables
$\boldsymbol{x}^*$	process state variables corresponding to optimal optimization variables
Z	feasible objective space
$\boldsymbol{\omega}$	vector of operational tasks

1 Introduction

1.1 Background

The first decade of the 21st century has been ground-breaking in the global forest industry, especially in the pulp and paper industry. Ten years ago, all seemed to be fine and the Finnish forest companies were successful and profitable. Then changes started to appear in the global markets and paper machines were run down one after another, both in Finland and in Europe. Even entire paper mills were closed down. The structural change forced the forest companies to develop both new products and new manufacturing processes in order to increase profitability. New processes are required to decrease the investment and production costs ensuring at the same time that the quality of products remains at an adequate level. In practice, the current products with the current quality criteria need to be produced at lower costs [1-3].

Greenfield investments of traditional papermaking applications are not likely to be profitable in Finland. This is because the fastest growing market for paper consumption is in Asia whereas the European markets have stabilized at the same time [1, 2]. However, there exist differences between the paper and board grades. To make changes in either the manufacturing process or the product of the Finnish paper mills, existing processes need to be rebuilt. This means that a part of the process is replaced with modern technology and a part is maintained. This enables changes to the product portfolio and more cost-efficient process lines (e.g., decreased raw material and manufacturing costs) increasing also opportunities in terms of global competition.

Besides the new ideas of processes and products, the process design procedures are also challenging. Sophisticated methods, such as model-based optimization, can be exploited in studying new processes and products. Computational models and simulation produce valuable information and illustrate the phenomena inside the process (see *Figure 1*). However, the models have their own limits and therefore cannot be applied to all problems. To increase the advantages of process modeling, the model can be coupled with mathematical optimization, which enables solving complicated problems related to either the process structure and controls or both, for example [4, 5].

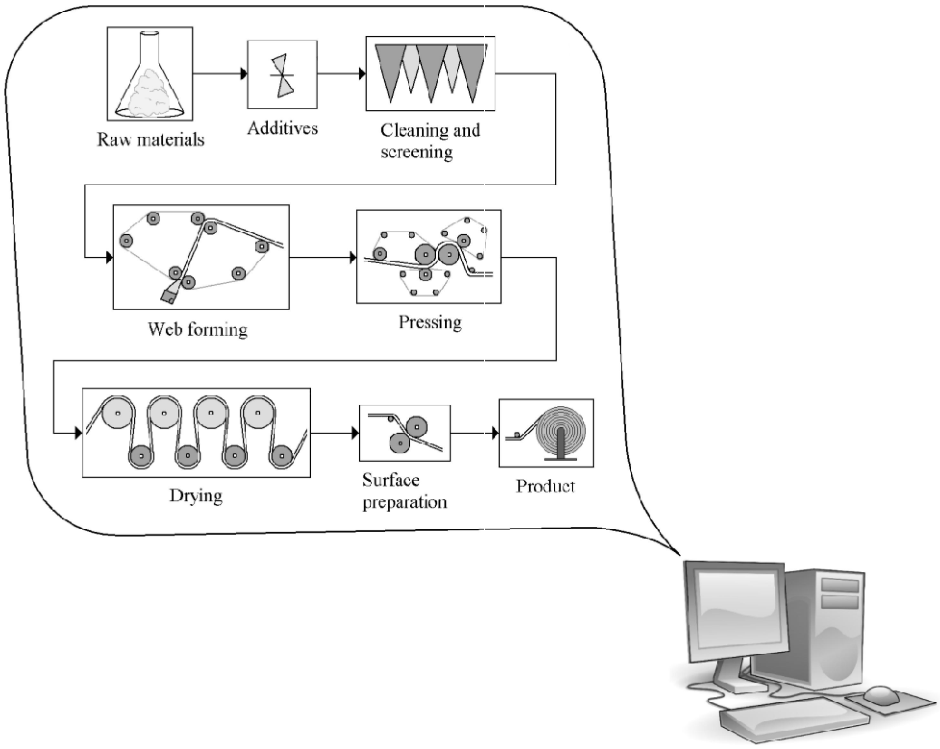

Figure 1: Computational methods are cost-effective tools enabling new possibilities in process design.

Chemical engineering has been a leader in the use of such methods but the paper industry is not as familiar with these possibilities. Therefore, the theory part of this thesis is derived from chemical engineering whereas the numerical experiments are applied to papermaking processes. Hopefully, new research programs and more broadminded ideas will enable the paper industry to take advantage of these tools [6, 7].

1.2 Scope and aims of this thesis

In this thesis, process modeling and optimization are applied to the paper industry. A process design methodology, utilizing process modeling and optimization in a wider spectrum compared to the traditional design methods, is developed. This approach applies bi-level optimization in which dynamic modeling and dynamic multiobjective optimization are coupled. With bi-level optimization, it is possible to simultaneously optimize both the process design and the operations. Regardless of the papermaking application, the methodology is generalized so that none of the individual elements, such as software or the problem formulation, is fixed. Hence, it is easily applicable to different industrial processes and purposes. In addition to bi-level optimization, efficient use of different process models is analyzed. The role of additional information produced to support the decision-making procedure, related to multiobjective optimization, is evaluated.

The novelty of this thesis lies in the new way of process design; bi-level optimization, familiar from other fields of industry, is tailored to the use of the paper industry. Existing methods are examined from the point of view of papermaking which significantly differs from the other industrial processes. Complicated processes may be one reason for lack of simulation and optimization tools in design of papermaking applications compared to chemical engineering, for example. Instead, papermaking applications are usually designed using traditional, well tried methods without too heavy computational aids.

A notable detail, generalization of all possible elements, enables applicability of the methodology to different problems. Hence, the new process concepts and products can be designed more efficiently.

2 Simulation and optimization of papermaking process

2.1 Papermaking process

Although the paper itself is a very familiar product and raw material for all of us, the papermaking process is more complex than it is usually considered. Firstly, paper consists of fibers, fines and additives, such as fillers, the size of which varies from nanometers to millimeters [8]. Hence, we are dealing with very small particles which should be correctly distributed over the paper web. Secondly, modern paper machines produce up to 400,000 tons of paper per year. This is equivalent to a paper web width of over ten meters and a speed of 1,500 to 2,000 meters per minute (90–120 kilometers per hour) in a paper machine [9]. Such huge paper machines should be able to produce sufficiently small and sensitive products with a reasonable quality, which sounds challenging. In this thesis, the papermaking concept analyzed contains all the main elements and sub-processes from the raw material inputs to the net production, as presented in *Figure 2*.

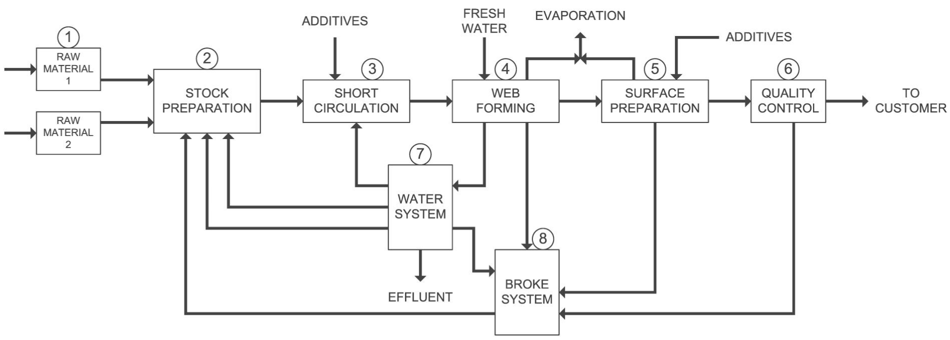

Figure 2: An example of the main components of a papermaking line.

In *Figure 2*, raw materials 1 and 2 include different pulps (wood fibers), both mechanical and chemical (1). Naturally, the number of pulp types used can differ from two, which is here selected only for illustration purposes. The stock preparation area (2) consists of towers and dilution water lines which are used to mix and dilute different raw materials into a usable form, to a dry solid content of approximately 3–4 wt-% in practice. In the short circulation (3), the stock suspension is further diluted to a dry solid content of approximately 1 wt-% and cleaned using different methods. Any additives, such as fillers and retention chemicals, are also mixed here with the stock suspension [10].

Web forming (4) consists of the following sub-processes: headbox, wire section, press section and drying section. The headbox is used to spread the stock flow exiting from a pipe to form a several meters wide web with optimal distribution and orientation of fibers and fillers. In modern paper machines, the web is formed between two running wires. This enables two-sided water removal in the wire section where most of the water is removed. The dry solid content increases up to ~15–20 wt-%. Next, the web is dried using mechanical work in wet pressing whereby the dry solid content increases up to 45 wt-%, approximately. During wet pressing, fiber bonding starts and the strength properties improve [10]. The final drying of the web is performed in the drying section where the web is traditionally heated with steel cylinders which themselves are heated with steam. In addition to multicylinder drying, other drying possibilities also exist, such as impingement drying [11]. At this stage the paper contains approximately 5–10 wt-% of water and is ready to be used in the finishing processes, such as calendering [12] or coating (5) [8], or it can be reeled to build up customer rolls. In paper finishing, large machine rolls are usually further divided into smaller rolls with a winder. Since the requirements for the paper quality are high, part of the production ends up in reject due to quality deviations (6).

In addition to the main process line, the paper mills have a water system (7). It consists of tanks and towers which are used to store different types of water. So-called white water is removed from the stock suspension in the wire section of the paper machine and used for dilutions in the short circulation. The rest of white water is collected to the white water tank (volume < 1000 m^3) and the white water tower (volume > 1000 m^3) from where it is taken to the fiber recovery process. In the wire section, where the paper web is formed, part of the solids goes through the wire and ends up in the water circulation. In papermaking, the term *retention* is used to refer to solids which remain on the wire and form the web. For example, fiber retention could be 80%, which means that 80% of the fibers forms the web and 20% goes to the water system. Filler retention is much lower ranging usually from 30% to 50%. Thus, valuable raw materials need to be separated from the water circulation. This is done with a disc filter which recovers most of the fibers and filler solids utilizing a filtration technique. In this way, the raw materials are recovered to be used in the paper machine again and, in addition, the water system is cleaned [10].

Another line running parallel to the main process line is the broke system (8) which is needed for the paper ending up in reject due to quality variations or other reasons. In practice, the paper machine cannot be run continuously and some web breaks occur unavoidably. During the web breaks, the web is fed to the broke system where it is kept in storage before being reused in the paper machine. The structure of the broke system depends on the paper produced. Usually there are separate lines for the wet broke (from the wire and press sections) and the dry broke (from drying and finishing) or, in case of coated paper production, there may be separate lines for uncoated and coated broke. In any case, in the broke system, the paper web is pulpered and diluted to a dry solid content of approximately 3–5 wt-% before the storage towers. From the towers, the broke is fed to stock preparation where it is again used as raw material. Because the broke dilution requires a lot of water, there is an interaction between the broke and water systems: when the broke towers are full, they bind up a lot of water and thus the water towers are empty, and *vice versa* [10].

2.2 Paper quality

Besides the process technical aspects described above, the paper quality properties also have a significant role during the process design procedure. New process concepts and products are compared to the quality properties of existing products, which are used as reference information. It is reasonable to maintain the quality, and the value, of the product but decrease the investment and operational costs of production.

If the papermaking process is complex, the paper as a material is even more complex. In addition to the basic material properties, such as basis weight, density/bulk, thickness, porosity and filler content, paper also has critical strength and optical properties. Tensile strength, tear strength, surface strength and out-of-plane strength, for example, define how the paper behaves both in the manufacturing process and in use. The web has to be strong enough to avoid web breaks in the paper machine but simultaneously soft, such as in case of tissue paper. By contrast, optical properties, such as brightness and opacity, do not affect runnability of a paper machine but they are critical in the printing house: printed text should not be visible through newsprint and images should be glossy in magazines [13, 14].

Many of the quality properties can be measured *on-line* from a running paper web. The measurement is conducted using a scanner with various sensors moving continuously over the web. In this way, several quality properties can be simultaneously measured. Usually, there are several scanners along the paper machine for analyzing the quality in the machine direction and cross machine direction. The information from the scanners is used in the process control system to ensure conformance with the quality requirements [15]. If a method for an *on-line* measurement, e.g., paper strength, does not exist, this property has to be measured in a laboratory. To this end, paper samples are collected from the reel and winder for an *off-line* analysis [13].

2.3 Modeling aspects

The papermaking process can be modeled using many different approaches. Firstly, the model can include only a single sub-process or the model can be mill-wide. Secondly, the process can be modeled either in a steady state or as a dynamic system. Traditionally, the processes are modeled in a steady state, which does not take into account the time horizon but examines only a single time stage [15, 16]. Steady-state models are useful in preliminary balance analyses, for example. Today, the most suitable method is dynamic modeling. This is because the processes are dynamic and it is usually desired to examine the process over a time horizon which can vary from minutes to weeks or months, for example [17-19]. In dynamic models, the process variables are considered as functions of time, i.e., the previous state affects the following state. Compared to steady-state models, dynamic models include transient features, such as delays and inertia [20]. This is why dynamic models behave more naturally and are also more realistic than steady-state models.

Dynamic models are widely used in the paper industry to study either a single phenomenon or operation of a specific sub-process, for example. The wet end and forming section have been examined by Bortolin *et al*. [21], Yeo *et al*. [22] and Cho *et al*. [23], the press section has been studied by Khanbaghi *et al*. [24] and Provatas and Uesaka [25], the calendering phenomena by Litvinov and Farnood [26], and different mass fractions in the paper machine by Yli-Fossi *et al*. [27]. In addition, process control systems exploiting dynamic models have been developed by Kokko [4], Lappalainen *et al*. [28] and Iso-Herttua *et al*. [29]. Along with the process technical approach, process modeling has also been used in economical studies [30], e.g., studies related to energy and fresh water savings [31-35].

As mentioned above, the paper quality properties are even more complex than the process. Hence, modeling of quality properties is difficult if not impossible. Coupling of quality models with a mill-level simulator is particularly challenging. While the models for the basic properties, such as basis weight and filler content, can be based on the paper furnish, modeling of strength and optical properties is very complicated. These properties depend on too many factors to allow reliable modeling. Thus, the lack of realistic models for the product quality and process runnability is a major issue in modeling discussions.

If the interest is focused on a single sub-process or another constrained area, the model accuracy can be very high and computational fluid dynamics (CFD), for example, can be exploited [36-41]. By contrast, when using a large and comprehensive model, accuracy may need to be decreased because high accuracy usually increases the computational capacity requirement. Hence, when dealing with large models, a compromise between accuracy, and reality, and the computational time is needed.

The modeling approach can also depend on the modeling software that is available and selected for use. In addition to the traditional programming languages, there are several commercial software applications for modeling pulp and paper processes, for example: BALAS [42], Apros [43], FlowMac [44], Metso WinGEMS [45] and Matlab/Simulink [46]. While the model can be programmed line by line, modern simulators also include a graphic user interface in which the model is built by creating a flow sheet. Since all tools have their own advantages and disadvantages, there is not only one right choice. Examples of the development of modeling software are presented by Niemenmaa *et al*. [47], Barber Scott [48, 49] and Jahangirian *et al*. [19].

2.4 Optimization methods

Like process modeling, optimization of papermaking processes is not a new research topic. During several years, different approaches have been presented and methods applied. There are approaches examining a single sub-process [50-54] and others with different areas of interests and the aim of optimization has been either technical or economical improvement of the application [33, 55]. Traditionally, steady-state models and/or single-objective optimization are used [54, 56-60]. However, since the papermaking processes are complex and usually require considering several conflicting objectives, the multiobjective approach has been a natural choice [60-65]. Hence, coupling the dynamic model and dynamic multiobjective optimization is at the moment the most promising way to study optimization problems related to industrial process applications [66-70]. With dynamic optimization, it is possible to optimize the process over a predefined time horizon in the same way as in dynamic modeling.

3 Bi-level optimization of papermaking process

As noted, dynamic multiobjective optimization is the most suitable way to handle optimization problems related to papermaking applications. When dealing with a process design case, the problem can be formulated as a bi-level optimization problem. Thus, the process structure is optimized on the upper level (design optimization) and the operations on the lower level (operational optimization). In bi-level optimization, dynamic multiobjective optimization and dynamic process models have a strong two-way interaction.

Previously, bi-level optimization was used for different purposes [71-73]; the first applications were in the chemical industry [7, 74-77]. Multiobjective cases are also discussed by Fliege and Vincent [78], Deb and Sinha [79], Li *et al*. [80] and Eichfelder [81], for example. By contrast, the papermaking applications are few and far between. Some examples related to broke system optimization are presented by Ropponen *et al*. [70]. There, both the broke tower design and the control operations are taken into account.

3.1 Dynamic multiobjective optimization

Dynamic optimization is used with dynamic process models in which the variable values change over time, and thus its solution differs from the steady-state case [82, 83]. The formulation of a single-objective dynamic optimization problem is shown in *Equation 1*.

$$\begin{aligned}&\underset{\boldsymbol{u}(t)}{\text{optimize}}\ f\left(\boldsymbol{x}(t_f),\boldsymbol{u}(t_f),\boldsymbol{p},t_f\right)\\&\text{subject to}\begin{cases}\boldsymbol{x}\in S_x\\\boldsymbol{u}\in S_u\\h\left(\dfrac{\mathrm{d}\boldsymbol{x}(t)}{\mathrm{d}t},\boldsymbol{x}(t),\boldsymbol{u}(t),\boldsymbol{p}(t),t\right)=0\quad\text{for all }t\in\left[t_0,t_f\right],\end{cases}\end{aligned}\qquad[1]$$

where f is the objective function, h is the system of the differential and algebraic equation constraints, $\boldsymbol{x}$ is the state vector, $\boldsymbol{u}$ is the control vector (optimization variables), $\boldsymbol{p}$ is the steady parameter vector, t_f is the length of the time horizon, and S_x and S_u are the feasible sets of $\boldsymbol{x}$ and $\boldsymbol{u}$, respectively, defined by all the constraints including box constraints and linear and nonlinear equality and inequality constraints. The steady parameter vector can also be ignored, if necessary, because it is constant from the point of view of optimization. Although the variables in dynamic optimization are continuous, the solution procedure typically requires at least partial discretization of the variables [84, 85].

Dynamic optimization in which multiple objectives need to be simultaneously optimized is called dynamic multiobjective optimization. This changes the problem formulation as shown in *Equation 2*.

$$\underset{\boldsymbol{u}(t)}{\text{optimize}}\left\{f_1\left(\boldsymbol{x}(t_f),\boldsymbol{u}(t_f),\boldsymbol{p},t_f\right),\ldots,f_n\left(\boldsymbol{x}(t_f),\boldsymbol{u}(t_f),\boldsymbol{p},t_f\right)\right\}$$
$$\text{subject to}\begin{cases}\boldsymbol{x}\in S_x\\ \boldsymbol{u}\in S_u\\ h\left(\dfrac{\mathrm{d}\boldsymbol{x}(t)}{\mathrm{d}t},\boldsymbol{x}(t),\boldsymbol{u}(t),\boldsymbol{p}(t),t\right)=0\quad\text{for all } t\in\left[t_0,t_f\right],\end{cases}\qquad [2]$$

where $\boldsymbol{f} = (f_1,\ldots, f_n)$ is the vector-valued objective function and $\boldsymbol{x}$, $\boldsymbol{u}$, $\boldsymbol{p}$ and t_f are the same as above. Here, all the objectives f_i need to be optimized simultaneously and thus the solution process differs from the single-objective case shown in *Equation 1*. For example, if the problem includes two conflicting objectives, f_1 and f_2, which both need to be minimized, there is a set of solutions, as illustrated in *Figure 3* [86, 87].

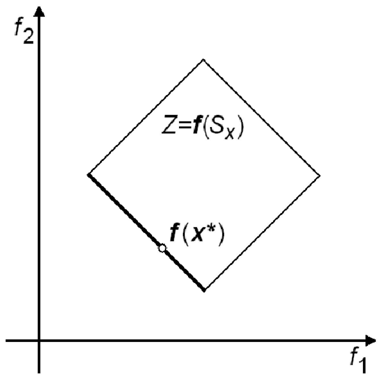

Figure 3: An example of conflicting objectives in a multiobjective optimization problem in which both objectives need to be minimized.

In *Figure 3*, $Z=\boldsymbol{f}(S_x)$ denotes the feasible objective space defined by the constraints. $\boldsymbol{f}(\boldsymbol{x}^*)$ and the white circle refer to a single Pareto optimal solution and the bold line refers to all Pareto optimal solutions, i.e., a Pareto optimal set. These are mathematically equally good solutions and thus cannot be ranked. Therefore, decision making is needed. In practice, the best solution is selected by using a numerical scalarization method and/or a human decision maker. A human decision maker is a person who can make the selection based on his/her knowledge of the optimization problem and the application. In turn, scalarization is based on predefined criteria which are exploited to rank the solutions by using numerical methods [64, 85-87].

3.2 Bi-level optimization problem

In bi-level optimization, both problems, upper and lower, are assumed to be dynamic and multiobjective. Hence, the formulation of a bi-level optimization problem consists of the same elements as the dynamic multiobjective problem shown in *Equation 2*. However, the upper-level problem includes the lower-level problem, as shown in *Equation 3*. This means that optimization of the upper-level problem requires optimization of the lower-level problem.

$$\underset{\boldsymbol{a}}{\text{optimize}}\left\{F_1\left(\boldsymbol{a}, \boldsymbol{x}\left(t_f\right), \boldsymbol{u}\left(t_f\right), \boldsymbol{\omega}\right), \ldots, F_k\left(\boldsymbol{a}, \boldsymbol{x}\left(t_f\right), \boldsymbol{u}\left(t_f\right), \boldsymbol{\omega}\right)\right\}$$

$$\text{subject to}\begin{cases}\boldsymbol{a} \in S_a \\ Eq.[4]\end{cases} \qquad [3]$$

where F_i, for all $i = 1,\ldots, k$, represents the upper-level objective functions, $\boldsymbol{a}$ is the vector of the upper-level optimization variables (design variables), $\boldsymbol{x}$ is the vector of the state variables, $\boldsymbol{u}$ is the vector of the lower-level optimization variables (control variables), $\boldsymbol{\omega}$ is the vector of the operational tasks, t_f is the length of the optimization horizon, and S_a is the feasible set of $\boldsymbol{a}$ defined by all the constraints. Here, operational tasks, $\boldsymbol{\omega}$, denote to the lower-level problem where they represent a change in the system state. The lower-level optimization problem can be formulated as shown in *Equation 4*.

$$\underset{\boldsymbol{u}}{\text{optimize}}\left\{f_1\left(\boldsymbol{x}\left(t_f\right), \boldsymbol{u}\left(t_f\right), \boldsymbol{\omega}(\boldsymbol{a}, t)\right), \ldots, f_l\left(\boldsymbol{x}\left(t_f\right), \boldsymbol{u}\left(t_f\right), \boldsymbol{\omega}(\boldsymbol{a}, t)\right)\right\}$$

$$\text{subject to}\begin{cases}\boldsymbol{x} \in S_x(\boldsymbol{a}) \\ \boldsymbol{u} \in S_u(\boldsymbol{a}) \\ h\left(\dfrac{\mathrm{d}\boldsymbol{x}(t)}{\mathrm{d}t}, \boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{\omega}(\boldsymbol{a}, t), t\right) = 0 \quad \text{for all } t \in \left[t_0, t_f\right],\end{cases} \qquad [4]$$

where f_j, for all $j = 1,\ldots, l$, represents the lower-level objective functions, $\boldsymbol{x}$, $\boldsymbol{a}$, $\boldsymbol{u}$, $\boldsymbol{\omega}$ are the same as above, S_x and S_u are the feasible sets of $\boldsymbol{x}$ and $\boldsymbol{u}$, respectively, and h is the system of dynamic differential and algebraic equations.

The formulation of the bi-level optimization problem in *Equations 3* and *4* shows that the values of the upper-level optimization variables affect the lower-level optimization problem. In addition, the solution of the lower-level problem affects the upper-level objective function values. Hence, the upper and lower levels of the optimization problem have two-way coupling, which is illustrated in *Figure 4*.

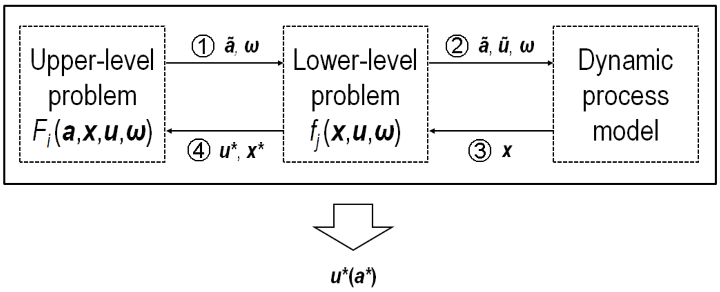

Figure 4: Two-way coupling between the optimization levels and a dynamic process model.

In *Figure 4*, the progress of solution of the bi-level optimization problem is illustrated with numbers 1–4. A detailed description of the solution procedure is given next.

3.3 Solution procedure for bi-level optimization problems

Bi-level optimization problems can be solved using either the simultaneous or the sequential method as presented by Mohideen *et al*. [7] and Deb and Sinha [79], for example. In this thesis, the solution procedure, described in *Algorithms 1* and *2*, can handle dynamic and multiobjective problems on both levels. Nevertheless, the procedure is abstract, which makes it easily applicable for different problems.

Algorithm 1 – Bi-level optimization

The solution procedure for the bi-level optimization problem, presented in *Equations 3* and *4*, can be defined as follows.

1. Initialize the optimization method selected for the upper-level optimization.
2. Define the objective functions, a vector of optimization variables and the constraints for the upper-level optimization problem (including the lower-level optimization problem parameterized by the upper-level optimization variables) and perform the optimization as follows.

Repeat the following steps until one (or more) of the stopping criteria is fulfilled:

(a) Let vector $\tilde{\boldsymbol{a}}$ contain the current values for the upper-level optimization variables. Define the corresponding lower-level optimization problem at $\tilde{\boldsymbol{a}}$.

(b) Find the optimal state for the lower level with the selected optimization method, i.e., perform the optimization based on *Algorithm 2*.

(c) Let $\boldsymbol{u^*}$ be the optimal solution of the lower-level optimization problem and $\boldsymbol{x^*}$ the corresponding vector of the state variables. In the multiobjective case, $\boldsymbol{u^*}$ is selected from a set of Pareto optimal solutions using either a human decision maker or predefined information.

(d) Based on $\boldsymbol{u^*}$ and $\boldsymbol{x^*}$, evaluate the objective functions $F_1,\ldots, F_k$ on the upper level and provide the objective function values to the optimization method.

End

3. The optimal solutions for the bi-level optimization problem are $F_1,\ldots, F_k$ at $\boldsymbol{a^*}$ with the corresponding optimal lower-level solutions $f_1,\ldots, f_l$ at $\boldsymbol{u^*}$.

Algorithm 2 – Lower-level optimization

The solution procedure for the lower-level optimization problem, presented in *Equation 4*, can be defined as follows.

1. Initialize the optimization method.
2. Define the objective functions, the vector of the optimization variables and the constraints for the given parameters $\tilde{\boldsymbol{a}}$. Start the optimization procedure as follows.

   Repeat the following steps until one (or more) of the stopping criteria is fulfilled:

   (a) Solve the dynamic process model with the current optimization variables $\tilde{\boldsymbol{u}}$.

   (b) Evaluate the objectives $f_1,\ldots, f_l$ at $\tilde{\boldsymbol{u}}$ based on the state variables $\tilde{\boldsymbol{x}}$.

End

3. Save the optimal values of the optimization variables ***u**** and the corresponding state variable values ***x**** as well as $f_1, ..., f_l$ which are needed in *Algorithm 1*.

The stopping criteria mentioned in both *Algorithms 1* and *2* can be based on the optimization algorithm used, e.g., the maximum number of iterations, the numerical accuracy required, the time horizon selected, or a model technical element, such as an undesirable process state, for example.

As discussed above, in multiobjective optimization there is a set of Pareto optimal solutions. However, in the practical optimization cases, only one solution needs to be chosen as the final one. In an investment case, we can build only one mill or process, for example. Therefore, some kind of decision making is needed, either a human decision maker or predefined information with a classical scalarization function.

3.4 Process models in bi-level optimization

To be able to optimize anything, a process model is required. In this study, a system of two different models is analyzed. A so-called nominal model is used inside bi-level optimization. It is a simplified model in which the process flows and dynamics are calculated using simple material balance equations. In turn, a more detailed model, the so-called verification model, is used after the optimization procedure to produce additional information about the solution options. The verification model is more accurate and reliable; it includes the first principles of physics, automation components, sub-models for a single phenomenon, etc. [88, 89].

Both models are based on the same flow sheet and the necessary definitions of operational specifications, such as product, production and hardware information. An example of a flow sheet is shown in *Figure 5*. Due to this, both models behave mainly in the same way. It is true, of course, that increasing details and controls in the verification model causes certain variations but this is expected and acceptable. In practice, the process models are built first and then coupled with the optimization algorithm. Hence, the optimization manipulates only some values of the model parameters depending on the problem definition. The fixed parameter values are based on the process know-how and measurements of the real process.

In this thesis, all the models are built with either Matlab or Apros. Matlab is used for the simplified models and Apros is used mainly for the more detailed models.

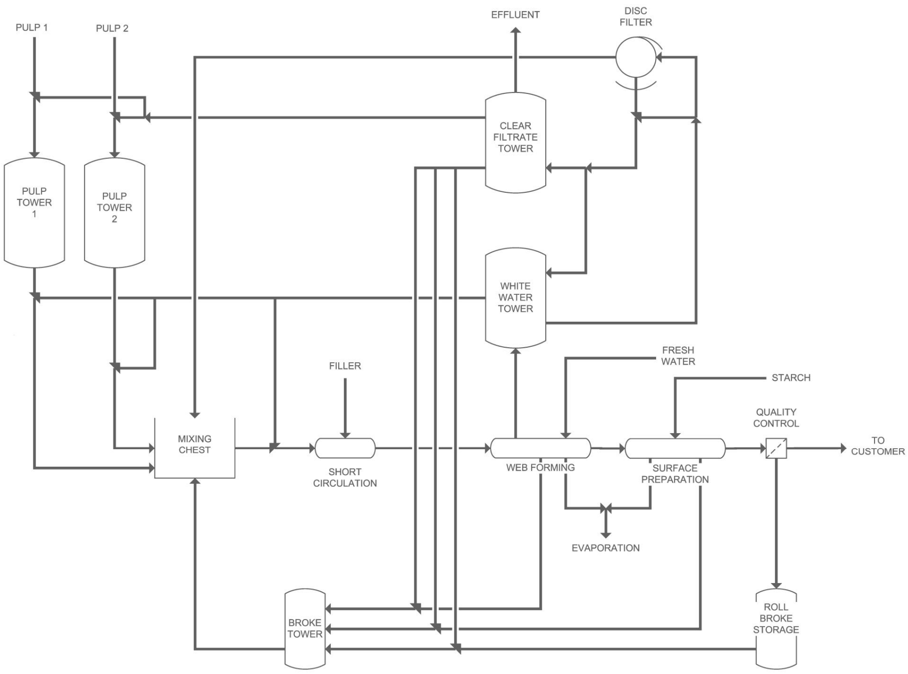

Figure 5: An example of a flow sheet of the papermaking line modeled.

The flow sheet includes all the elements and sub-processes shown above in *Figure 2*. However, the flow sheet is a more detailed description of the process compared to the block diagram, including numerous flows and tanks which are not contained in the block diagram.

4 Main results and discussion

The optimization problems presented in this thesis had some consistent characteristics (see Publication II for more details). Firstly, the dynamics were handled using the receding horizon prediction principle which is one type of a model predictive control [90]. The optimization horizon was discretized and the problem was solved proceeding one time stage after another as illustrated in *Figure 6*. First, the prediction horizon, T_{pred}, was used to predict and optimize the controls. After optimization, the controls were used to simulate one time stage, T_{sim}, forward. This loop was repeated until the total time horizon, t_f, was simulated. Secondly, the optimization problem was solved using a differential evolution algorithm [91, 92] which belongs to the group of evolutionary algorithms [93, 94]. Thirdly, the numerical experiments of bi-level optimization were limited to handle only the structure and operations of the broke and water systems.

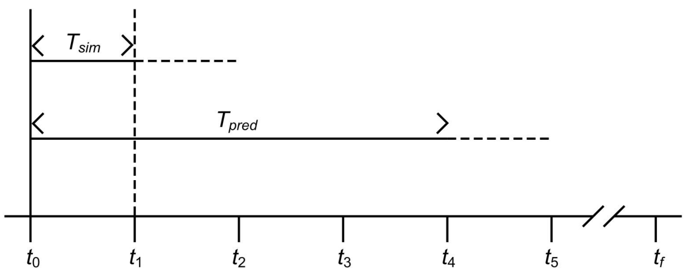

Figure 6: An example of the receding horizon prediction principle. T_{sim} is the simulation horizon, T_{pred} is the prediction horizon and t_f is the total optimization horizon.

4.1 Dynamic multiobjective optimization applied to papermaking

In this thesis, process modeling and optimization were developed to provide a tool for more efficient process design in the paper industry. The research was started by coupling a dynamic process simulator (Apros) and single-level dynamic multiobjective optimization (in Matlab). A sufficiently large and heavy process model was used to optimize the operations of the filler content and basis weight controllers during a simulated retention disturbance. In practice, two PI-controllers were tuned trying to minimize variations in the tensile strength ratio and *β*-formation. The main results of this study are illustrated in *Figure 7*.

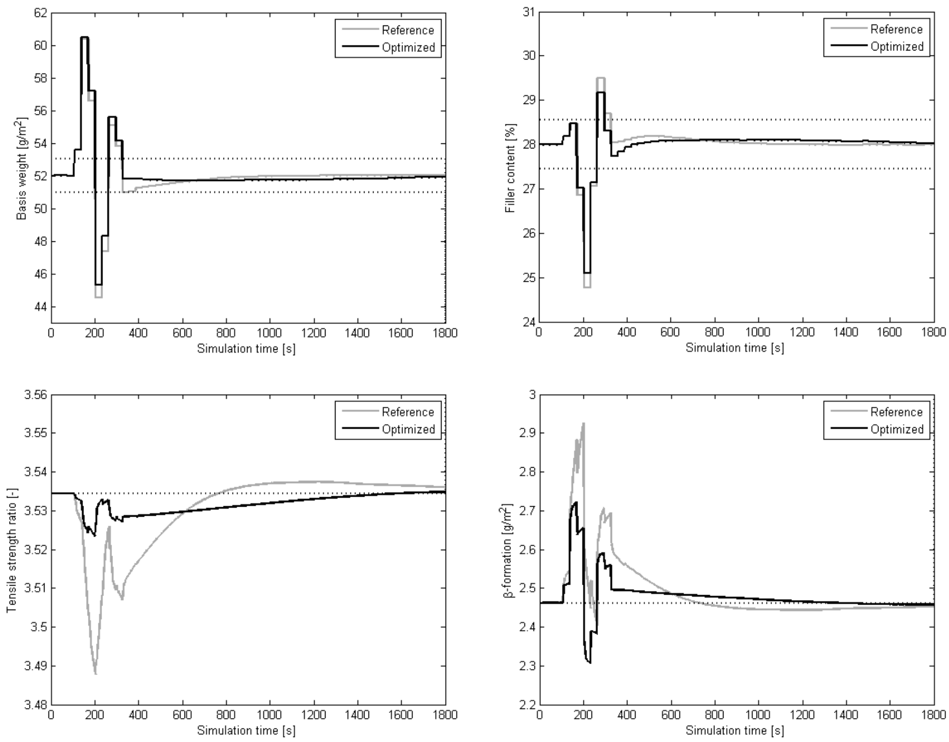

Figure 7: Variations in basis weight (upper left), filler content (upper right), tensile strength ratio (lower left) and *β*-formation (lower right) during a simulated retention disturbance. The figure is from Publication I.

Figure 7 shows that after optimization, the variations in the tensile strength ratio and *β*-formation were much smaller than in the reference case. In addition, the variations in basis weight and filler content decreased even though they were not included in the objective functions.

Hence, the main target of Publication I, coupling the dynamic process model and dynamic multiobjective optimization (single-level problem), was successfully met.

4.2 Bi-level optimization applied to papermaking

After the studies conducted with the single-level optimization problem and its successful solution, it was possible to define the bi-level optimization problem (Publication II). A formulation of the bi-level optimization problem and a solution algorithm for such problems were created. The related theoretical part is presented in the previous section.

The bi-level optimization procedure has been illustrated with several examples in Publications II, III and IV. In general, the main target of the design optimization on the upper level was either to keep the process stable or to minimize the investment costs of the broke and water towers. The process stability was illustrated via the broke tower fill percentages. Multiobjective optimization led to a set of Pareto optimal solutions which are illustrated in *Figure 8*.

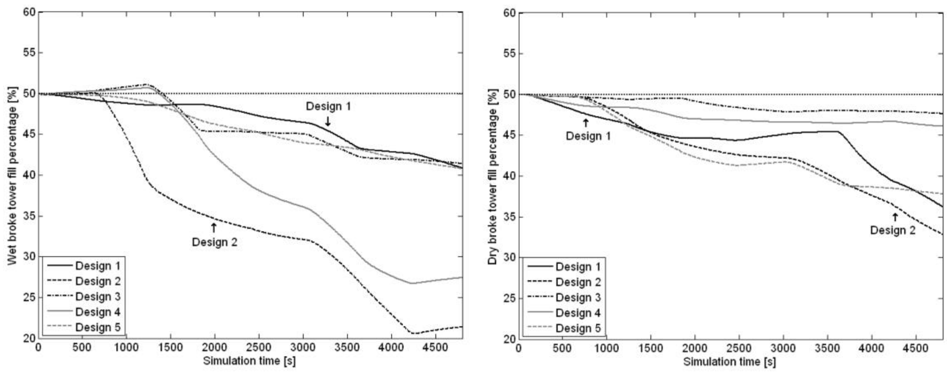

Figure 8: Fill percentage variations in the wet broke tower (left) and dry broke tower (right). Designs 1-5 illustrate mathematically equally good, Pareto optimal solutions. The figure is from Publication II.

Figure 8 shows that although the process designs were equally good from the point of view of optimization, the differences between them were significant. Further, the investment costs were calculated based on the tower volumes according to a generalized form of the so-called six-tenths rule [95, 96] which is shown in *Equation 5*.

$$\text{cost} = p_1 \times \text{capacity}^{p_2} \quad [5]$$

where p_1 and p_2 are constant parameters. In this thesis, $p_1 = 1$ and $p_2 = 0.7$, which values were approved by the industrial partners. Differences in the investment costs are illustrated in *Figure 9* using normalized objective function values.

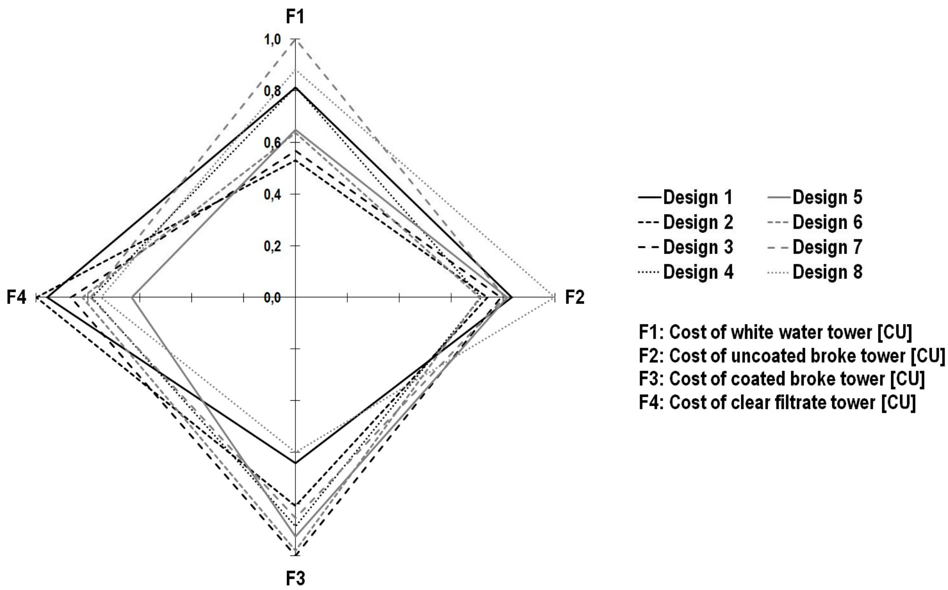

Figure 9: Normalized objective function values of the upper-level optimization problem. CU refers to an undefined currency unit. The figure is from Publication IV.

The visualization of different solutions is challenging as *Figure 9* shows. When the number of solutions increases, it is easier to analyze them in smaller parts. Conflicts appearing between two different designs are illustrated in *Figure 10* which shows only designs 2 and 3 of *Figure 9*.

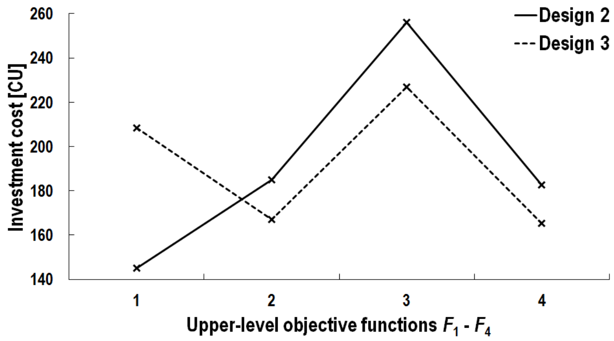

Figure 10: An example of two conflicting upper-level objectives. The figure is from Publication IV.

Figures 9 and *10* prove the nature of multiobjective optimization; handling of several conflicting objectives requires some kind of decision making. In bi-level optimization, also the lower-level objectives need to be taken into account during the decision-making process. Because the experiments were related to the broke and water systems, the lower-level objectives involved broke dosage, production and product quality variables. Maximization of both the broke dosage and the paper machine production were conflicting objectives because the wet end break frequency was dependent on the broke dosage. The hypothetical break model was based on amount and composition of broke but age and physic-chemical properties, for example, were not taken into account. In practice, a higher broke dosage increased the probability of web breaks, which further decreased the cumulative production. This conflict is illustrated in *Figure 11*.

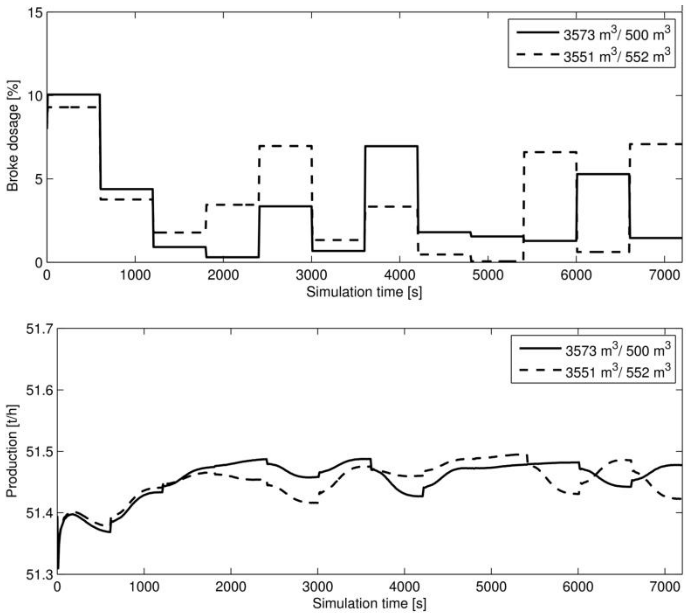

Figure 11: Variations in broke dosage (upper) and production (lower). The figure is from Publication III.

Figure 11 shows that a transient change in the broke dosage affected the production of that time. Therefore, maintaining a balance between the maximal production and the process stability was sensitive and required continuous control. However, variations in production were equivalent to about 0.2% of production which is not significant if compared to break frequency, for example.

An analysis of the bi-level optimization experiments also highlighted conflicts between the upper-level objectives and the lower-level objectives. When the investment costs were included in the upper-level objectives and the broke tower liquid levels in the lower-level objectives, there existed clear correlation between them. In practice, the process stability was dependent on the tower capacity: when the tower volumes were high enough, the process was more stable than while using smaller tower volumes. Hence, cost savings led to an unstable process. This correlation is illustrated in *Figure 12*. It is true, of course, that also other aspects, such as energy efficiency and broke delay in towers, should be considered when the final tower volumes are decided.

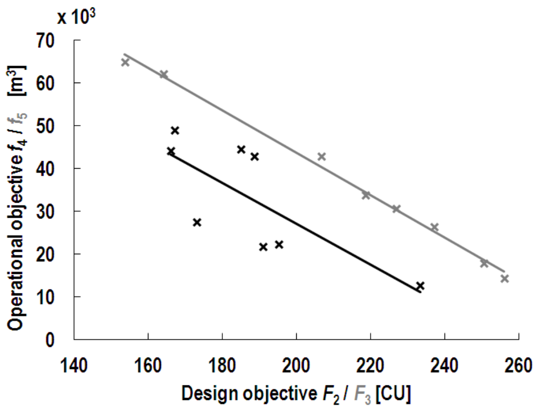

Figure 12: Correlation between the upper-level and lower-level objectives. F_2 and F_3 are the investment costs of the broke towers and f_4 and f_5 are the liquid level variations in the broke towers. Black color refers to the uncoated broke tower, grey color to the coated broke tower. Numerical results are illustrated with the crosses in which the linear functions are fitted. The figure is from Publication IV.

Numerical experiments prove that the method is usable for different kinds of process design problems. By using suitable models and problem definition, bi-level optimization method is applicable for any industrial process. Generality enables use of any modeling software as well as use of different optimization algorithms; only current application and problem definition fix the elements.

In the experiments, the method illustrated such properties that additional value compared to traditional design methods is clear. Briefly, the method relies on mathematical facts instead of trials and errors. The results, process structure and operational principles for papermaking applications, are achieved using modern computational tools, simulation and optimization. Hence, the main target of the thesis, development of tailored but still generalized process design method, is fulfilled.

4.3 Utilization of different process models

In the optimization studies, two different model types were used. Experiments were started by using a more detailed, advanced and heavy model which was later changed to a simplified model consisting of the material balance equations. The more detailed model produced more accurate and realistic results but the computational time was long. By contrast, simplification decreased the model accuracy but also the computational time. Thus, the aim was to show which of the two model types was more efficient.

Previously, a model called verification model has been used to test different operational scenarios and modifications of model reality. The verification model includes, for example, certain sub-processes, such as dilution and thickening, which are not taken into account in the simplified model. However, the different solutions of the bi-level optimization problem, which are achieved with the simplified model, can be repeated with the verification model. The process design and controls are the targets of optimization and the stochastic elements, such as break frequency, are also the same. Interactions of the bi-level optimization procedure and the roles of process models are shown in *Figure 13*.

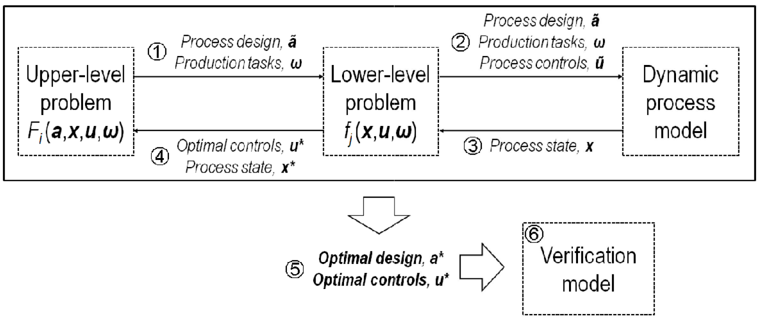

Figure 13: A general overview of bi-level optimization procedure.

The use of the verification model after optimization may reduce the number of possible solutions facilitating the decision-making process. At least some of the solutions can be ignored relying on the simulation data.

In general, the different approaches of process modeling and the advantages of various modeling software applications should be considered during the formulation and planning of the bi-level optimization problem.

5 Conclusions

Modeling and optimization tools and methods are widely used in the process industry, including the paper industry. However, both methods are continuously being developed and the paper industry lags behind the chemical engineering industry, for example, in the use of these applications. In this thesis, one step forward has been taken and bi-level optimization has been successfully applied to papermaking processes. Simultaneous optimization of both the process structure and the operations has been proved possible.

A bi-level optimization problem is formulated in a generalized form, i.e., it can be easily applied for different purposes. The focus is on dynamic and multiobjective optimization, because it is the best way to handle the complex papermaking processes. Furthermore, the formulation of the bi-level optimization problem and the solution procedure for the problem are described. The methodology is developed without too tight limitations. In practice, it is possible to use the same structure of the bi-level optimization problem and the solution algorithm even though the application, objectives or software used would differ from those presented in this thesis. In the future, the same process design methodology could be applied to the design of new process types, such as biorefiners, for example.

The forest industry is seeking for new business ideas and cost-effective methods for developing the processes. The methodology presented here is a significant option for that purpose. In this way, profitability, sustainability and energy efficiency, for example, of the papermaking processes can be improved. Although the numerical experiments presented in this thesis handled generic process models and limited aspects, such as process stability and product quality, potential of the methodology is much higher.

6 Summary of papers

I In this publication, a dynamic mill-wide process model was coupled with dynamic multiobjective optimization. The interaction between the software and the practical optimization procedure was created for a single-level problem. The method was illustrated by numerical experiments in which the basis weight and filler content controllers (PI type) were tuned to operate more accurately. A process model of a supercalendered (SC) papermaking line was built up using Apros software in cooperation with VTT Technical Research Centre of Finland.

II After single-level optimization, the focus of the research was turned to the theoretical formulation of a bi-level optimization problem. The upper level consisted of the structural design optimization and the lower level of the operational optimization. The background was the same as in Publication I: dynamic multiobjective optimization. In addition, a solution algorithm for bi-level optimization problems was presented. The bi-level optimization procedure was illustrated by a numerical experiment in which the process stability was considered on the upper level and the quality and production aspects on the lower level.

III In this publication, the research around the bi-level optimization was continued but the numerical experiments were more realistic. The main difference between Publications II and III was the cost function for the investment cost and a more economical approach. The investment costs were considered on the upper level and the operational costs on the lower level. However, the operational costs were handled through the process parameters, such as broke dosage and net production.

IV In this paper, the application was changed from SC paper to light-weight coated (LWC) paper. The process was modeled using the

Matlab software and therefore the model was simplified and computationally not as heavy as the Apros model in the previous publications. In addition, the design problem included both the broke system and the water system. Hence, the upper-level objectives consisted of the investment costs only while the lower-level optimization problem focused on the process stability and efficiency.

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PUBLICATION I

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Bi-level optimization for a dynamic multiobjective problem

Mikko Linnala[a]*, Elina Madetoja[a], Henri Ruotsalainen[a] and Jari Hämäläinen[b]

[a]*Department of Applied Physics, University of Eastern Finland, P.O. Box 1627, FI-70211 Kuopio, Finland;* [b]*Centre of Computational Engineering and Integrated Design, Lappeenranta University of Technology, P.O. Box 20, FI-53851 Lappeenranta, Finland*

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In this article, a bi-level optimization problem covering upper (design) and lower (operation) levels is defined and a solution procedure for bi-level optimization problems is presented. This is devised as a dynamic multiobjective optimization problem, *i.e.* the values of the control and state variables change over a predefined time horizon and several competing criteria are optimized simultaneously. Moreover, the interaction between the upper and lower levels is analysed. The benefits of bi-level dynamic multiobjective optimization are illustrated in detail by examining an industrial case in which the design of a paper mill (upper level) and the mill operation (lower level) are optimized at the same time. However, the problem definition and the solution procedure are not limited to any specific application but can be exploited in many different industrial areas.

Keywords: bi-level optimization; dynamic multiobjective optimization; dynamic process simulation

1. Introduction

A bi-level optimization makes possible the simultaneous optimization of design and operation. A bi-level optimization problem has two levels where the upper-level (*e.g.* process design) problem is the leader and the lower-level (*e.g.* process operation) problem is the follower. Thus, the upper-level solution affects the lower-level solution and vice versa. For example, the optimization variables of the upper level are used as constants in the lower lever. If the objective function on one or both of the levels is vector-valued, the problem is called a bi-level multiobjective optimization problem (Eichfelder 2010). Bi-level multiobjective optimization makes it possible to conduct an efficient optimization of complicated practical applications, such as a papermaking process.

Bi-level optimization can be applied in many fields and for different kinds of problems. For example, in chemical engineering bi-level optimization is exploited to optimize the design and control of processes (Mohideen *et al.* 1996b, Bansal *et al.* 2000a,b), in electricity markets, it is applied to strategic pricing (Fampa *et al.* 2008), and in supply chain problems, production–distribution interactions are studied (Calvete *et al.* 2011). Bi-level optimization methodology was developed

*Corresponding author. Email: mikko.linnala@uef.fi

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by Mohideen *et al.* (1996b) who proposed an algorithm for solving integrated design and operation problems including dynamic mathematical models, uncertainty parameters, time-varying disturbances and robust stability criteria. Subsequently, Bansal *et al.* (2000b) described both simultaneous and sequential solution procedures for bi-level problems. In the sequential procedure, the process design and operation are optimized in turn until optimal design with optimal operation is achieved. Multiobjective bi-level problems have been studied by Fliege and Vicente (2006) as well as Deb and Sinha (2008), and Li *et al.* (2010) solved multiobjective bi-level problems by using evolutionary algorithms. Different cases and useful background to bi-level optimization were reviewed by Colson *et al.* (2005).

Practical optimization problems in industrial processes can usually be considered as being both dynamic and multiobjective. In addition, solution methods may be based on process models (Kameswaran and Biegler 2006), in which case they are referred to as model-based problems. As well as bi-level optimization, dynamic multiobjective optimization has been widely applied in chemical engineering. For example, Cervantes *et al.* (2002) have considered optimal control strategies of an industrial low-density polyethylene plant, and Barakat *et al.* (2008) have presented dynamic multiobjective optimization as applied in batch separation processes.

In the paper industry, although dynamic process modelling has been used for a long time (Niemenmaa *et al.* 1998, Barber and Scott 2007), process optimization has mainly been simply single objective (Höfferl and Steinschorn 2009, Ropponen and Ritala 2010) or multiobjective with steady-state models (Madetoja and Tarvainen 2008, Hämäläinen *et al.* 2010). However, there are examples of dynamic multiobjective approaches being used in single-level optimization (Linnala *et al.* 2009, 2010). Bi-level multiobjective optimization has already been exploited so that the design and operation of one sub-process ('broke' system) are optimized simultaneously (Ropponen *et al.* 2010). In this article bi-level multiobjective optimization is applied for the broke system similarly to previous studies, but as far as is known the process model used is more exact, realistic and larger than those used in previous studies. In this way the results of the optimization are more reliable for implementation in real processes, which is one important goal of this kind of research.

In this study, dynamic and multiobjective properties were taken into account in both levels of a bi-level optimization problem unlike in previous studies of bi-level optimization. That is because several of the practical optimization problems in the process industry are dynamic and multiobjective, and those problems have not been discussed extensively from a bi-level optimization point of view. Here, the definition of the bi-level problem as well as the solution procedure is generalized, *i.e.* they are not limited to any specific application, algorithm or solver. Since the optimization problem is formulated in the bi-level multiobjective mode, it is possible to handle both long-term and short-term objectives simultaneously and efficiently. In the long-term, one can decrease capital expenditure in the process as well as raw material costs, and in the short-term one can assure optimal operation during different production tasks. In addition to handling different problems, a similar approach can be exploited for the design of both new processes and for the revision of existing processes.

The article is organized as follows: the next section handles the theoretical background and presents a solution procedure for a bi-level optimization problem. Then, there are numerical experiments and the results are presented in Section 3. Finally, conclusions sum up the results in Section 4.

2. Problem setting and solution procedure

Here a bi-level optimization problem in which the upper (design) and lower (operation) levels are taken into account will be defined. There are several articles on this topic (Mohideen *et al.* 1996b, Deb and Sinha 2008). However, certain aspects presented in this article have not been considered previously, where the emphasis of the research may have been different. Deb and Sinha (2008) have described an algorithm that uses a multiobjective evolutionary algorithm on both levels of a bi-level optimization problem. Thus, there are some similarities with this solution procedure. For instance, Deb and Sinha emphasize that the upper-level control variables do not change in the lower-level optimization. The same assumption is also used in this approach. In addition, both levels have separate objective functions and control variables. Moreover, Deb and Sinha highlighted one important issue: Pareto optimal solutions of the lower-level optimization problem become feasible solutions to the upper-level optimization problem. Pareto optimal solutions are mathematically equally good solutions of a multiobjective optimization problem (Sawaragi *et al.* 1985). However, this approach can use different optimization methods and algorithms whereas their algorithm was developed as a multiobjective evolutionary algorithm.

Similarly to this approach and Deb and Sinha's algorithm, Mohideen *et al.* (1996b) also attempted to find an optimal design on the upper level with feasible and efficient operation on the lower level. They proposed a framework for solving integrated design and control problems that included dynamic mathematical models similar to this approach. Moreover their framework also takes into account uncertainty parameters and time-varying disturbances as well as robust stability criteria. These two last features are not taken into account to the same extent in this approach, though this optimization can also cope with some time-varying disturbances (Linnala *et al.* 2010). The main difference between this approach and the algorithm of Mohideen *et al.* (1996b) is that their solution procedure can only manage a single objective function.

Since there are two important aspects in this approach – multiobjectivity and dynamics – next a dynamic optimization problem and its solution procedure are defined, and then a dynamic multiobjective optimization problem is studied.

2.1. *Dynamic optimization*

A dynamic optimization problem involves a dynamic process model where dynamic variable values change with time (Biegler and Grossmann 2004). Thus, its solution differs from the steady-state problem. The dynamic optimization problem can be formulated as follows:

$$\begin{aligned} &\underset{\boldsymbol{u}(t)}{\text{optimize}}\ f(\boldsymbol{x}(t_f), \boldsymbol{u}(t_f), \boldsymbol{p}, t_f) \\ &\text{subject to} \begin{cases} \boldsymbol{x} \in S_x \\ \boldsymbol{u} \in S_u \\ h\left(\dfrac{\mathrm{d}\boldsymbol{x}(t)}{\mathrm{d}t}, \boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{\omega}(t), t\right) = 0 \quad \text{for all } t \in [t_o, t_f], \end{cases} \end{aligned} \tag{2.1}$$

where f is an objective function, h is a system of the differential and algebraic equation constraints, which can also be divided into two separate systems (Cervantes and Biegler 2000, Biegler and Grossmann 2004), $\boldsymbol{x}$ denotes the differential and algebraic state vectors (these can also be presented separately), $\boldsymbol{u}$ is the vector of optimization variables, also known as a control vector, $\boldsymbol{p}$ is a steady parameter vector, and t_f is a length of time horizon. Sometimes the steady parameter vectors can be ignored, because they are constants from the optimization point of view. Since dynamic optimization has been studied for years, there are several different solution approaches for problem (2.1). Typically some of the solutions require at least partial discretization of the originally continuous variables (Biegler and Grossmann 2004, Grossmann and Biegler 2004).

In the case when several objectives need to be optimized simultaneously and objectives and/or variables change with time, the optimization problem is called a dynamic multiobjective optimization problem and can be formulated as follows:

$$\underset{\boldsymbol{u}(t)}{\text{optimize}}\ (f_1(\boldsymbol{x}(t_f), \boldsymbol{u}(t_f), \boldsymbol{p}, t_f), \ldots, f_n(\boldsymbol{x}(t_f), \boldsymbol{u}(t_f), \boldsymbol{p}, t_f))$$

$$\text{subject to} \begin{cases} \boldsymbol{x} \in S_x \\ \boldsymbol{u} \in S_u \\ h\left(\dfrac{\mathrm{d}\boldsymbol{x}(t)}{\mathrm{d}t}, \boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{p}(t), t\right) = 0 \quad \text{for all } t \in [t_o, t_f], \end{cases} \tag{2.2}$$

where $\boldsymbol{f} = (f_1, \ldots, f_n)^{\mathrm{T}}$ is a vector-valued objective function. In this case, the solution process is different compared to (2.1) because all the objective functions f_i, for all $i = 1, \ldots, n$, need to be optimized at the same time. Thus, there does not typically exist a unique solution, but instead, there can be a set of solutions that are mathematically equally good. These solutions are called Pareto optimal or non-dominated or efficient solutions (Sawaragi *et al.* 1985).

2.2. *Bi-level optimization*

Based on the dynamic multiobjective optimization problem (2.2), the problem setting can be extended such that there are two separate levels in the optimization problem; the upper level and the lower level. The assumption is that both levels have multiple objectives and the upper level includes the lower-level optimization problem. In other words, optimization of the upper level requires that the lower level is optimized. The optimization problem considered on the upper level can be given as follows:

$$\underset{\boldsymbol{a}}{\text{optimize}}\{F_1(\boldsymbol{a}, \boldsymbol{x}(t_f), \boldsymbol{u}(t_f), \boldsymbol{\omega}), \ldots, F_k(\boldsymbol{a}, \boldsymbol{x}(t_f), \boldsymbol{u}(t_f), \boldsymbol{\omega})\}$$

$$\text{subject to} \begin{cases} \boldsymbol{a} \in S_a \\ (2.4), \end{cases} \tag{2.3}$$

where F_i, for all $i = 1, \ldots, k$, are the upper-level objective functions, $\boldsymbol{a}$ is a vector of the optimization variables on the upper level (design variables), $\boldsymbol{x}$ is a vector of the state variables, $\boldsymbol{u}$ is a vector of the optimization variables on the lower level (control variables), $\boldsymbol{\omega}$ is a vector of the operational tasks, t_f is the length of the optimization horizon and S_a is a feasible set of $\boldsymbol{a}$ defined by all the constraints including box constraints as well as linear and nonlinear equality and inequality constraints. In problem (2.3), the operation tasks ($\boldsymbol{\omega}$) are related to the lower-level optimization problem and they typically present some assignment or modification of the system state. One should note that compared to some other formulations in (2.3), steady parameters are ignored.

The problem (2.3) becomes dynamic because the lower-level optimization problem includes a system of transient differential and algebraic equations that is a dynamic system. The optimization problem on the lower level can be given as follows:

$$\underset{\boldsymbol{u}}{\text{optimize}}\{f_1(\boldsymbol{x}(t_f), \boldsymbol{u}(t_f), \boldsymbol{\omega}(\boldsymbol{a}, t)), \ldots, f_l(\boldsymbol{x}(t_f), \boldsymbol{u}(t_f), \boldsymbol{\omega}(\boldsymbol{a}, t))\}$$

$$\text{subject to} \begin{cases} \boldsymbol{x} \in S_x(\boldsymbol{a}) \\ \boldsymbol{u} \in S_u(\boldsymbol{a}) \\ h\left(\dfrac{\mathrm{d}\boldsymbol{x}(t)}{\mathrm{d}t}, \boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{\omega}(\boldsymbol{a}, t), t\right) = 0 \quad \text{for all } t \in [t_o, t_f], \end{cases} \tag{2.4}$$

where f_j, for all $j = 1, \ldots, l$, are the lower-level objective functions, $\boldsymbol{x}$, $\boldsymbol{a}$, $\boldsymbol{u}$ and $\boldsymbol{\omega}$ are the same as above, S_x and S_u are the feasible sets of $\boldsymbol{x}$ and $\boldsymbol{u}$, respectively, and h is the system of dynamic differential and algebraic equations, similar to (2.1) and (2.2).

As (2.3) and (2.4) show, in this problem formulation, the current optimization variable values on the upper level affect the lower-level problem setting. They appear not only in the operational tasks but also in defining the feasible sets of the state variables and the optimization variables. On the other hand, the solution of the lower-level optimization problem (optimal values of the optimization variables) affects the objective functions on the upper level. Thus, the optimization problems on the upper and lower levels have two-way coupling which is presented in Figure 1. Here, the assumption is that the objective functions and optimization variables are different between the levels, and the optimal variable values are denoted by *.

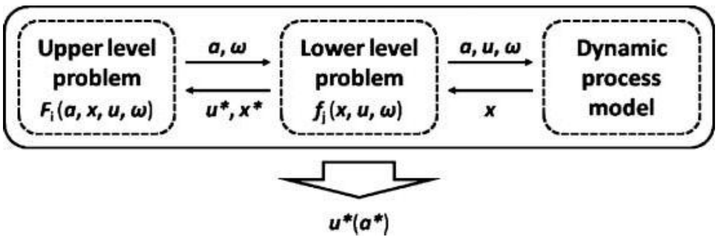

Figure 1. Interactions between the optimization levels and a dynamic process model.

2.3. *Solution procedure*

Next a solution procedure for the bi-level optimization problem given in (2.3) will be presented. As described, this approach has a few similar features to simultaneous and sequential optimization procedures presented by Mohideen *et al.* (1996a) and the algorithm of Deb and Sinha (2008). In practice, this approach is able to handle dynamic and multiobjective optimization problems on both levels. The main emphasis is given to the definition of an abstract solution procedure that can be applied and modified easily for different problems. In the following section, an example of how it is applied for solving a bi-level optimization problem from the paper industry will be presented.

Algorithm 1 – Bi-level optimization

Let the bi-level optimization problem be defined as in (2.3) and (2.4). Then the solution procedure for such a problem can be defined as follows.

1. Initialize the optimization method selected for the upper-level optimization.
2. Define objective functions, a vector of optimization variables and constraints for the upper-level optimization problem (2.3) (including the lower-level optimization problem parametrized by the upper-level optimization variables) and perform optimization as follows. Do until some stopping criterion is fulfilled, as follows.
   (a) Let vector $\tilde{\boldsymbol{a}}$ contain the current values for the optimization variables on the upper level. Define the corresponding lower-level optimization problem (2.4) at $\tilde{\boldsymbol{a}}$.
   (b) Find the optimal state for the lower level with the selected optimization method, *i.e.* perform the optimization based on Algorithm 2.
   (c) Let $\boldsymbol{u}^*$ be the optimal solution of the lower-level optimization problem and $\boldsymbol{x}^*$ the corresponding vector of state variables. In the multiobjective case $\boldsymbol{u}^*$ is selected from a

set of Pareto optimal solutions using even a human decision maker or some predefined information.

(d) Based on $\boldsymbol{u}^*$ and $\boldsymbol{x}^*$, evaluate objective functions $F_1, \ldots, F_k$ on the upper level and provide the objective function values to the optimization method.

End Do

3. The optimal solutions for the bi-level optimization problem are $F_1, \ldots, F_k$ at $\boldsymbol{a}^*$ with the corresponding optimal lower-level optimization solutions $f_1, \ldots, f_l$ at $\boldsymbol{u}^*$.

Algorithm 2 – Lower-level optimization

Let a lower-level optimization problem be defined as in (2.4). Then the solution procedure is as follows.

1. Initialize the optimization method.
2. Define the objective functions, a vector of the optimization variables and constraints in (2.4) for the given parameters $\tilde{\boldsymbol{a}}$. Start the optimization procedure as follows.
   Do until some stopping criterion is fulfilled, as follows.
   (a) Solve the dynamic process model with the current optimization variables $\tilde{\boldsymbol{u}}$.
   (b) Evaluate objectives $f_1, \ldots, f_l$ at $\tilde{\boldsymbol{u}}$ based on the state variables $\tilde{\boldsymbol{x}}$.
   End Do
3. Save the optimal values of the optimization variables $\boldsymbol{u}^*$ and the corresponding state variable values $\boldsymbol{x}^*$ as well as $f_1, \ldots, f_l$ which are needed in Algorithm 1.

In this approach, the bi-level optimization problem is multiobjective in both optimization levels. If the objectives are conflicting, a set of mathematically equally good solutions (Pareto optimal solutions) is obtained on both levels. In the work of Deb and Sinha (2008) bi-level Pareto optimality was analysed and their algorithm could handle the Pareto optimal solutions produced on the lower level. However, in many situations only one solution has to be chosen as the final one. This choice can be done by a decision maker who is capable of comparing the Pareto optimal solutions based on her/his expert knowledge of the current problem. Sometimes computational time becomes unacceptably long and that precludes participation of the decision maker. Then some kind of predefined information with classical scalarizing functions can be used to choose the best solution during the bi-level optimization process (Miettinen 1999).

3. Numerical experiment

Here a numerical experiment where a bi-level optimization was applied to the process of papermaking is presented. To be precise, a broke system in which the rejected paper is being collected and re-circulated back into the process as a raw material is considered. Briefly, the aim was to optimize the capital costs and the operating costs simultaneously. The capital costs were described by the broke tower volumes that were minimized, and the operating costs were minimized by maximizing the broke dosage (in order to minimize the need for virgin raw material) and the net production. In order to highlight the special features of this problem, the application will be introduced.

3.1. *Dynamic multiobjective optimization related to papermaking*

In this experiment a dynamic process model of a supercalendered (SC) papermaking line was used. The model consists of a TMP (thermomechanical pulp) mill where the mechanical pulp is produced, an approach system where the raw materials are mixed and diluted, a broke system where the rejected paper is being collected, a paper machine where the paper web is formed and dried, and a reel where the ready paper is packaged for post processing. The dynamic process model was conducted with Apros software (VTT 2010) in co-operation with the VTT Technical Research Centre of Finland.

The problem became a bi-level one because the design and operation of the broke system had to be considered. The broke system had its own subsystems for a wet broke (paper rejected before drying having approximately 50% moisture content) and a dry broke (ready paper being rejected). Hence, the broke system consisted of the elements presented in Figure 2.

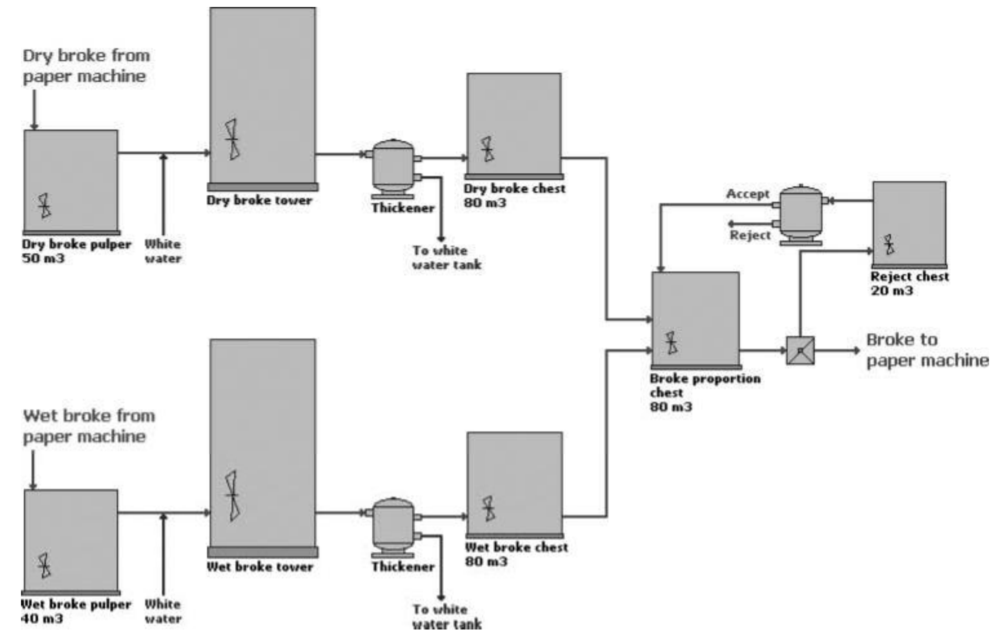

Figure 2. Broke system of the papermaking line modelled.

When the broke is recycled back into the process, its properties differ from those of the virgin raw materials and therefore this affects the paper properties. For example, when the dosage of broke increases, the strength properties of the paper web decrease and, furthermore, the risk of production failure, referred to as a break, increases significantly. Should a break occur, all the paper needs to be rejected and fed back to the broke system (which creates the need for a larger broke tower volume). This phenomenon was modelled such that, when the broke dosage increased, a larger part of the paper web was rejected, but no actual break occurred. This illustrated the growing risk of break caused by the increased broke dosage over the long-term. On the other hand, broke is a much cheaper raw material than virgin raw materials such as TMP or chemical pulp. Therefore the dosage of broke should be kept as high as possible. Hence, on the lower level (operation of the broke system) there were conflicting objectives: maximize both dosage of broke and net production. On the upper level (process design) investment costs (broke tower volumes) which depend on the operations of the lower level were tried to be minimized. Overall, there were multiple objectives at both levels which had very strong interactions with each other.

3.2. *Optimization problem setting*

At the operational level, there were two continuous control variables; dosage of broke and the wet broke proportion of total broke dosaged. Instead, at the design level different tower volumes as control variables were considered and they were defined as integer variables in order to limit the search space. The objective functions optimized on the operational level consisted of production loss (f_1), variation of fill percentage of the dry broke tower (f_2), variation of fill percentage of the wet broke tower (f_3), and broke dosage (f_4). From these functions, f_1, f_2 and f_3 were minimized, and f_4 was maximized. The objective functions on the operational level were defined as follows:

$$f_j = \sum_{t=t_0}^{t_f} |x(t) - x_{\text{target}}|, \quad \text{for all } j = 1, \ldots, 4. \tag{3.1}$$

On the design level, the objective functions consisted of the fill percentages of wet broke (F_1) and dry broke (F_2) towers and both functions were minimized. The objective functions were defined as follows:

$$F_i = \max_{t \in [t_0, t_f]} |x(t) - x_{\text{target}}|, \quad \text{for all } i = 1, 2. \tag{3.2}$$

In this way, the tower volumes could be minimized, but runnability and stability were able to be maintained with the buffer volume needed. This can be seen in the objective functions f_2, f_3, F_1 and F_2, which were based on the same state variables. At the operational level (f_2 and f_3), the process stability was the most important parameter, whereas at the design level (F_1 and F_2) maximum values were the most important. Numerical values for the design, control and state variables are presented in Table 1. The upper and lower limits of the design and control variables were defined based on expert knowledge. The initial values of the variables represented a stable process situation (reference point).

Table 1. Numerical values of the design, control and state variables. Lower and upper limits or step size were not needed for the state variables and target values were not needed for the control variables. Thus, they are marked '–'.

	Control variables		State variables	
Operational level	Wet broke prop. [%]	Broke dos.[a] [%]	Prod. [t/h]	Fill-% [%]
Initial value	60	15	51.39	50
Lower limit	0	0	–	–
Upper limit	100	75	–	–
Target value	–	75	53.69	50
	Design variables		State variables	
Design level	$V_{\text{wet broke}}$ [m^3]	$V_{\text{dry broke}}$ [m^3]	Fill-% [%]	
Initial value	2000	4000	50	
Lower limit	250	250	–	
Upper limit	6000	6000	–	
Step size	250	250	–	
Target value	–	–	75	

[a] Broke dosage was both a control and a state variable. Its target value was used only in the objective function formulation.

The optimization problem on the operational level was multiobjective, and thus, a set of Pareto optimal solutions was obtained. Here only one solution was wanted to be brought to the design level. To achieve that goal, a scalarizing function was used to select a single solution. The method of global criteria was applied as a scalarizing function (Deb 2001):

$$S(\boldsymbol{f}, \boldsymbol{z}) = \left(\sum_{m=1}^{l} |f_m(\boldsymbol{u}) - z_m|^p \right)^{1/p}, \tag{3.3}$$

where $\boldsymbol{f} = (f_1, \ldots, f_l)^{\mathrm{T}}$ is a vector of the objective functions, $\boldsymbol{z} = (z_1, \ldots, z_l)$ is the reference point defined close to the ideal point based on expert knowledge, and here p was 2. After the scalarizing, a solution which corresponded to the smallest value of the scalarizing function was brought to the design level.

Since the optimization problem on the operational level was dynamic, a receding horizon prediction principle (model predictive control) was applied (Rawlings 2000). In this example, the same dynamic process model was used for both prediction and simulation. Therefore two different time horizons were defined. The longer time horizon, $T_{\mathrm{pred}} = 3000$ s, was used for prediction of the control sequence, and the shorter time horizon, $T_{\mathrm{sim}} = 600$ s, was used to simulate one time stage forward with the first controls predicted. This loop was repeated until the end of the total time horizon, 4800 s, was achieved ($T_{\mathrm{end}} = T_8$). The principle of receding horizon prediction is presented in Figure 3, and an example of this has been presented previously (Linnala *et al.* 2010).

In this example, the optimization problem on both levels was solved by using the differential evolution algorithm (DE) implemented in MATLAB™. DE belongs to the group of evolution strategies, *i.e.* it simulates natural evolution. The simulation is based on generations and populations as in other evolution algorithms (Coello Coello 2000, Lampinen 2002, Price *et al.* 2005). The DE algorithm can be formulated to solve multiobjective problems with linear and nonlinear equality and inequality constraints. The solution of the problem begins with the definition of the initial vector population (target vectors) from the permitted search space. After the initialization, differential mutation produces a population of mutation vectors such that the scaled difference of two randomly sampled vectors is added to the third vector. The scale factor is used to control the rate at which the population evolves. After a mutation, DE performs a uniform crossover or discrete recombination. Subsequently, trial vectors are built by copying parameter values from two different vectors, *i.e.* each target vector is crossed with a corresponding mutant vector. The crossover probability is used to control the proportion of parameters copied from the mutant vector. The defined crossover probability is compared to the output of a random number generator and if the probability is greater than the random number, then this parameter is copied from the mutant vector. Otherwise, the parameter value is copied from the target vector. Still, at least one parameter value is copied from the mutant vector in order to avoid duplication of the target vector. Finally, the DE selects the vectors for the new population. If the trial vector is equally good or better from the objective function point of view, it will replace the target vector in the new generation. In the multiobjective case, the non-dominated vector is selected for the new generation. In this way, the search moves toward the optimal solution in a step-by-step manner (Price *et al.* 2005).

Even if the same solver was used on both levels, some parameter values of the DE differed. The mutation rate was 0.3 and the crossover rate was 0.6 on both levels. The number of generations and the population size were five at the design level. At the operational level, the number of generations was five also, but the population size was eight in order to increase variation in the set of optimal solutions.

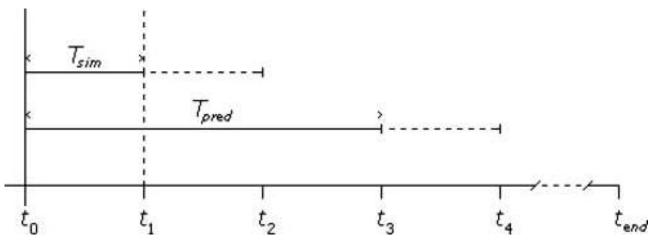

Figure 3. Receding horizon prediction principle.

3.3. *Results*

After the optimization problem was solved, several different design candidates with the optimal operation were obtained. Since the design optimization problem was multiobjective and the operational level affected the design level, design candidates differed from each other. As an example, the objective function values of two chosen design candidates are presented in Table 2. Here, the conflicts between the objectives can be appreciated: at the design level, if F_2 decreased then F_1 increased, and vice versa. At the operational level, conflicts were more complicated because several variables affected several objectives. Nonetheless, it could be considered as a conflict between the dry broke and wet broke line operations, as can be seen in Table 2. If f_3 (wet broke tower variations) decreased, f_2 (dry broke tower variations) increased (candidate 1) and vice versa, if f_2 (dry broke tower variations) decreased, f_3 (wet broke tower variations) increased (candidate 2).

Table 2. The objective function values of two different solution candidates.

	Candidate 1	Candidate 2
f_1, sum of production loss [t/h]	1149	1200
f_2, sum of dry broke tower liquid level [%]	2587	3377
f_3, sum of wet broke tower liquid level [%]	1672	7489
f_4, sum of broke dosage [%]	408	385
F_1, maximum liquid level of wet broke tower [%]	25.00	24.93
F_2, maximum liquid level of dry broke tower [%]	24.98	25.00

Each optimal process design had its own optimal control sequence defined by the operational optimization over the time horizon T_1–T_8. Table 3 presents the previous two design candidates including the design variable values (tower volumes) and control variable values (broke dosage and wet broke proportion of total broke).

Table 3. Design and control variable values of two design candidates.

				Control variables [%]							
Design variables [m^3]				T_1	T_2	T_3	T_4	T_5	T_6	T_7	T_8
Candidate 1	a_1	4000	u_1	15.0	7.6	2.3	18.7	3.9	38.6	8.5	27.5
	a_2	1000	u_2	60.0	57.4	23.7	80.8	95.7	95.4	39.0	65.2
Candidate 2	a_1	1000	u_1	0.5	61.0	7.2	7.7	3.9	40.7	25.7	12.4
	a_2	2750	u_2	37.5	58.5	38.5	38.4	50.4	42.2	46.3	2.8

a_1: Wet broke tower volume. a_2: Dry broke tower volume.
u_1: Broke dosage. u_2: Wet broke proportion of the total broke.

The optimization results can be visualized with the time series of different state variables used in the objective functions as presented in Figures 4 and 5. Here, five optimal solutions are shown in order to illustrate the variation between the different designs and operations. The dotted lines mark the target levels, *i.e.* the objective function values are better the closer the state variable values are to the target level. For the sake of clarification, design candidates 1 and 2 presented above are marked with arrows in Figure 4.

Figure 6 presents variation in basis weight and filler content, which are very important paper quality parameters. These parameters were not included in the objective functions but produce interesting additional information for the decision maker because the quality parameters should stay within the target interval (marked with dotted lines).

As the results show, there was variation between the solutions both in design and in operation. At the operational level, variations in the broke tower liquid levels (Figure 4) differed rather markedly

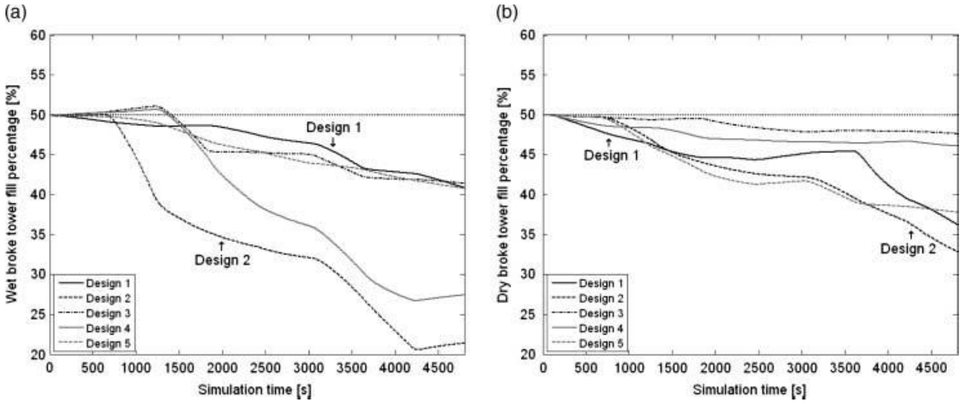

Figure 4. Fill percentages of wet broke (left) and dry broke (right) towers during the simulation. The dotted line represents the target value.

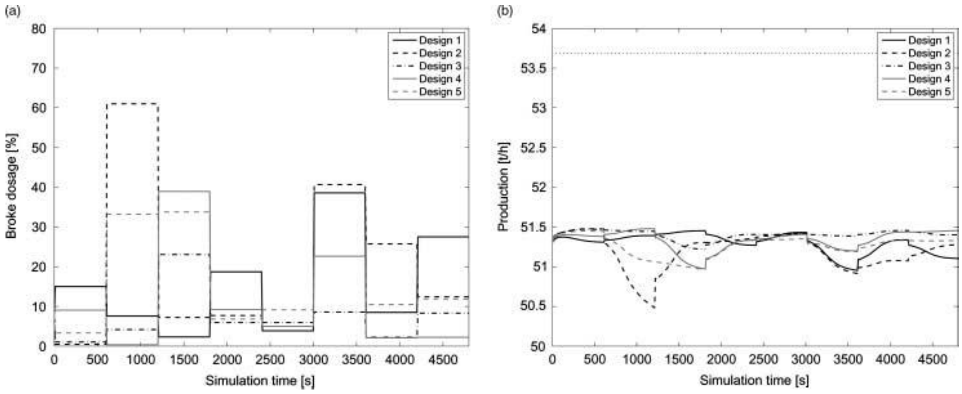

Figure 5. Broke dosage for each of the eight time stages (left) and production (right) during the simulation. The dotted line represents the target value.

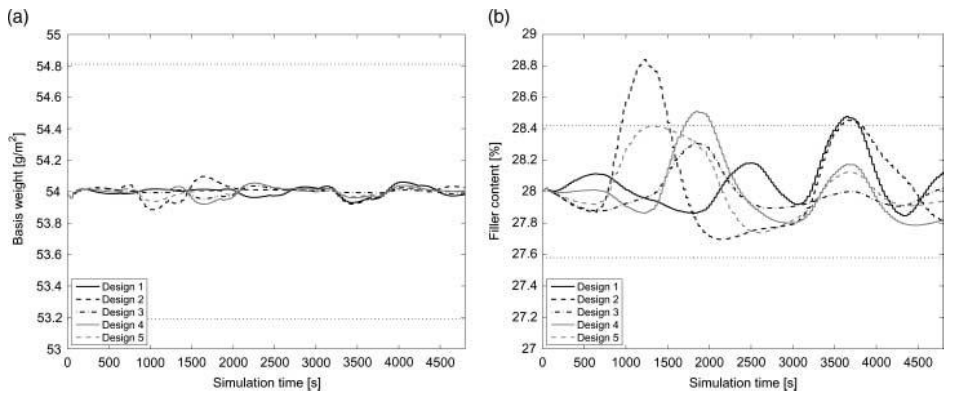

Figure 6. Basis weight (left) and filler content (right) during the simulation. The dotted lines represent the target intervals.

between the design candidates. For example, designs 2 and 4 show that too strong operations lead to loss of process stability. The same phenomenon can be seen in Figure 5, in which too high a broke dosage leads to production losses (design 2). In addition, some solutions, such as designs 2 and 4, could be discounted in practice based on expert knowledge because paper quality would not stay in the target interval, as can be seen in Figure 6. Since paper quality was not included in the objective functions, all the solutions presented are equally good from the optimization point of view. Therefore, a decision maker is the best individual to compare the various solution candidates and choose the best one to be realized.

Above, only one control sequence for each design is presented. Nonetheless, depending on the method used at the operational level, different control sequences are also possible. Here, the scalarizing function selected the best controls for eight time stages, one after another. When the first controls were implemented, the next control possibilities were fixed, because the next stage depended on the previous stage. Note that if the scalarizing function or the value of the reference point were changed, the optimal control sequence could be different. This is the challenge of dynamics in a bi-level case, which has not been considered previously in the literature. Overall, this numerical experiment shows that dynamic and multiobjective bi-level optimization can be applied in practical optimization problems, but it requires expert knowledge to understand the relationships between different optimization levels, objectives and variables.

4. Conclusions

In this article a real life optimization problem, being dynamic, multiobjective and bi-level by nature, was discussed. All these special features set requirements for the solution process as well as the problem formulation. Thus, the generalized formulation for a dynamic multiobjective bi-level optimization problem was defined, and a solution procedure for such problems was presented. Subsequently, the approach was illustrated with a real life example in which the process design and operation were optimized simultaneously in place of theoretical test case examination. The results showed that this approach was successful and could be implemented in practical optimization problems. Moreover, this complicated problem cannot be solved efficiently as a single-level optimization problem. Here, the bi-level optimization problem was solved by using a differential evolution algorithm, but other techniques can be implemented as well. It would be interesting to apply this approach with different optimization problems and algorithms. Furthermore, this generalized approach could be implemented in some industrial, even more complicated and challenging, optimization problems in order to demonstrate the real advantages of the approach.

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PUBLICATION III

Improvement of the cost efficiency in papermaking with optimization tools

M. Linnala and J. Hämäläinen

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IMPROVEMENT OF COST EFFICIENCY IN PAPERMAKING WITH OPTIMIZATION TOOLS

MIKKO LINNALA*, JARI HÄMÄLÄINEN

ABSTRACT

This paper presents a bi-level optimization approach for process design of the broke system in which both design and operation are optimized. On the design level, the capital costs invested in the process are minimized, and on the operational level, raw material costs, process runnability, and product quality are optimized simultaneously. The set of solutions consists of the optimal process designs with their optimal control sequences.

INTRODUCTION

As has been clear to all, the global paper industry has come to a turning point in the 21st century. Paper companies are interested in higher process profitability and lower capital costs at the same time. Various kinds of investments made to increase productivity are presented in [1], where a number of unidentified North American and European pulp and paper companies are analyzed from the investment point of view. In [2], the economic benefits of industrial symbiosis are evaluated using an optimization model. Other, more process engineering points of view are presented in [3], which considers the utilization of excess heat, and in [4], which describes energy savings achieved with filler addition.

Because papermaking processes are very complex and equipment is expensive, process improvements are usually tested first using simulators. With simulation results in hand, it is easier to make decisions about possible laboratory or pilot plant trials. Nowadays, paper mill modeling and simulation are performed using dynamic models and simulators. An extensive survey on the use of pulp and paper simulation software in Europe is presented in [5], and a review of the state of the art in modeling and simulation in the pulp and paper industry is presented in [6]. A more detailed description of paper machine modeling is presented in [7,8]. This research did not involve the development of new software, but a large paper mill model was constructed using the Apros™ dynamic process simulator. The entire papermaking process is modeled, including a TMP (thermomechanical pulp) mill, stock preparation system, the short circulation, and a paper machine from the headbox to the drying section. This model is very realistic and more inclusive than the models previously used in this kind of study.

Coupling of this process model with an optimization algorithm enables model-based optimization. Usually, optimization problems must be formulated with multiple objectives because papermaking processes are highly complex. In addition, process dynamics must be taken into account, which leads to a dynamic multiobjective optimization problem formulation. Many existing studies describe papermaking process optimization, but usually a steady-state model is used, or the optimization addresses only one objective, as in [9] and [10], for

MIKKO LINNALA
University of
Eastern Finland
Department of
Applied Physics
Kuopio,
Finland
*Contact: mikko.linnala@uef.fi

JARI HÄMÄLÄINEN
Lappeenranta University
of Technology
Centre of Computational
Engineering and
Integrated Design
Lappeenranta,
Finland

example. However, some studies of dynamic multiobjective optimization in papermaking can also be found in the literature. In [11], process operations are optimized during different production tasks, and in [12], broke system management is optimized.

This paper describes the application of bi-level dynamic multiobjective optimization to the papermaking process, or more accurately, to the broke system. In a bi-level optimization, there are two optimization levels: the upper level consists of design optimization, and the lower level consists of operational optimization. On the upper level (design), the costs of capital investment in the process are minimized, and on the lower level (operations), the operations are optimized so that the process maintains stability, runnability, and high product quality. A similar approach was studied previously in [12], but the process model used here is more exact, more realistic, and broader in scope than those used in previous studies known to the authors. The tradeoff is in computing time which is longer than with simplified models, but the results are more reliable and better suited for application to real processes, which is one important purpose of this kind of research.

This kind of optimization approach can be used for design of both new mills and rebuilds. Moreover, this approach is not limited to papermaking processes only. In the past few years, the paper industry has become interested in new products that require new production lines, such as biorefineries. A corresponding bi-level optimization problem can be formulated for the process design of biorefineries as well.

BI-LEVEL OPTIMIZATION APPROACH

As mentioned above, optimization tasks related to papermaking are usually formulated as dynamic multiobjective optimization problems. After numerous conflicting objectives have been solved for simultaneously, the result is a set of Pareto optimal solutions [13]. These solutions are mathematically equally good solutions, i.e., if one objective improves, another objective is degraded, and vice versa. However, usually a single solution must be chosen as the final one. Therefore, a decision-maker is needed who can compare the solutions and choose the best one based on his/her expertise. Sometimes the decision-maker is not needed because the best solution can be selected based on some kind of predefined information using classical scaling functions [14].

This paper considers a bi-level optimization problem with multiple conflicting objectives on both levels and over some predefined time horizon (dynamics). The term "bi-level optimization problem" means a problem having two levels in which the upper-level (design) problem includes the lower-level (operational) problem. Therefore, the upper-level solution affects the lower-level one, and vice versa. For example, the optimization variables on the upper level are used as constants on the lower level. Hence, the upper and lower optimization levels exhibit two-way coupling, as shown in Fig. 1.

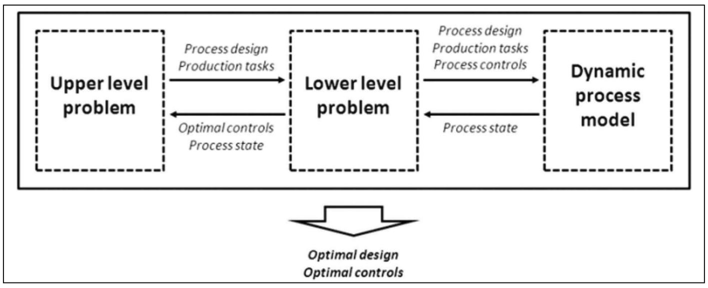

Fig. 1 - Interactions between the optimization levels and a dynamic process model.

The upper-level optimization defines the process design parameter values (e.g., tower dimensions) and the production tasks (e.g., grade changes), which are fed to the lower-level optimization as parameters. The lower-level optimization defines the process control parameters (e.g., setpoint values for the controllers), and these three variables are fed to the process model. After the simulation, the process state (e.g., time series of state variable values) is returned to the lower-level optimization, and the values for the operational objectives are calculated based on the state variables. After that, new values for the process control parameters are fed to the process model for simulation. This loop between the lower-level optimization and the process model is repeated until the optimal process control parameters are achieved. The optimal control parameters and the process state are then returned to the upper-level optimization, where the values of the design objectives are calculated. Based on the objective values, new process design parameter values are fed to the lower-level optimization. This loop between the upper-level optimization and the lower-level optimization is repeated until the optimal process design is achieved. Finally, the output of the bi-level optimization problem is the optimal process design with optimal control parameters.

On the lower level (operational optimization), process control parameters are optimized over some predefined time horizon. This can be done, for example, using a receding-horizon prediction principle such as model predictive control [15]. In this approach, the total time horizon is discretized, and two different time horizons are used. First, the control sequence is predicted over a longer time horizon (prediction horizon). Second, a shorter time horizon is used to simulate one time stage forward with the first set of control parameters predicted (simulation horizon). This loop is repeated until the end of the total time horizon is achieved. Such a receding-horizon prediction principle is illustrated in Fig. 2.

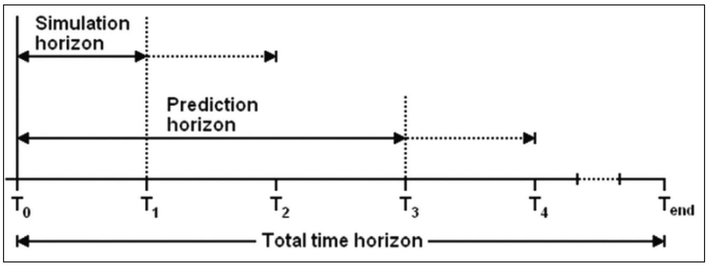

Fig. 2 - **Receding-horizon prediction principle.**

PAPERMAKING CASE STUDY

This case study illustrates how the bi-level optimization approach can be applied in practice. The case study involves design and management of a broke system with the aim of minimizing both capital and operating costs. The bi-level optimization procedure was based on a dynamic process model of a papermaking line generated using the Apros™ software. The model was a generic one, without reference to any real mill, but the process and product were comparable to a state-of-the-art supercalendered papermaking line. The model consisted of numerous submodels which represented the main process components from TMP production to the reel, as presented in Fig. 3. Because only the design and management of the broke system were studied here, the components of the broke system are presented below the overall process block diagram.

In this case, the broke system consisted of two parallel lines: one for wet broke and another for dry broke. The two broke lines were merged just before the broke was fed back to the process. This made it possible to control both the total broke dosage and the relative proportion of the broke types, which is interesting from both process design and quality points of view (effect of drying on fibers).

On the design level, the capital costs of the wet and dry broke towers were minimized (approximation: cost = $V^{0.7}$). On the operations level, broke dosage was maximized, production losses were minimized, and variations in basis weight and filler content were minimized. All objective functions were implemented so that the differences between the current parameter values and the predefined target values were minimized. The optimization problems were solved using a differential evolution algorithm [16] on both levels. The population size was five on both levels, but the number of generations was eight on the design level and five on the operations level. The bi-level optimization procedure was carried out as described in the previous section. Relatively small populations were used to limit the computing time, but larger population sizes should produce more accurate results and

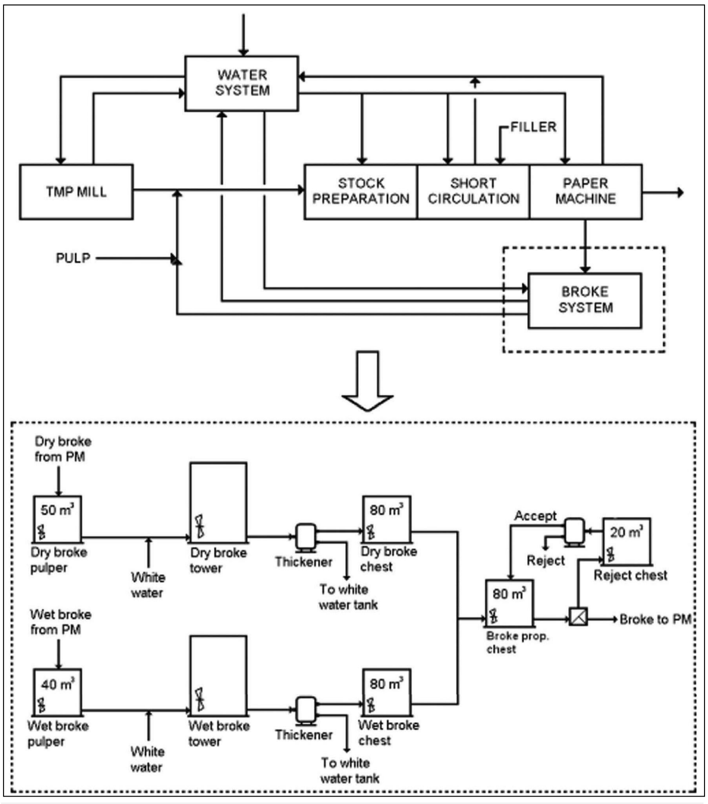

Fig. 3 - **Models of the components of the papermaking line (upper) and the broke system (lower).**

TABLE 1 Optimal values of the design objectives and their corresponding tower volumes.			
	Initial	Design 1	Design 2
F_1: Cost wet broke tower [CU]*	332.2	307.0	305.7
F_2: Cost dry broke tower [CU]*	204.5	77.5	83.1
V wet broke tower [m^3]	4000	3573	3551
V dry broke tower [m^3]	2000	500	552

* CU = currency unit (approximation: cost = $V^{0.7}$)

improve the efficiency of the optimization procedure.

RESULTS

The bi-level optimization yielded two conflicting process designs, as presented in Table 1.

Because the designs are conflicting, a decision-maker is needed to choose the best one based on expert knowledge. Additional information about the process designs can be obtained from the results of operational optimization. Both process designs had optimal control parameters for broke dosage (Fig. 4) and for wet broke proportion of total broke which were defined by operational optimization over the time horizon T_0-T_{12}. The objective on the operational level was to minimize operating costs by maximizing broke dosage and minimizing production losses, as illustrated in Fig. 4.

Figure 4 shows that the operational optimization was difficult because the objectives were conflicting. When the broke dosage was increased, production decreased, and vice versa. Therefore, variations in broke dosage were kept to a minimum, and production was increased as much as possible. Another operating objective was to minimize variations in basis weight and filler content, as shown in Fig. 5.

As Fig. 5 shows, paper quality remained well within the target intervals. Figures 4 and 5 show only one alternative to the optimal operations scenario because a scaling function was used on the operations level. The interrelationship between the operating objectives can be changed using different scaling parameters. In addition to the objective functions, the stability of the different process designs can be compared using the time series of liquid levels in the broke towers, as shown in Fig. 6.

Although the tower volumes were decreased, process operations were able to maintain stability without risk of over-

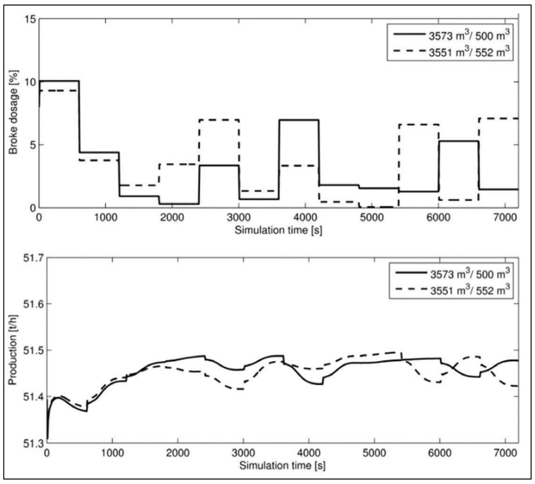

Fig. 4 - Variations in broke dosage (upper) and production (lower) during the simulation.

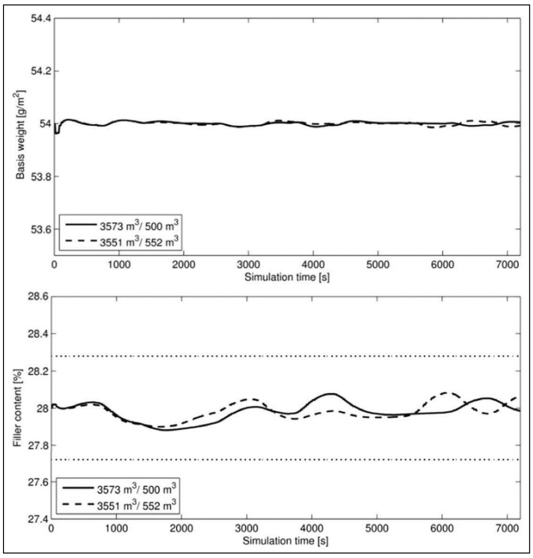

Fig. 5 - Variations in basis weight (upper) and filler content (lower) during simulation. Target interval is marked with dotted lines.

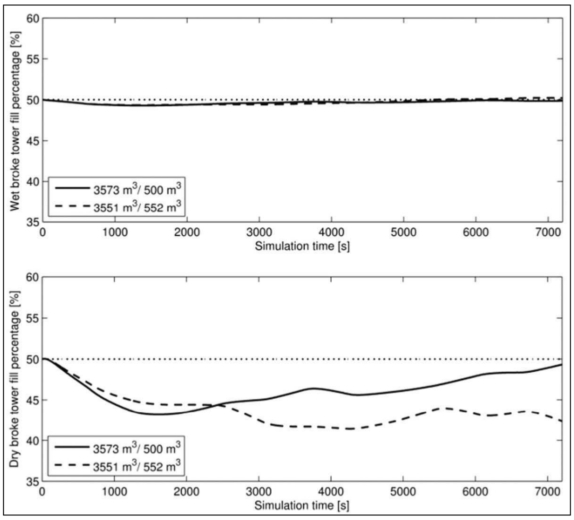

Fig. 6 - Variations in fill percentage of wet broke tower (upper) and dry broke tower (lower) during the simulation.

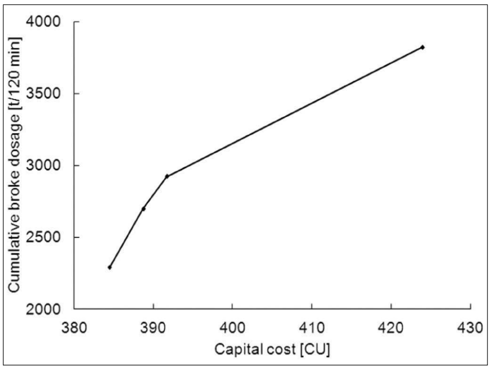

Fig. 7 - Estimated tradeoff between upper-level and lower-level objectives. CU = currency unit.

flow or runout. This kind of tradeoff between upper- and lower-level objectives is interesting and reveals how much the values of the design-level objectives can be decreased without losing too much on the operations level. A tradeoff between capital costs and cumulative broke dosage over the total time horizon is illustrated in Fig. 7.

CONCLUSIONS

This paper has presented a bi-level optimization approach and its application to cost-efficiency improvement in the broke system. The results show that the approach was successful: capital costs were decreased while maintaining adequate process stability. However, the computing time requirements were relatively high; to reduce them, the operational optimization on the lower level could be performed using a slightly simplified process model. However, the differences between the upper-level model and the lower-level model should be as small as possible to maintain the accuracy and efficiency of the bi-level optimization. In future research, this bi-level optimization approach could be expanded outside the broke system, and more complex problems could be studied. In addition, it would be interesting to apply this approach to a practical process optimization problem.

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