Dynamic optimization in business-wide process control

Dynamic optimization in business-wide process control

PROEFSCHRIFT

ter verkrijging van de graad van doctor
aan de Technische Universiteit Delft,
op gezag van de Rector Magnificus prof. dr. ir. J.T. Fokkema,
voorzitter van het College voor Promoties,
in het openbaar te verdedigen

op dinsdag 12 november om 10:30 uur

door

Robertus Leonardus TOUSAIN

werktuigbouwkundig ingenieur
geboren te 's Gravenhage

Dit proefschrift is goedgekeurd door de promotoren:
Prof.ir. O.H. Bosgra
Prof.dr.ir. A.C.P.M. Backx

Samenstelling promotiecommissie:

Rector Magnificus	voorzitter
Prof.ir. O.H. Bosgra	Technische Universiteit Delft, promotor
Prof.dr.ir. A.C.P.M. Backx	Technische Universiteit Eindhoven, promotor
Professor J.D. Perkins	Imperial College, London
Prof.dr.-Ing. W. Marquardt,	RWTH Aachen
Prof.dr.-Ing. H.A. Preisig	Technische Universiteit Eindhoven
Prof.ir. J. Grievink	Technische Universiteit Delft
Dr.-Ing. M. Friedrich	Bayer AG, Leverkusen

Published and distributed by: DUP Science

DUP Science is an imprint of
Delft University Press
P.O.Box 98
2600 MG Delft
The Netherlands
Telephone: +31 15 27 85 678
Telefax: +31 15 27 85 706
E-mail: DUP@Library.TUDelft.NL

ISBN 90-407-2354-0

Keywords: chemical processes, optimization, supply chain

Printed in The Netherlands

Voorwoord

Halverwege 1997 ruilde ik, enthousiast gemaakt door Okko Bosgra en Ton Backx, de nogal klinische mechanische wereld die ik tijdens mijn afstudeerwerk bij Philips had leren kennen in voor de naar verluidt wat minder klinische wereld van de procesregeltechniek. Ik kreeg een pioniersrol in het INCOOP project, een project samen met interessante bedrijven, met grote, uitdagende, industrile problemen en veel reisgeld. Toen ik na anderhalf jaar nog steeds geen chemische plant (spreek uit: *plent*, beetje op z'n Haags zoals in het Delftse INCOOP clubje te doen gebruikelijk) had aangeraakt, nog niet verder was geweest dan Antwerpen, en al sterk begon te geloven dat INCOOP stond voor INdustriële COnflicten en OPonthoud, besloten Okko en ik de verdere promotieplanning wat minder afhankelijk te maken van externe factoren. Rond die tijd werden de eerste leuke resultaten met dynamische optimalisatie behaald, dus het leek een goede zet om op dat spoor verder te gaan, maar dan wel met een supply-chain-brilletje op. Meer daarover in de rest van dit boekje. Rest mij nog een halve pagina om een aantal mensen te bedanken.

Ik wil allereerst Okko bedanken: je inspirerende begeleiding, onuitputtelijke kennis van literatuur en je vertrouwen in mijn handelen heb ik enorm gewaardeerd. Ik hoop nog vaak met je van gedachten te mogen wisselen. Ton, bedankt voor je al minstens zo inspirerende houding, niet alleen naar mij toe maar ook naar de afstudeerders die zich met deelvragen van mijn onderzoek bezig hielden. En dat *waren* afstudeerders. Joeri, Joris, Camile, Wilbert en ook Johan, Justine en Mari. Jullie bijdrage aan het onderzoek zowel als aan de lol die ik had in het werk is enorm. Als ik aan jullie denk, zie ik doorbraakgebak op zaterdagmiddag en polymeren die maar blijven groeien als haren aan mijn hoofd. Lol in het werk, daar spelen collega's natuurlijk de belangrijkste rol in. Ad, A3, Branko, Carsten, Cor, David, Debby, Edwin, Eduard, Els, Frits, Gideon, Guus, Jacqueline, Jogchem, John, Joost, Judi, Camile, Marco, Maria, Maria M., Marjolein, Les, Martijn S., Paul, Peter H., Peter R. de Valk, Piet, Sjirk, Sjoerd, Thomas, Ton. Bedankt voor een fantastische tijd in de vakgroep. En jij natuurlijk ook Dennie! (kneep je hem al?). Ook diegenen waar ik in projectverband mee heb samengewerkt wil ik bedanken: Wim van Brempt, Jobert Ludlage, John Perkins, Wolfgang Marquardt en zijn Aachen boys, Gregor Fernholz en nog vele anderen. Tenslotte, lol in het werk gedijt natuurlijk alleen maar goed als de kantoortijden ingebed zijn in een prettig sociaal leven. Pap, mam, Heid, Bas, Ron, Vicky, zuipmaatjes, familie, Peus, en Mirtje in het bijzonder, jullie hoef ik niet te vertellen hoe blij ik met jullie ben.

Rob Tousain
Eindhoven, September 2002

Contents

Chapter 1

Introduction

This thesis concerns the development of advanced process control and optimization solutions for chemical process industries. Over the past decades the marketplace for chemicals has undergone major changes. To define the current and future requirements of advanced operating strategies for chemical plants it is foremost essential to investigate the main consequences of these changes, which will be done in this chapter (1.1). This chapter will further review the current industrial state of the art in process operations as well as recent, academic developments in the field of process control and optimization (1.2). Finally, a justification of our research approach is given in 1.3.

1.1 Chemical manufacturing

1.1.1 The chemical marketplace

Chemical industry has grown significantly during the post-second world war period. The cheap and limitless supply of oil, combined with a post-war era of unparallelled economic growth resulted in a major expansion of the chemical industry, based on oil and supported by rapidly evolving technology. This growth was catalyzed during the 1950's by the enormous increase in demand for synthetic polymers. Production capacity for commodity chemicals was largely expanded during the 1950's, reducing the gap between demand and production significantly and resulting for the first time in oversaturation in parts of the chemical marketplace. Large investments of the oil industry in commodity chemicals during the 1950's-1960's brought on the next surge of competition: the building of large and modern plants resulted in excess production capacity which stimulated the chemical companies to diversify into other fields of more specialized chemicals. The relation between the gradual saturation of the market since the 1950's and the decrease in chemical industry's profitability during this very time span can not be a coincidence.

The chemical industry is believed to have gone through its most difficult era so far during the 1970's as it was shaken up rudely by successively the report of the Club of Rome in 1972, the oil crisis of 1973 and the world wide recession of 1979. In a report by the steering committee of the European Federation of Chemical Engineering (EFCE) from 1981 [9] the commotion within the chemical industry was expressed as follows: "It is no overstatement that the changes which hang over the industry are more basic and far reaching than at any time since 1945". A main concern of the chemical industry at that time was its critical dependence on the availability of oil which was then expected to cease dramatically during the coming years. In response to the pessimistic predictions of availability of oil, the EFCE concluded that the chemical industry should continuously enhance the quality and utility of its finished consumer products to enable the industry to bid away and conserve crude oil for raw material rather than for energy uses.

The finding of large oil reserves during the past decades and the increased efficiency in the exploration of existing fields reduced the necessity for major interventions. However, the strong dependency on fossil fuels remains a threat for the chemical industry. Tightening legislation with respect to air and water pollution forced chemical industry to choose between investing in costly modifications of processes and process operations to meet the rules or to pay huge fines for violating them.

Global competition

During the past decades the chemical industry has been faced with a major change in its marketplace: the local competition which had its roots in the 1950's expanded to *global* competition in a rapid pace. Several factors contributed to this development. In the beginning of the 1990's many of the basic processes for producing key intermediates such as alkanes and aromatics were mature as they had been operated for more than 20 years. This meant that patent protection had expired so that countries with reserves of crude oil (such as Korea, Mexico, Saudi Arabia) could enter and quickly expand the production of these intermediates for the world market. Other examples are the entrance of the world market for Potassium Chloride by government-controlled (and largely subsidized) companies from Israel, Russia and Canada in the mid 1980's [30] and the production of basic chemicals (e.g. ammonia) from natural gas in Alaska, Mexico and Venezuela. The manufacturing cost advantage due to cheap resources began to outweigh by far the freight costs to ship the products to end users. Next to being confronted with global competition, many chemical com-

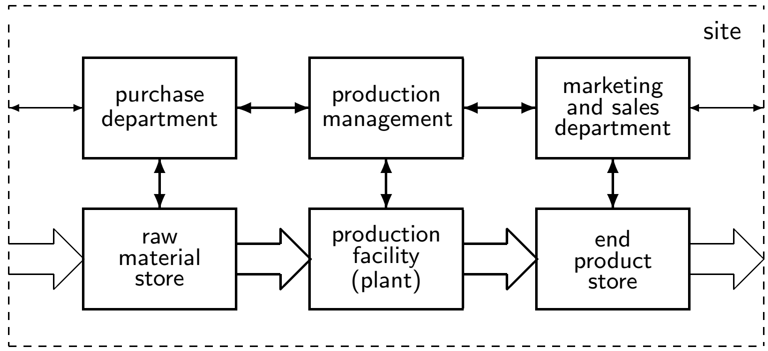


Figure 1.1: The internal supply chain of a chemical manufacturing site.

panies have been or are on the verge of taking a worldwide view on production and marketing themselves. Political developments such as the formation of the European Union have encouraged this. Additionally, products requiring large Research and Development costs such as pharmaceuticals, pesticides and specialty polymers cannot possibly recoup these costs in their home market: they must hence be sold worldwide.

A global marketplace creates a threat for some companies, yet an opportunity for others. Those companies that deal best with the changing requirements the marketplace puts on the company's organization and automation are expected to be the most viable ones.

1.1.2 Towards flexible, demand driven operation

During its early years chemical manufacturing was largely *supply-driven* which was logical because the demand for chemicals exceeded the production. Most companies were practically run by the production managers and process operators, who viewed the plant as being isolated from its environment, interpreting most influences from outside (such as market changes) as disturbances. Sales and purchasing departments played minor roles as being subjected to the consequences of the production manager's actions. The slowly emerging situation of oversaturation in a large part of the chemical marketplace forced chemical companies to adopt a *demand-driven* mode of operation. Companies are required to respond quickly to changing market situations and to meet the more and more diversified demands customers have regarding product specifications. Clearly this puts high demands on the effectiveness and speed of the company's decision making. The fact that decision making is distributed amongst different players in the company, such as purchasing managers, production managers and sales managers complicates matters. The latter is illustrated in Figure 1.1 where the typical internal supply chain of a chemical manufacturing site is depicted [8].

Effective decision making requires a continuous process of gathering, storing, and processing information. The information and decision management is nowadays supported by revolutionary developments in the area of information technology and enterprise automation. As an example consider Enterprise Resource Planning systems as offered by e.g. SAP and Baan. The often company-wide availability and accessibility of crucial information regarding the company's operation creates new opportunities for supply chain management and company-wide decision support. One of the main challenges in this respect, and also the key to demand-driven operation, is the allocation of production resources to comply with orders and physical constraints such as plant capacity, storage capacities etc. Such problems are generally referred to as *scheduling* problems. Literature on scheduling in relation to process industries is rather extensive and the role of scheduling in the internal supply chain is broadly acknowledged. An overview can be found in [70].

Rather surprisingly however, despite the large share of *continuous* chemical manufacturing in chemical industry and its economic attractiveness, most of the scheduling literature focuses on *batch* operations. Typical batch scheduling problems concern the timing of batch operations on parallel processing units so as to meet certain production dead lines. The type of scheduling problem one encounters in continuous manufacturing is of a different nature. Most continuous manufacturing plants can process different feedstocks and/or produce different grades or combinations of grades[1] of products. The scheduling task concerns the timing of feedstock and grade changes. Obviously, production scheduling interferes largely with purchasing and sales decision making and process control and optimization. True flexible operation of the company may require to integrate these. To the author's knowledge, such integrated solutions to production management do not exist to date.

This is certainly reflected in today's operation of multi-grade plants. Most of those plants are still operated according to a predetermined sequence of product grades, called a *product slate* or a product wheel, see Figure 1.2 [77]. The sequence is constructed such that the necessary grade changes are relatively easy, safe and well-known by the operating staff. Remaining degrees of freedom in the determination of the sequence are used to minimize for example the total grade change time. The choice of the grade slate and the duration of the grades is a trade-off between the costs of inventory and the costs of grade changes. Observe that the product-slate type of operation is largely supply-driven and

[1] A product 'grade' is a certain quality of the produced chemical that meets specific customer demands. An example of a product grade is a 'grade of High-density Poly Ethylene' which is typically characterized by the polymer's density and melt index.

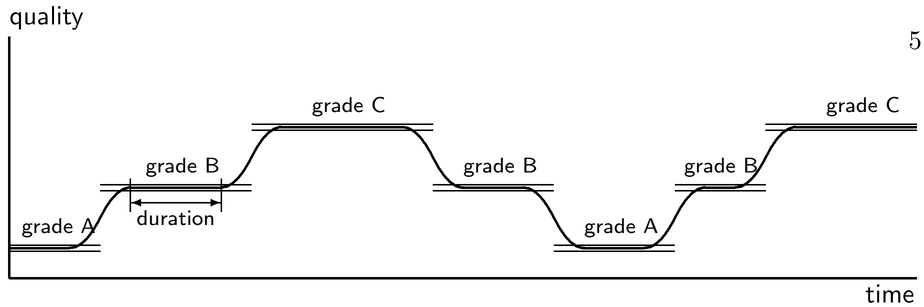


Figure 1.2: A product grade slate A-B-C-B-A with on-spec-ranges.

hardly allows to account for changes in the market.

The lack of systematic approaches to production scheduling for continuous chemical manufacturing is one crucial observation that contributes to the motivation behind our research.

A primary reason for the inflexible operation of continuous chemical plants is the moderate quality of process control systems that are currently implemented in chemical plants. Observe that fast, accurate control of the plant, especially during changeovers between different grades or production rates, is required in order to facilitate demand-driven operation of the plant. A description of the *status quo* of process control technology in chemical manufacturing as well as a critical evaluation of the role of *advanced* process control will be given next.

1.1.3 Production management and control

In this section we will discuss the operation of chemical plants nowadays, ranging from operator control to fully automated process control. We will describe the successful role of advanced control technology in (mainly) refinery applications and why its success in chemical applications is still lagging behind. Also, a description of what we consider to be the current industrial state of the art in process control and optimization will be given, mainly for reference purposes.

Operator control vs. automated control

The operation of chemical processes has always been an intricate task, which is inherent to the scale, the complexity and the potential danger of chemical processing plants in general. The role of process control in the operation of these processes is considered essential. The primary role of process control is to contribute to guaranteed safe operation of the plant. Most processing plants contain hundreds of local control loops and logical devices which help to maintain the plant at a safe and reliable status at all times. Nowadays, these local controllers are often digitalized and implemented on a so-called Distributed

Control System (DCS).

Despite the presence of advanced implementation technology for basic control, the level of automation in most chemical industries is still rather low. Brisk [11] stated in 1992 that most computer-based control systems were being used to at most 25 % of their potential. At present, the use of computer control in the process industries is without doubt more extensive. However the potential of computer-based control systems has grown exponentionally during the past decade so the current figures are probably hardly any better. Illustratively, governing of setpoints for the basic controllers is in many processes still done manually. This traditional, operator-controlled mode of operation is represented schematically in the left part of Figure 1.3.

The performance of an operator-controlled plant is clearly limited by the operator's understanding of the plant's behavior. Although operators can be expected to have at least a so-called "mental model" of the plant's behavior on the basis of which they determine their decisions, the limitations of such mental models are obvious: they are mostly based on past observations of the plant's operation and, because of the enormous dimension and complexity of the true plant's behavior, bound to govern only a small part of the plant's potential behavior. As a logical consequence, operators tend to control the plant in a sequential fashion: prioritizing different control goals and attempting to achieve one after the other. Also, different operators have different mental models and different priorities which implies that there will hardly be any consensus with respect to the operation of the plant: the plant will be operated differently depending on the shift of operators that controls it.

Advanced process control in refinery applications - the success story

In the recent decades there has been, especially in the refinery industries, a growing consciousness of the benefits of Advanced Process Control (APC) technologies such as Model Predictive Control (MPC). The main driver for this development was an economical one: it was observed that many refinery plants were not operated at or close to the maximum throughput. Also, changes in the feedstock composition caused large upsets of the total plant with related losses due to decreased productivity.

In the late 1970's these problems were identified to be operational (control) problems instead of structural (process technology related) ones and solutions were sought in the area of advanced process control. The result was the development of the first generation MPC's in industry, among which IDCOM (Identification and Command) and DMC (Dynamic Matrix Control) were the very first to become known to literature [25, 24]. The main feature of these multi-variable control algorithms is their ability to handle process interactions and constraints.

The great success of the first few advanced control projects stimulated a more widespread application of this technology, bringing the status of APC in refinery applications to what it is now: proven technology. The success of advanced process control in refinery industries triggered the introduction of another major technology: Real-Time Process Optimizeration (RTPO). RTPO optimizes in a recursive fashion the static operating conditions of the plant such that the economic optimum is tracked continuously. Descriptions of such on-line optimizing structures in literature are numerous, see e.g. [96, 1].

APC in chemical industries - the best is yet to come

The booming number of MPC and RTPO applications in refinery industries contrasts with the small number of applications in chemical industries. The primary reason is an economical one: while commissioning costs for MPC and RTPO in refinery applications are often a factor smaller than the annual pay-backs, the costs of APC projects in chemical industries can often not be justified. Two main reasons can be given. First, the throughputs of most chemical plants are a lot smaller than in refinery applications, total revenues and profit margins are often proportionally smaller. Second, commissioning costs for APC in chemical applications are often rather high due to the specific technological requirements most of these applications put. In refinery applications the main task of APC and RTPO is to optimize the stationary behavior of the plant, in chemical applications process transitions (e.g. grade transitions, feedstock changes) occur frequently which must be handled by the APC. This means that process nonlinearity will be encountered during the operation which must be taken into account in controller design and process modeling. System identification-based modeling, the preferred approach in refinery applications of (linear model based!) MPC, seems not adequate for this task, physical process modeling will be required. Obviously, this requires much higher modeling efforts, both technically and financially.

It is important to note that all of this does not mean that there is no incentive for APC in chemical industries. The lack of experience-based indicators for pay-back times and benefits simply makes the implementation of APC on many chemical plants a risk-investment that many companies are not willing to make.

State of the art in advanced process control

Despite the non-uniform penetration of advanced operation technology in processing industries in general it seems opportune to define a *state of the art* operating strategy for reference purposes. The current state of the art in process operations consists of a structure with different control layers, which are separated according to the time scale and the spatial distribution at which they

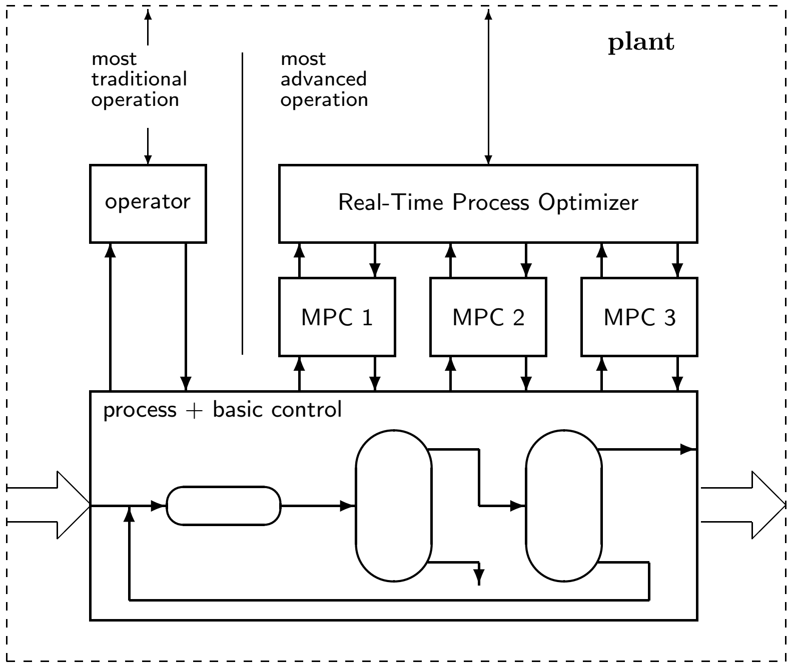


Figure 1.3: The most traditional (left) and the most advanced process control configuration (right) in continuous chemical manufacturing.

operate. In literature, a great inconsistency exists as to the division and nomenclature of control layers, however we will strictly stay to one model that divides the structure in three layers as in [71, 17], see the right part of Figure 1.3:

- Real-Time Process Optimization
- Model Predictive Control
- Basic Control

The *Real-Time Process Optimizer* computes the plant's operating conditions that are deemed optimal taking into account the process behavior, the process constraints and the process economics. The process behavior is described by a steady state plant-wide process model which is often a derivative of the flowsheet process models that were used in the plant design. Parameters in the model are updated on the basis of process measurements to make the model track the actual process behavior.

The role of *Model Predictive Control* is to realize the optimal conditions computed by the RTPO while obeying the process constraints. MPC computes control moves towards the “optimal” operating conditions by solving a constrained, finite-horizon optimal control problem each sample time. The process behavior is described using linear, discrete time models that are often determined via a system identification procedure. The control moves are implemented according to the so-called *receding horizon principle*: only the first move in the horizon is really implemented, then the horizon is shifted and a new optimal control problem is solved for the next move. To limit the computational complexity of the MPC problem and also for maintenance reasons, often several MPC's are installed on a plant where each MPC controls one or two process units. The MPC layer implements its control moves either directly on the control valves or on the setpoints of the basic controllers.

The *Basic Control layer* consists of a decentralized system of low level control loops. The role of these loops is to control locally certain elementary process variables (levels, pressures, temperatures, flows) in order to yield safe, stable and reliable operation of the whole plant.

As to the relation between the different layers in the control hierarchy it is important to recognize that the three layers were developed in separate stages after which they have been added together. The division of tasks is therefore not always very logical and inconsistency between the different layers and their control actions is likely to occur. An example of this inconsistency is the fact that economic optimization is done only with regard to the *static* operation of the plant. Obviously, in case of flexible operation of the plant, the optimization of the *transient* behavior becomes (at least) equally important. *This is a second crucial observation that contributes to the motivation for this research.*

1.2 Trends in chemical manufacturing and control

In the previous section we sketched the basic developments in the chemical marketplace which have lead to the position of chemical industry as it is. Next we will investigate some trends that are expected to characterize the future development of chemical industry and the role of process control therein.

1.2.1 The process and its environment

Market developments

The ongoing developments in modern communication technology in general and internet in particular have a major impact on the supplier-customer relationship, also in the chemical marketplace. Already, virtual chemical marketplaces are in place on which suppliers and customers are brought together. An example of such a chemical marketplace is ChemUnity, which was one of the few B2B (business to business) internet companies that ended the year 2000 (according to many "the year of the truth" for internet trading companies) successfully and has bright prospects for the future. The role of virtual marketplaces such as ChemUnity is believed to grow significantly in the nearby future, making the chemical marketplace eventually more transparent and truly global.

Besides globalization, a tendency to make production more customer-specific is expected, both with respect to delivery contracts and product diversity. Long term contracts will become rare and will be replaced by shorter term contracts and eventually by delivery on demand. The requirements these changes put on the operation of processing plants are completely different from those defining the current operation of for example refinery applications. Optimization and control technology, which is at present largely based on the situation encountered in refinery applications, must be fitted to those requirements.

Changes in plant design

Chemical plants change as well. Luyben [51] mentions some characteristics of many (new) chemical plants which he finds to be at the basis of the need for plant-wide process control:

- material recycles,
- energy integration.

Material recycles, though undesirable from a control perspective, arise frequently for various reasons, e.g. to increase conversion, to improve economics, to improve yields, or to minimize side-reactions. The fundamental reason for the use of *energy integration* is to improve the thermodynamic efficiency of the process and thereby to reduce utility costs. Another reason for energy integration is located in the environmental legislation which sets increasingly strict constraints and/or penalties on the plant's environmental burden.

Another trend in process design is the *minimization of inventory*. The reason for this is twofold. First, a large inventory of raw materials and intermediate products in the process is disadvantageous from an economic point of view. Second, intermediate storage is often considered dangerous and hence necessitates expensive safety precautions. The absence of intermediate storage results in processes that exhibit strong dynamic interaction between different process units, making the application of plant-wide, multi-variable control techniques opportune.

Tightening legislation regarding environmental protection

Environmental care and sustainability have been more and more predominantly present on the European and American political agenda during the past decades. Tightening legislation will continue to set hard boundaries on the operational requirements for chemical industries. Where the focus in the past was often on production maximization, future challenges in process control will be oriented more and more towards quality control and waste minimization.

1.2.2 Process control research and development

Above-mentioned trends will put new requirements on the operation of chemical manufacturing facilities in the future. Fortunately, several promising developments in the field of process control make us believe that an extension of the currently available control and optimization methods towards solutions that meet these requirements is feasible. The ones that are most essential in view of advanced process control and optimization are outlined here.

Modeling large scale process systems

Essential in any model-based control and optimization approach is the availability of a model. At present, modeling is still a time-intensive, specialistic task. However, noting from the development of the last generation of professional modeling packages (AspenTech's *Aspen Custom Modeler*, PSE's *gPROMS*) there is a trend towards making the modeling process systematic and feasible also for less-experienced users. A good example of such an attempt was the development of Dynaplus, a tool which supported the user in transferring Aspen Plus static models (which are often readily available from the process design stage) into dynamic models. Further developments which support the modeling effort are to be expected in the nearby future. Eventually, dynamic process modeling may turn from an *art* into *common practice*. This may enable the use of rigorous models or derivatives there-of (for example so-called grey-box models, rigorous models in which parameters are fit to experimental data) in model-based control, relaxing to some extent the need for system identification which is expensive, time-consuming and very difficult especially for nonlinear chemical plants.

Numerical integration and optimization

Various applications of plant models can be distinguished: simulation studies to the dynamic behavior of the process, off-line and on-line optimization of the process, or controller synthesis. Since most process models are of large scale and nonlinear, the role of numerical methods in all model-applications is imperative. Efficient integration methods have been developed (many on the basis of DASSL, a result of the pioneering work by Petzold [64]) which enable to simulate large systems of Differential-Algebraic Equations (DAE) at desired accuracy. Also, different strategies for the optimization of large DAE's have been developed. Most of the proposed methods use a smart parametrization of the input and/or state trajectories to end up with a NLP [89, 45]. Optimization methods have been developed and tailored for the solution of these (e.g. [80, 81]). During the past decade there has been a large renewed interest in convex optimization, mainly due to the success of *interior point optimization methods*. The efficiency of these methods in solving large-scale convex programmes, as well as their role in speeding up non-convex optimization creates new opportunities for amongst others *real-time* optimization, where computation time is inherently critical.

Robust stability of MPC systems.

Performance and stability analysis of control systems is often considered to be of academic interest only. This may be true when experimentation is so cheap that proof of principle can be derived from practice or when the stability and performance properties can be made plausible on the basis of dozens of successful similar applications. When it comes to the application of advanced process control in chemical applications however, both arguments do not hold. The availability of theoretical stability and performance results could help a lot in increasing the acceptability of these new technologies. Up to the present no general theoretical basis exists for stability and performance analysis of MPC schemes operating in the presence of disturbances and plant-model mismatch. Important progress has been made however, see e.g. [58, 74, 42].

Nonlinear MPC

Steady state optimizers use *static nonlinear* models, current MPC technology uses *dynamic linear* models. The current state of the art operating strategy obviously entails model inconsistency. Nonlinear MPC (NMPC), using *dynamic nonlinear* models, has the potential to overcome this inconsistency. In the past decade, developments in the field of NMPC have been extensive. The basic properties of NMPC have been studied and nominal stability proofs were proposed. Also, efficient optimization approaches have been developed which already make real-time application feasible for small problems or problems with very slow nonlinear dynamics. For an overview, refer to [32] and for a nice review of emerging topics to [54]. It must be noted however, that at present there is a significant gap between process control theory and practice, resulting in a disappointing number of true applications of advanced nonlinear control solutions. This is only partially due to conservatism in process industries, academia can also be blamed. The motivation behind a large part of the control research is purely theoretic and as a result many solutions address problems that are, to put it nicely, not so apparent to process control practicers. To avoid this a rather practical approach to defining and designing new control solutions for process industries is taken in this thesis, necessarily sacrificing the theoretical contribution.

1.3 Research justification

The current chapter contains a rather dense and necessarily incomplete review of past, current and future developments in chemical manufacturing and plant operation in particular. For the sake of our research project we have translated these observations into a set of research questions which will be outlined in the next chapter. We like to believe that these research questions touch upon many problems that are indeed currently visible in industrial practice. Nevertheless we must be so modest to alert the reader that no end-solutions to true practical problems are to be expected from our research. This is a sheer consequence of the fact that we were, for generality of the results as well as feasibility of our efforts, forced to leave out a significant level of detail in the formulation of our research questions. The results of this research should hence be interpreted as being partial solutions, concepts and tools that may, when properly extended to case-specific solutions and combined with existing technology, indeed improve the operation of many plants.

Embedding

This research was started as a preliminary investigation prior to the European Union research project INCOOP[2] in which the Mechanical Engineering Systems and Control group of the Delft University of Technology participates. INCOOP stands for "INtegration of process unit COntrol and plant-wide OPtimization" and aims to deliver new technologies for plant-wide optimization and control of non-stationary processes, such as batch processes and continuous multi-product or multi-grade processes. Other participants in the INCOOP project are Bayer A.G. (Germany), Shell International Chemicals B.V. (The Netherlands), IPCOS Technology B.V. (The Netherlands), MDC Technology Ltd. (United Kingdom), RWTH-Aachen (Germany), Technical University of Eindhoven (The Netherlands), and the Process Systems Engineering group from the Delft University of Technology (The Netherlands). Preliminary discussions between the part-

[2]Project number: GRD1-1999-10628. Project funded by the European Community under the 'Competitive and Sustainable Growth' Programme (1998-2002).

ners and in particular between the originators of the project, Ton Backx (IPCOS/TUE), Okko Bosgra (TUD) and Wolfgang Marquardt (RWTH) during the preparatory phase (see e.g. [53]) were of inspiration to this research.

Some results from this research were submitted to the IMPACT project. IMPACT stands for "Improved Polymers Advanced Control Technology" and is a so-called Eureka project[3]. Participants in the IMPACT project are Dow Belgium N.V., Dow Benelux N.V., ISMC N.V., Katholieke Universiteit Leuven, and IPCOS Technology B.V. Discussion with the IMPACT participants on the particular requirements of improved control of polymers processes were helpful in the formulation of the research problems and in the definition of a realistic industrially relevant case study for our research.

Prior to the IMPACT project, the author spent 3 months at the Imperial College of Science, Medicine and Technology (London) as part of a joint investigation of IPCOS Technology B.V., PSE (London), Imperial College and the Delft University of Technology into the dynamic optimization and control of a High-Density Poly Ethylene (HDPE) process, using gPROMS for process modeling and INCA for multi-variable process control. This work was done under the supervision of John Perkins. The results of this short collaboration were presented at the PSE User Group Meeting in April 1999 and thereafter used as a basic framework for the development of a simulation and optimization configuration with gPROMS and MATLAB.

We would at this point like to emphasize the importance of collaborations between industry and academia in process control and optimization studies as described here. Such collaborations are potentially fruitful for all partners and may help to bridge (at least a little bit) the theory-practice gap in process control.

[3] Project number: E! 2063. Eureka is a pan-European network for cooperative industrial research and development.

Chapter 2

Problem formulation

This chapter defines the research problems which will be addressed in the remainder of this thesis. We will sketch the operational demands for the future in the light of the developments in chemical industry which were described in the previous chapter (2.1). On the basis thereof, the technological requirements for the operation of chemical manufacturing plants today and in the future shall be outlined. These technological requirements are translated into two main research questions (2.2). A brief overview of the contributions of this thesis shall be given (2.3) and finally the outline (2.4).

2.1 Defining the operational demands for the future

In the previous chapter, we identified the main changes in the chemical marketplace to be the merger of several local markets into a global one and the saturation of demand for many of its products. An interesting question is what it takes for a chemical company to remain competitive. One possibility is to develop new products or production methods. Another possibility is to streamline, and optimize existing production facilities. This is the possibility we consider in our research.

A key requirement for a chemical manufacturing company's strategy to be viable is that it should be largely *market*-oriented. In the end, the value a company adds to the raw materials depends largely on its ability to make good prices for the end products. Making good prices means being *responsive* to the market situation and changes therein. In order for a company to be *responsive* its internal supply chain must be well-organized and its decision making should be fast and efficient. The restrictions and the potential of the processing plant have to be taken into account in a non-conservative manner so that the limit in addressing the market is in the true plant limitations and not in the effects of ill-communication between sales managers and plant managers. Further, a responsive company does not require large stocks of its products to be able to cope with varying demands: it will handle those through operating *flexibility*, maintaining only the minimum required stock levels. Customer satisfaction is prioritized and this is put in practice by responding flexibly to specific quality demands and by guaranteeing short delivery times.

The transition of a company to a market-driven, responsive and flexible mode of operation requires investments in the organization and information technology. Yet, if the company's organization is highly responsive to market variations but the plant is not half as responsive, then *market-driven operation* remains but a line in the company's mission statement. Hence, there is a big technological challenge in making the plant a reliable and predictable part of the company.

Market-oriented production and plant management One of the most important technological issues to be resolved is the development of decision support systems which enable to control the main decisions in the internal supply chain in such a way that the performance of the company is optimized. Such a system should guarantee consistency between the management of production, marketing, purchasing and sales. Regarding the type of purchasing and sales decisions that we aim to take into account, we must be so modest to admit that the focus of this thesis will be on *short term* decisions, related to factual purchasing and sales transactions. Marketing and concurrency strategies are left outside our considerations and are assumed to be part of a longer term decision making problem. In short term decision making regarding purchasing, production and sales it is crucial to predict accurately the true potential of the production plant; how we do this is considered the main extension of our work on production scheduling compared to existing approaches.

Predictable and economically viable plant operation The second main technological issue involves the improvement of reliability, predictability, and flexibility of production. In a responsive company the material flows are continuously dictated by the motions of the market. The plant must be able to deal with all these changes. Load changes and grade changes will happen more frequently which requires an *intentional dynamic*[1] operation of the plant. In present-day practice, dynamic operation of the plant is often avoided, relying on the well-known and predictable steady state operating characteristics of the plant. This can lead to strongly inflexible operation, as in the case of product

[1]The notion of intentional dynamics was introduced in a similar discussion in [53].

wheels [77]. The operation of the chemical plant in accordance with the notion of intentional dynamics requires a new and fresh view on process control and optimization. The role of the operators should shift to one of monitoring and supervision, rather than governing the actual process control, since no operator can be expected to meet the control requirements the intentional-dynamics-approach put. Instead, automated control technology with a guaranteed and predictable performance is required. These considerations are particularly relevant for the class of multi-grade or multi-feedstock continuous chemical processes on which hence the focus of this thesis will be.

Overlapping time scales Chemical industries should deploy process dynamics to serve the market better. A consequence of this 'intentional dynamics' view is that the borders between process control and production management become vague. Interesting market opportunities that we would like to be responsive to may occur on a day-to-day basis, a time scale which may well interfere with the dominant time constants of the process itself! Although process control and production management time scales may overlap, the resolution of these two types of decision making is clearly distinct: control decisions will need to be taken on a minute-to-minute basis, whereas smart production management may require to consider future purchasing and sales transactions during several weeks or longer and typically involve day-to-day decisions. How to deal in a consistent and practically feasible manner with overlapping time scales in purchasing, sales and production management and process control is a big challenge that is taken up partly in the writing of this thesis.

2.2 Research problem formulation

There is a strong need for a decision support tool which enables a chemical production site to bring the plant operational management in agreement with the status and developments in the marketplace. Such a tool should process information from within and outside the internal supply chain (see Figure 1.1) to support the management of production, purchasing and sales. To this end it should reconcile delivery orders resulting from partner contracts and foreseen opportunities in the market with the present and future production capacity.

Further, it should provide a realistic representation of the potentials and the limitations of the process operation in such a way that the process becomes a predictable, well-understood link in the supply chain and true supply chain integration becomes possible. In the remainder, we will refer to such a tool as a *scheduler*. The scheduler, by assumption, sets the boundary conditions for the process control problem. This decomposition of the plant operation problem into a scheduling problem and a control problem is common practice in current process operations, however it may at this point seem artificial and indeed requires further motivation which will be given in Chapter 4. The reason why we introduce this decomposition as an assumption rather than a result from our research is a practical one: it enables to further structure and specify our research problems.

For the scheduler to act as a true decision support system it must combine all the information available and separate on the basis of those, presumably via optimization, the preferred decisions from the undesirable ones. The development of such a scheduler is the first problem addressed in our research:

problem 1

How can we schedule the production of continuous chemical processes in compliance with market demands and the capacity of the process, and to a company- (or supply-chain-wide-) optimum ?

Related to this problem, we can define several research questions. To enable the scheduler to make its decision making or decision support consistent with the entire supply chain it should dispose of an internal representation of the essential behavior of the supply chain which is updated on the basis of information available throughout the supply chain. The act of combining and filtering all this information to end up with a consistent and compact representation of all relevant aspects of the supply chain operation is referred to as *supply chain modeling.* Although a lot of literature on supply chain modeling is available, e.g. [82, 14], most studies are qualitative and extremely general. In this research, we focus on chemical manufacturing and continuous chemical processing plants in particular. The formulation of models for this specific class of chemical manufacturing sites is our concern. The related research question is:

1.1 *How should we model a continuous chemical manufacturing site for the purpose of supply-chain-conscious scheduling ?*

The ultimate goal of the scheduler is to control the behavior of the entire internal supply chain. To this end, it should continuously select the most desirable decisions with respect to company-market interaction and production. To define which decisions are most desirable, we must first define what *is* desirable, hence we must quantitatively define the economic performance of the company. When such an objective is defined, we can formalize the selection process by viewing it as an *optimization problem.* The next research question refers to the formulation of such an optimization problem:

1.2 *How should we define the operating objective for a continuous chemical manufacturing site and how can we optimize this subject to the relations* *imposed by the supply chain model ?*

We motivated the need for a scheduler from a consideration of the current and future characteristics of the chemical marketplace and the role of chemical manufacturing sites therein. However, we did not discuss where such a scheduler should fit in the organization. This organizational issue contains many different aspects as it concerns the interaction with the process control system and thereby the role of operators as well. The relevance of this issue has been recognized by many researchers before, e.g. [5, 52] and we will address it for the specific class of continuous chemical processes:

1.3 *How should the scheduler fit in the supply-chain organization and the process control hierarchy ?*

It was argued previously that a prerequisite for market driven operation is reliable, predictable and flexible operation of the process. Reliability and predictability must be guaranteed for the production scheduling to make sense at all. Flexibility must provide the key to increased responsiveness of the company to market changes. The advanced control and optimization technology which is currently available was primarily designed to control and optimize plants in single operating conditions, dealing only with fast disturbances and slow parameter variations. Essential contributions to the development of this technology are by P.D. Roberts [72]. The steady state optimization concept seems not ideally suited for achieving the intentional dynamic operation of the plant which we envision. Instead we will consider *dynamic optimization* methodologies. The use of off-line dynamic optimization was studied in relation to grade changes, e.g. [56], and batch operations, e.g. [50]. Promising results from these research activities indicate the potential of *real-time* dynamic optimization strategies. The development of a *real-time* control and optimization strategy (hereafter often bluntly referred to 'control') which takes the process dynamics into account as an opportunity rather than a nuisance is the second main problem that we want to address.

problem 2

How can we control the operation of a continuous chemical plant subject to disturbances in compliance with the production schedule and to an economic optimum ?

The traditional process control hierarchy constitutes a clear separation of static economic optimization (RTPO) and advanced control (MPC). In this traditional setting MPC mainly has a regulatory task, where the desired steady state conditions are determined by the RTPO. In case of intentional dynamic operation, including grade changes, load changes and alike, the distinct separation between optimization (statics) and control (dynamics) seems not be a logical choice. One of the research questions we would like to address is hence:

2.1 *How can we integrate real-time economic optimization of the process with advanced control in case of intentional dynamic operation of the plant ?*

The control problem incorporates nonlinear plant dynamics. In literature, several general control solutions have been proposed for dealing with plant nonlinearity amongst which NMPC seems to be the most attractive since it can also deal with process constraints. However, the optimization problems that are to be solved in the NMPC scheme are often extremely large and probably too large to handle on-line. Approximate, linearization-based strategies were proposed in literature such as the Nonlinear Quadratic Dynamic Matrix Control strategy [27] or the constrained pseudo-Newton control strategy [46]. However, the development of such approximate control laws in relation to dynamic real-time optimization has not yet been studied. Our next research question is hence:

2.2 *How can we approximate the nonlinear control laws needed for intentional-dynamic operation so as to maintain feasible computation times?*

A main ingredient of receding horizon nonlinear control schemes is a *dynamic optimization* algorithm. Also, dynamic optimization is the key to finding efficient trajectories for grade and load change problems. To make on-line implementation of advanced control and optimization techniques feasible efficient computational tools need to be developed. A first step therein is to tailor existing computational approaches to the specific characteristics of the control configuration. The corresponding research question is:

2.1 *How can we tailor existing optimization methods for the purpose of real-time control and optimization of continuous chemical processes?*

Cases

To illustrate the relevance of the problem formulations and to demonstrate the potential of the methodology that is described in this thesis we will discuss several cases. Case 1 is the simulation of a simple blending process that operates in interaction with an end product market. This case will be used to indicate the different time scales that occur in a production management problem and to illustrate the working of the production scheduling solution that is developed in this thesis. Case II comprises the operation of a binary distillation column. This case will be used to demonstrate the potential of the tailor made optimization methods developed in this thesis and the real-time control and optimization approaches. Case III involves the operation of a HDPE plant and its interaction with the end product market. In this case, a semi-large scale simulation model of a HDPE reactor is used in the optimization studies. This case is believed to represent well the benefits of the 'intentional dynamics' approach, and will be elaborated on a bit further next.

Motivating example - HDPE production There are several reasons why the case study of HDPE production is relevant to our research. First, the market for HDPE is a true global market that is subject to strong fluctuations in volume and price. Currently, the market is characterized by over-capacity. For a supplier this means that it is hard to exercise control over price levels and delivery times: the need to respond flexibly to emerging opportunities is obvious. Main customers for HDPE are automotive industries. The yearly volume of polymers that is required by these industries is quite predictable, however since just-in-time production is common practice in automotive manufacturing the fluctuations in demand on a short term can be significant. Most of the transactions between polymer manufacturers and customers proceed according to longer term contracts, where the actual orders are placed a few weeks prior to the date of delivery. Interesting and often attractive opportunities arise for example when competitors fail their contractual obligations. Naturally, these opportunities become known to the manufacturer on a very short notice, however the bonus on in-time delivery can be attractive enough to motivate, if feasible, corresponding changes in the production schedule.

Those manufacturers who are best able to deal with the increasing demands on quality and flexibility that the market puts will have a significant advantage in comparison with the others. Currently, most HDPE plants are operated according to so-called slate schedules (explained in Section 1.1.2). The technological solutions presented in this thesis may provide a competitive edge.

A process-related reason for our interest in HDPE production is that the dynamics of large HDPE plants are generally slow, so that market dynamics and process dynamics should ideally be regarded simultaneously, as advocated in this thesis. Typical durations for grade changes lay in the range of 6-14 hours. Obviously, grade change time and costs play an important role in the operation of these processes. Another reason why advanced control is beneficial in HDPE production is the fact that due to the high viscosity of polymers, product quality does not or or only poorly *mix*. This makes it necessary to produce within tight specifications.

A practical advantage of considering this case is its comparatively small scale: instead of considering a largely integrated processing plant, we will consider a single processing unit only, retaining however the interesting interaction with the markets. This makes it possible to implement in a straightforward fashion the solutions presented in this thesis without getting stuck in problems that have to do solely with dimension and complexity.

2.3 Contributions of this thesis

The problems that are posited in the previous section are derived from considerations regarding the future needs of process operation and are hence new in many aspects. One consequence of this is that the problems cannot so easily be classified as being naturally related to specific academic disciplines. Indeed, production management problems are studied by many different disciplines, with no intention to be complete we mention ‘operations research (OR)’, ‘logistics’, ‘management studies’, and ‘systems and control’. Another consequence is that there is not yet an unambiguous and generally agreed upon formulation of the research problems. To avoid getting stuck in generality and to make the results of our research concrete and meaningful, we will especially in the first chapters of the remainder of this thesis make further assumptions regarding the scope and the level of details of the specific problems that we consider. The further remarcation and sharpening of the research problems mentioned above is the first contribution of this thesis. Really, to define market-focused operation of chemical processes in terms of a set of formal, smaller research problems is a pioneering effort.

For the ‘trimmed down’ problems that result from this effort, formal and technical solutions will be presented. These technical solutions form the second contribution of this thesis. Because the technical part of the work presented in this thesis touches upon activities from many different disciplines in academia and we can hardly expect our readers to be an expert in all of those we deem it instructive to outline the main contributions next.

Scheduling continuous multi-grade chemical plants. The first technical contribution is the definition of a modeling framework and a corresponding Mathematical Programming (MP) formulation for the scheduling of continuous, single-machine, multi-grade, chemical plants. Chemical plant production scheduling is studied by researchers from the fields OR and chemical engineering as well, however most of the present work focuses on the scheduling of batch operations. Our way of including the effect of process transitions on the material flows appears new. Further, most scheduling studies assume the order base to be fixed in advance and strive for for example ‘minimum makespan’ or ‘minimum lateness’. In our approach, the negotiation of sales orders and purchases is an integral part of the decision making that is supported by the scheduler, and to this end the scheduler selects a set of appealing purchase and sales transactions from a larger set of possible transactions (denoted *opportunities* in the remainder of this thesis). Besides a few guidelines for the tuning of Branch and Bound (BB) solvers and the demonstration on two examples, not much attention is paid to the solution of the Mixed Integer Linear Programme (MILP) that the scheduling problem results in.

Economics-based process control To make intentional dynamic operation of continuous chemical plants possible the process control system must be designed in such a way that it can cope with demands on product quality and quantity that result from the tight connection of the company to the market, while maintaining economically attractive operating conditions. The traditional control hierarchy is not suited for this purpose

The solution that we propose builds on the Extended Kalman Filter based NMPC scheme that is described in e.g. [41]. Our main contribution is in the formulation of the deterministic optimization problem that NMPC solves. Traditional NMPC objectives include quadratic penalties on the deviation of a selected set of performance variables from their setpoints, our objective is economic. In traditional NMPC only process constraints are considered, we include constraints on the desired production levels as well in order to ensure a consistent coupling with the scheduler. Finally, we propose several decomposition and approximation schemes that are specific to our control configuration in order to guarantee feasible computation times. It must be noted that our solutions builds on existing tools and methodology and can best be seen as a creative variation to those. No fundamental contributions to control theory are claimed, neither are stability and closed loop performance aspects considered.

Grade change optimization strategies Different customers may have different demands regarding the product quality, in which case a variety of product grades need to be made at the same production facility. To switch production from the specifications of one grade to those of another grade in an economically attractive fashion we promote the use of model-based grade change optimization. Our formulation of the grade change problem includes a truly economic objective in contrast to the use of rather arbitrary quadratic weightings in other approaches to grade change optimization.

This thesis considers control parametrization methods only. The grade change optimization problem is hard to solve using standard gradient-based numerical optimization due to the fact that the production rate of a certain grade depends discontinuously on the quality variables. We introduce two new optimization approaches to circumvent these problems. The first, named the SSQP method (for Successive Sequential Quadratic Optimization), uses a smooth approximation of the definition of the grade region and exploits the structure of the problem in the definition of a Nonlinear Programming (NLP) based inner loop optimization to compute accurate search directions. The second approach uses integer variables to describe the grade regions and solves a sequence of MILP's to converge to a solution.

The grade change problem is non convex and both methods can be expected to converge to local minima only, however they are believed to do so a lot faster than the conventional control parametrization method, a supposition that is confirmed by the two optimization case studies (case II and case III).

2.4 Outline of this thesis

This thesis is organized as follows. In **Chapter 3** we will introduce a simplistic chemical manufacturing supply chain framework on which the research is based. This chapter also analyzes how the production management can be geared to other activities that determine the behavior of the internal supply chain such as purchasing and sales. A 'scheduler' is introduced as a decision support system which enables the different players in the internal supply chain to cooperate in such a fashion that close-to-optimal supply chain operation can be achieved.

Chapter 4 deals with the question how the process control hierarchy should be organized such that the production management becomes an integral part of the cooperative supply chain management structure. Two possible approaches shall be outlined. The first, a single level approach is mainly of academic interest. The second, a conceptual decomposition approach decomposes the production management into a *scheduling problem* and a *real-time control* problem and is the basis for the remainder of the thesis.

The definition and mathematical formulation of the scheduling problem is the subject of **Chapter 5**. For the aim of scheduling a description of the plant in terms of quasi-static tasks and transition tasks is proposed. The scheduler is to determine a sequence of production tasks and purchasing and sales decisions that is optimal with respect to a company-wide objective. How the different elements that constitute the internal supply chain are modeled mathematically for the purpose of this scheduling algorithm is described in this chapter. The scheduling problem formulation results in a MILP and its properties are demonstrated on case I.

Chapter 6 presents the definition of the real-time control problem in compliance with the conceptual decomposition of the production management problem as proposed in Chapter 4. A decomposition of the plant-wide control into several control layers is proposed on the basis of an analysis of the different time scales that arise due to the presence of different types of disturbances (fast vs. persistent disturbances). The proposed strategies are implemented on case II.

The development of efficient dynamic optimization strategies for the specific dynamic optimization problems encountered in the previous chapters is the subject of **Chapter 7**. Dynamic optimization plays an important role in the derivation of the dynamic production tasks for the purpose of scheduling (Chapter 5) as well as in real-time economic optimization (Chapter 6). Due to the focus on multi-grade processes, the dynamic optimization problems encountered have a very specific structure that makes them hard to handle by standard Newton-type optimization strategies. Two tailor-made methods that exploit the structure of the problems are presented. One uses a smooth approximation of the definition of the grade region and exploits the structure of the problem in the definition of a NLP based inner loop optimization to compute accurate search directions. The second approach uses integer variables to describe the grade regions and solves a sequence of MILP's to converge to a solution.

The feasibility of all methods that are presented in Chapters 5 to 7 is demonstrated by means of an industrial-scale simulation study on a HDPE reactor (case III) in **Chapter 8**.

Conclusions regarding this thesis as well as recommendations for further research are given in **Chapter 9**.

Reading guidelines

Although there is a strong interplay between the different chapters some readers who have a specific interest in one of the topics may find it more effective to read selected chapters only. Attempts have been made to guarantee (independent) readability of the individual chapters where possible. Naturally, the link between Chapters 5 and 6 is rather strong due to the fact that the scheduler and the real-time control system described in these chapters result from a conceptual decomposition of the production management problem.

Essential assumptions and choices that are made in this research are typeset in boldface fonts and are indicated by means of an asterisk]*.

Chapter 3

Business wide process modeling

This chapter proposes a simple framework for modeling the plant and its environment on the basis of which company-market interaction and the consequences thereof for the operation of continuous chemical plants can be studied. The supply chain as a basic modeling framework shall be introduced in (3.1). Production management and sales and purchasing management shall be discussed from an organizational point of view (3.2), with the incentive to lay the foundation for a decision structure in which the plant operational management becomes an integral part of the company's ambition to serve the market to its best potential. The different elements in the supply chain model are described and an approach to modeling the decisions and the decision making in these elements is sketched (3.3). The contribution of this chapter shall be summarized in 3.4.

3.1 Introduction

Traditionally, process control and optimization focuses on the process equipment only. This may be sufficient to guarantee effective plant operation in the case where purchasing, production and sales decision making is only weakly coupled. However, in most cases economic optimization and control of the plant cannot contribute optimally to the company's performance unless purchasing and sales decision making is taking into account as well. This requires a new, broader scope on *process control*. In this chapter we will define this broader scope and outline the basic elements therein. The result will be a reference *supply chain model* that is used as a basic description of our to-be-controlled plant in the remainder of this thesis.

The *supply chain* concept is very useful in the study of manufacturing and company-market interactions. A *supply chain* is, according to Stevens [78], in its essence defined as 'a system whose constituent parts include material suppliers, production facilities, distribution services and customers linked together by the feedforward flow of materials and the feedback flow of information'. Supply chains are often too complex to be modeled even qualitatively. Still, considering the supply chain may help a lot in understanding the complex behavior of the whole of company market interactions, competition, logistics and so on[1]. Further, taking the supply chain view helps to put the company role and its operation in the right perspective, as being one link in an often lengthy supply chain rather than merely adding some value to raw materials which matches clearly our incentive to broaden the scope on process optimization. For these reasons, we will throughout this thesis make extensive use of the supply chain concept in describing and modeling company-market interaction and company organization.

The modeling framework that is supposed to combine a sufficient level of realism with effective simplicity is represented schematically in Figure 3.1 and is the result of combining the elementary *internal supply chain model* of Figure 1.1 with markets on both sides. This simple model captures some of the main mechanisms which appear in practical chemical supply chains:

- company-market interactions,
- inventory control,
- process dynamics (transitions, load changes),
- internal supply chain organization.

The horizontal scope of the reference supply chain model is somewhat limited: the role of for example handling and transportation is not made explicit, which implies that well-known dynamic supply chain phenomena such as demand amplification [23] are not considered. Also, competition will not be modeled explicitly, although we will later see that the consequences of competition can be accounted for through an appropriate modeling of company-market interaction.

The supply chain model will be used as as basic framework for describing the material flows and related information flows between the different players

[1]The study on dynamic behavior of supply chains was pioneered by Forrester [23]. Using elements of systems theory, control, management sciences, and decision making theory he examined quantitatively how organizational structure, amplification and time delays interact to influence the success of enterprises. His working arena was referred to as the area of *industrial dynamics*. Later, the use of supply chain modeling and analysis for the purpose of supply chain management and redesign was taken up amongst others by Towill [87] and, at present, the area of supply chain modeling and managament is a popular research area in amongst others management sciences and OR.

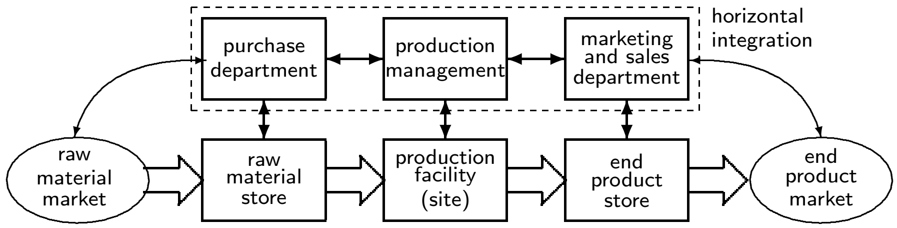


Figure 3.1: A simple supply chain model for a continuous chemical manufacturing site.

that produce, sell and buy a certain product or class of products. **Our main focus will be on multi-grade processes**]★ because for this class of processes the interplay between the different supply chain elements is naturally rather intensive. Consider for example the production of different grades of a certain polymer where interesting conflicts between production and sales management occur due to the inevitable trade-off between performing costly changeovers and maintaining high storage levels [77].

Guidelines for quantitative modeling of supply chains are abundantly available in literature, see e.g. [14, 82, 53, 87]. Although most of the proposed approaches differ in details, the general supposition is that supply chain modeling is best done in a hierarchical fashion, where one should start to consider the supply chain as a whole and then model its different elements based on the understanding of the most elementary and essential behavior of the entire supply chain. The perspective from which we will start to consider the chemical manufacturing supply chain will be mainly operational and organizational. Our main interest is in the decision making within the different supply chain elements and how this influences the performance of the supply chain as a whole.

3.2 Business organization

The performance of the internal supply chain is measured against a so-called company-wide objective. In most cases, it requires but a few lines in the company's mission statement to define such an objective. Nevertheless, if the different subsystems that form the company strive for local objectives this company-wide objective cannot be achieved unless the decision making process is controlled in some way: the act of gearing the local activities to one another is referred to as *horizontal integration*, see Figure 3.1. Horizontal integration is an essential aspect in relation to our first research goal being the production scheduling in compliance with market demands. In literature on decision making, a lot of attention is paid to the multi-person decision problems that

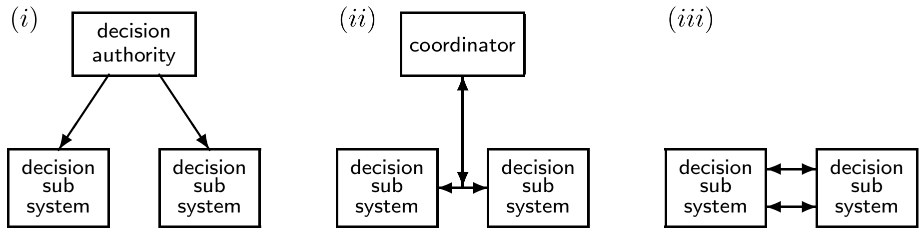


Figure 3.2: Centralized (i), Coordinated (ii) and Cooperative (iii) decision making.

horizontal integration entails and several approaches are presented. The most commonly mentioned variants are depicted in Figure 3.2. In the *centralized approach* (often called hierarchical control), e.g. [20], all relevant information is gathered centrally and the optimal strategy is issued over all subsystems. Although this structure is theoretically optimal, no realistic management structure is perceived to fit all the organizational, information-processing and computational demands of centralized decision structure. The *coordination approach* recognizes the need for decision authority for the different players. The decision making of the decision subsystems (purchase management, sales management, production) is coordinated by influencing how they perceive reality (model coordination) or how they interpret the company wide objective (price coordination) [76]. However, the problem of coordinating decision making by control of the interaction between the players (e.g. price coordination, [76]) is still perceived to be too heavy for a realistic successful implementation. Practically, the most suitable organizational concept is *cooperation* (or the *team decision concept*). In this setting the players are authorized to make decisions regarding their subsystem while agreeing to operate according to a common company-wide goal. This will generally lead to a suboptimal mode of operation, but Prasad [67] convincingly explains that it may be the best achievable one.

Cooperative decision making

Each player in the cooperative team has two tasks. First, he should gather information with respect to the state of the subsystem he controls and provide this information to the other players. Second, he must decide on the operation of the subsystem based on his information and information from the other players. The interpretation of these tasks as to contribute to the evolution of information will be discussed in the following.

The *first task* relates to the selection and communication of information that is deemed relevant in view of the supply chain operation. It may seem artificial to view interpretation and communication of data as a decision, but then consider that it is indeed an active task to decide where to investigate and how to evaluate the data that is locally available. Further it is also decided whether or not and how to communicate the information to the rest of the supply chain. As an example let us consider a case where the maximum production capacity of a plant is decreased due to a technical problem. For the supply chain operation it is essential that the plant managers communicates the decrease in production capacity and the expected duration of the problem to the other players. However, detailed information on the technical problem is not relevant to the other players and should thus be filtered out. If this first task is being executed adequately this will result in each player having a complete and accurate view on his potential role in the internal supply chain. The actions he will conceivably take in relation to this role will be denoted *opportunities* in the sequel.

The *second task* is the transformation of opportunities to *confinements*. This task refers to the actual action-taking. Examples of such decisions are the commitment of the sales subsystem to a customer's order, or the decision of a production manager to switch to a different set of operating conditions. For such decisions to be made properly[2], each player must have, based on his information and the information from other players, an accurate perception of the sensitivity of the company-wide objective to his decisions. Furthermore, this perception of the company-wide objective should be made sufficiently concrete so that each player can start to effectively view it as his own objective. In other words, the company-interest should be interpretable as a player's self-interest [67].

To achieve this we suggest that a **decision support system provides feedback to each subsystem regarding which opportunities could be best turned into confinements**]*. Clearly, we limit the scope of the decision support to decisions that were previously identified as being the *second task* each player in the team has. Actions corresponding to task 1 are left out of consideration although it must be understood that with respect to the information supply we require at least a cooperative attitude of the players to make the proposed decision support meaningful at all. The decision support system shall hereafter be denoted a *scheduler*.

The obvious way to have the scheduler reconcile foreseen actions with the company-wide objective is to make it solve a simplification of the company-wide problem based on all the opportunities brought in by the subsystems and with the union of all decisions as degrees of freedom. This vision on role of the scheduler complies with the main philosophy underlying other integration studies. For example Bassett et al. [5] state that one of the principle advantages of computer integration is to provide a basis for organizational units to assess the value of local decisions and initiatives.

---

[2] *Properly* here means "in such a way that close-to optimal operation of the internal supply chain is achieved".

We want to stress the static and centralized character of the scheduler's problem perception as opposed to the dynamic, a-synchronous and decentralized decision problem that characterizes the complete behavior of all players in time. Next we will investigate the main decisions that are to be taken in the different supply chain elements and how these can be modeled.

3.3 Reference supply chain model

3.3.1 Production subsystem

The production subsystem imposes strong limitations on the behavior of the entire supply chain. First, of course, production capacity is limited by the physical constraints of the process. Further, due to inherent process dynamics the response of the plant to external changes (feedstock changes, grade changes) is comparatively slow. This last property distinguishes chemical processing plants from mechanical manufacturing machines of which the dynamics are often considered negligibly fast compared to other dynamic supply chain phenomena.

Characterization

The production subsystem is defined to contain all processing steps within a particular site that are deployed for the manufacturing of the particular product or class of products under consideration. In general, the manufacturing site will contain several plants, possibly interconnected via intermediate storage. This situation is depicted in the left image of Figure 3.3. The presence of intermediate storage has an important consequence, namely that the dynamics of the different plants are to some extent decoupled. This decoupling provides an important degree of freedom in the site's operation and should be modeled adequately. The interconnection of two different plants via piping is of a different nature: dynamic effects in one plant will propagate to the other. From a supply-chain-dynamics point of view it is undesirable and maybe even impossible to view these two plants as separate supply chain elements. It is therefore proposed as a modeling guideline to model the composition of processing units that are interconnected via piping as a single plant. Observe that the application of this reasoning to the illustrative configuration depicted in the left image of Figure 3.3 would lead to the decomposition of the site in *two* plants which are partly interconnected by an intermediate storage.

In few occasions it may suffice to consider a single manufacturing plant or, in the OR jargon, a 'single machine', as depicted in the right image in Figure 3.3. The single machine consists of a continuous processing plant which is connected to storage facilities and it can hence be used as a building block for more general

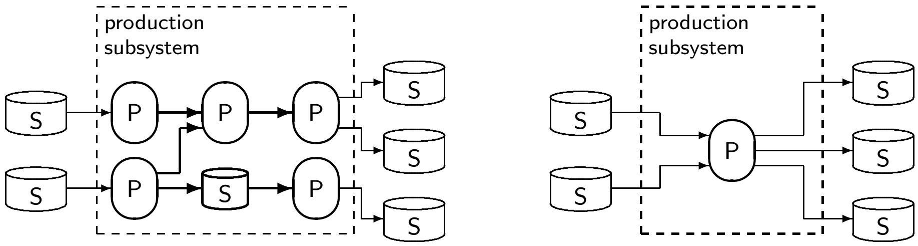


Figure 3.3: Production subsystem with several plants (P) and intermediate storage (S) (left) and single-machine production subsystem (right).

manufacturing sites. In the remainder of this thesis **we will study the single machine case only**]★. Extensions to more general manufacturing sites are believed to be rather straightforward, though probably computationally more demanding.

To properly account for the plant's behavior - and in particular the response to grade changes and load changes - in modeling the supply chain, **we will assume a dynamic model of the process to be available**]★. In the next chapters we will analyze which are the basic properties of the plant that such a model should capture.

Decisions

The operation of the plant subsystem is managed by the production managers and further established through its interaction with the process control system. Operational decisions can be described in different levels of details and on different time scales. For example, the intention to switch to a different set of operating conditions may be characterized as being an operational decision. However, to switch to different operating conditions many valve positions need to be adjusted on a second to second basis. The manipulation of these valves may just as well be considered to be operational decisions, though much more detailed and on a much shorter time scale than the intention to switch. In order to include the operational decisions in the scheduling formulation they need to be modeled in such a way that, for feasibility of the computations, abundant details are omitted while the main impact on the entire supply-chain behavior is retained. *How this is done is a crucial and decisive choice in our approach to supply-chain-conscious plant optimization.* This will be discussed in more detail in the next chapter.

3.3.2 Storage subsystem

The feedstock of the manufacturing plant is either supplied continuously via a pipeline connection or it is stored on-site. Equivalently, end products are transported to the customer via a pipeline connection or stored on-site before transportation. Storage units are amongst the most basic elements of supply chains. The storage of raw materials or end products provides for a means to suppress the effect of market fluctuations on the production requirements. Ultimately, in the case of very large stock levels, the dynamics of the end product and raw material market would be *decoupled* from the manufacturing dynamics, which would make supply-chain conscious production scheduling abundant. The financial consequences of large inventories are in general undesirable: stored products or raw material are considered 'dead capital' and costs related to the storage infrastructure are often significant. It is mainly for this reason that the most recent trends in manufacturing management sciences point towards *production on demand*. Although production on demand might be the optimal operating philosophy in theory, its practical implications are far-reaching and reasonable arguments for maintaining non-zero storage levels are found easily. For example in chemical manufacturing there will always be an incentive to keep a minimum amount of raw materials in stock to control the risk of an obliged shut-down in case raw material supply falls short unexpectedly. Also, in order to enable the negotiation of attractive 'delivery on demand' contracts with customers it may be necessary to retain a minimum level of end product storage. Obviously, inventory control cannot be seen separately from production scheduling, sales forecast etc. and it will hence be an integrated part of the operational methodology that we develop.

Characterization/decisions

For simplicity, we will **consider no other but the effect of production and sales/purchase actions on the storage levels**]*. Storage capacity for each of the different end products and feedstocks is lumped and no separate storage management is considered. As a consequence the characterization of the storage in our supply chain model is passive and very simple.

3.3.3 Company-market interaction

The part of the supply chain that is most difficult to model is the interaction with the raw material and end product markets. In the sequel we will focus on the company-*end product market* interaction only. The results are not essentially different for the interaction with the *raw materials market*. The interaction between a company and the market is of a bilateral nature. In case of a *pull* market, a price for the end product is determined by the sales decision makers and the market determines the demand. An appropriate pull market description should hence be able to answer the question: *"What unit price is offered by the market for a certain amount of product taking into account previous transactions?"*. Similar market descriptions can be derived in case of a *push* market.

No general market model was found in literature that meets these requirements, which may be explained from the severe difficulties that one encounters when trying to derive such a model. First, predicting market behavior is an intricate act. Although the sales department can be expected to have some intuition on (short term) future demands and prices, catching this intuition in hard mathematical relations seems very awkward. Second, there are many aspects in company-market interaction which cannot or not easily be included in relations as described above. Examples are *contracts, partnerships*, etc. Moreover, many markets will not have purely pull or push characteristics but a mixture of these two. For these reasons, we decided to look into different ways of modeling company-market interaction. The proposed market description is treated below.

Characterization: a transaction-based market description

The observation that sales managers are often remarkably well able to formulate their expectations with respect to future sales transactions despite their limited insight in the underlying market behavior, suggests a **transaction-based framework for modeling the company-market interaction**]*. In such a transaction-based framework, not the interaction between the company and the market itself but only the expected result of this interaction, i.e. the factual sales transactions, are modeled. These sales actions can be categorized as follows:

orders originate from long term sales contracts or short term commitments to customers. They should be communicated to the scheduler and will constrain the scheduling to those solutions which meet the delivery requirements. The main order attributes are the quantity, the price and the time span during which the order can be delivered;

opportunities arise from predictions of the market-company interaction made by the sales decision makers. In opportunities they express their estimate of future sales deals. The attributes of the opportunities are the same as those of the orders.

The set of orders and opportunities (ord./opp.) is constructed by the sales decision makers who are deemed best fitted to do so, based on their experience in and intuition for dealing with the market. The problem of modeling and predicting market behavior is hence partly shifted towards the responsibility of the sales decision makers to make good predictions. They will predict the outcome of their interaction with the markets based on probably a mental model of the market behavior which we believe might be even better able to incorporate all *soft* aspects of market behavior than any mechanistic market model.

Different market behaviors The transaction-based market model captures a broad spectrum of market behaviors. Some extreme cases which may well be the vertices of all market forms encountered in continuous chemical manufacturing are described below.

Perfect competition. In a market with perfect competition the trading prices are determined every day or hour such that demand is balanced against production. This is for example the situation many electricity markets are left with nowadays after the completion of the very recent liberalizations. For a company operating in such a market it may be advisable to negotiate a number of long term contracts to secure a certain income; the corresponding sales transactions will appear in the ord./opp. database as *production orders*. The remaining production capacity will be used to follow the trends in demand with the ultimate incentive to adjust the production continuously to the most favorable market segment. The sales managers are confronted with the challenging task to represent their estimation of the trends in the development of the equilibrium prices in terms of a set of appropriately tuned *sales opportunities*.

Pure oligopoly. In an oligopoly long term contracts will be more predominantly present than in a market characterized by perfect competition. In an *oversaturated* oligopoly the negotiation of long-term contracts may even be the only way to guarantee a minimum amount of sales on the long term. Hence, for companies operating in an oligopolistic market a substantial fraction of the production capacity will be reserved for contract-based production which will be reflected in the composition of the ord./opp. database. Long-term contracts come in many different appearances. For the most traditional long-term contract time and quantity of the deliveries are fixed. Other contracts may involve the commitment of the manufacturing company to maintain a minimum level of inventory of the sold material at the customers location. Such contracts demand a more active role of sales managers since they must predict the product deliveries so as to meet the minimum inventory constraint. In such a case it may even be opportune to extend the simple supply chain model with the raw material inventory of the concerned customer. Sales opportunities will arise in case of a sudden increase in demand for specific products *or* when competitors fail to deliver a certain order due to technical problems or bad planning.

Monopoly. Due to the absence of competitors there is no benefit to be gained from long term contracts in a monopolistic market. Hence, a monopolistic market description will mainly consist of sales opportunities. The main handle to control the company-market interaction in a monopolistic market is the product price. The task for sales and marketing managers is to predict how the demand will vary with the product price. This dependency can be modeled by the introduction of several sets of sales opportunities of different quantity and with different prices. For example let it be assumed that in a period of two weeks 2000 tons of a certain product can be sold at an average price of 2 Euro or 2500 tons at an average price of 1.7 Euro. This would lead to the introduction of two sets of sales opportunities, one containing sales actions summing up to a total of 2000 tons and with an average price of 2 Euro and one summing up to a total of 2500 tons and with an average price of 2.5 Euro.

Penalty on delayed delivery The introduction of additional relationships *between* sales opportunities or orders makes it possible to model many practical situations which may occur in company-market interaction. For example consider the case where a certain product lot cannot (or only at the expense of very high losses) be delivered in time. For such situations the manufacturer and the customer will generally agree on a penalty on delayed delivery where the height of the penalty will depend on the delay. The consequences of this agreement can easily be included in the ord./opp. database through the introduction of copies of the concerned sales order at later time instances and at a lower price. An additional constraint should then be added to ensure that exactly one of these sales orders is fulfilled.

Decisions

The main decisions that need to be considered in relation to the supply-chain-wide scheduling are *i.* to assign delivery dates to sales orders and *ii.* to turn, when possible and presumably after negotiation with the clients, attractive sales opportunities into sales orders. Whether a sales opportunity is attractive or not is decided on basis of the feedback from the scheduler.

3.3.4 Operating objective

In its role as a decision support tool, the scheduler will select and return to all players the set of decisions that optimizes some company-wide objective. In this section we will define such an operating objective in general terms. The main supposition is that **the company's intentions are to maximise an economical criterion**]*. Other objectives such as social, environmental or strategic ones are not considered, although they could be imposed as constraints where necessary.

Added value

A chemical manufacturing company uses its equipment and expertise to transform raw materials to intermediates or end-products. This way it can be seen to *add value* to the raw materials. The *cumulative added value* of a company or a manufacturing site will be used as an economic criterion to measure the company's performance. In its most simplistic form, the cumulative added value (CAV) is computed as the difference between all revenues through sales of end products and all expenses on raw materials over a certain period of time. This basic form is not of much use in our optimization since it does not honor variable production costs and for example interest. These factors will be discussed next.

Manufacturing costs

Raw material costs account for only part of a chemical company's expenses. The whole lot of expenses can be divided in two main categories: plant costs and manufacturing costs. The *plant costs*, which comprise the costs of equipment, instrumentation, piping, buildings, fire protection, construction and engineering and many more small categories [26], are considered irrelevant in this study since we focus on operation of existing processes only, not on their design or re-engineering. *Manufacturing costs* can be subdivided in fixed costs and variable costs. The fixed costs contain depreciation, taxes, insurance, licensing fees, administrative expenses, corporate overhead, patents and royalties. Fixed costs are considered not *controllable* during operation and hence not relevant to take into consideration in our optimization. Variable manufacturing costs *are* controllable to some extent and should hence be taken into account where relevant. Variable costs include raw materials (including additives and catalysts), utilities (fuel, electricity, water, steam, air, telephone, sewage), labor, indirect labor charges (health insurance, retirement etc.), maintenance, transportation and freight, distribution, packaging, storage, R&D, and corporate costs (office, books, travel, meetings, etc.). Most of these are outside the scope of our decision problem because they are not sensitive to the actual controls (purchase/sales/production actions) that we assume to have at our disposal.

Time-value of money

A very important aspect that must be included in the formulation of the objective is the loss of interest due to the investment of capital in raw material and end product stock. Would the same capital be available in the company's bank accounts, then investing it in business, savings or at the stock market would yield a certain profit. For this reason the value of raw materials and end products in stock is referred to as 'dead capital'. Losses due to capital destruction can be rather significant. To prevent capital destruction (and some other related disadvantages of keeping large storages), companies attempt to reduce the time raw materials and end products reside inside their organization. Of course, the process operations solutions that we develop should conform to this incentive which means that we must take the negative effects of capital destruction into account in the formulation of our objective function. A straightforward way of doing so is to account for interest on the net capital balance. A mathematical formulation of the CAV including interest on the net capital balance will be presented in the following chapters.

3.4 Contributions of this chapter

This chapter introduces a simple supply chain model using which we can study the consequences of market-driven production management on the operation of continuous chemical plants and lays the foundation for a decision structure which enables to bring operational management of the plant in agreement with purchasing and sales management. Several important choices with respect to the system boundaries and the modeling of decision making are made which we will briefly review here.

First, a simple, internal supply chain model is introduced as a basic framework for our qualitative and quantitative studies. The chain consists of a single, multi-grade continuous plant with raw material storage and end product storage and it interacts with raw material market and end product markets only. Decision making in such a chain is by nature distributed. Three major players are distinguished: purchasing managers, production managers and sales managers. In order for a company to address the market flexibly and with maximum economic benefits it *does not* suffice to optimize the behavior of the individual players, instead we need to gear the activities of the players to one another in such a way that their composite behavior approaches the theoretical company-wide optimum. This being the ultimate goal we suggest that a flexible manufacturing company should have a cooperative decision structure in which all players have two main roles. One is to provide foreseen possible actions, denoted opportunities to a decision support tool, denoted *scheduler*, which considers the union of all opportunities and selects preferably via optimization of a company-wide objective an attractive sequence of actions. The second is to implement their actual decisions based on the information they receive from the scheduler.

The scheduler due to its company-wide perspective provides an impartial and well-interpretable feedback to each player regarding which of his foreseen actions is indeed opportune. The formulation of the company wide decision making problem that the scheduler needs to solve proceeds via an investigation of the main decisions that the three above-mentioned players face. For *purchase* respectively *sales* managers we suggest that the factual decisions can be modeled as the act of turning purchasing and sales opportunities into *orders*. The introduction of new opportunities or the modification of old ones on the basis of insight in the market behavior is a decision of a different type which the scheduler will not support and which remains outside the scope of our research. The decisions related to production are not explicitly modeled in this chapter. How this is done depends on the implementation of the process control and operations hierarchy, which will be studied in the next chapter.

The definition of a quantitative company-wide objective completes the conceptual formulation of the problem that is to be solved by the scheduler. We choose to consider the CAV as the basic economic performance index. In this added value computation all variable production costs are included. Interest on the net capital balance is included to indicate the attractiveness of short residence times.

Chapter 4

Production management decision structures

This chapter analyzes the demands supply-chain-conscious operation puts on the process control hierarchy. First, we motivate why a reconsideration of the process control hierarchy is required in light of intentional dynamic operation (4.1). Then we discuss mainly for reference purposes how the process control hierarchy is organized nowadays (4.2) and why this is not the right framework to build upon. The use of mathematical models in the integration of different operational tasks is advocated next and three model-based integration strategies are described (4.3). Finally, the single level approach (4.4) and the conceptual decomposition approach (4.5) are discussed in more detail and it is described how these can be of use in the (re-)organization of production management to meet the requirements of market-oriented production.

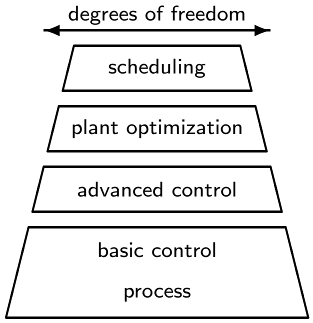
4.1 Vertical integration

From the previous chapter we concluded the need for a *scheduler* as a tool which supports decision making of purchase, production and sales managers. It is obvious that decision support for the production management is of a different nature than that for the sales and purchase managers. Purchase and sales decisions are often of the binary type: the deal *will* or *will not* be made. Production decisions factually involve the manipulation of process valves or control setpoints on a seconds or minutes basis and thus have a distinct dynamic and continuous character. In traditional operation (see Figure 1.3), the production decisions are implemented by the operators who modify the setpoints of basic controllers manually; in the most advanced implementations of process automation systems, the main moves are made by process optimizers. How should this change with supply-chain conscious production? Should the operator be surpassed at all? Should the operator be supported by presenting him *suggested* setpoints? In case of a process optimizer: should we manipulate the RTPO's cost function? Underlying these questions is a more fundamental one: should we stay with the traditional hierarchical control system with its historically developed division into several different layers, or should we try to develop one integrated control system which deals with the slow dynamics of the market as well as the fast plant dynamics? This issue of structuring the process operations hierarchy is believed of great importance; some more considerations to this subject will be given next.

4.2 The process operations hierarchy

Conventionally, the tasks related to the operation of a plant are viewed to be related in a hierarchical fashion. This means that high level decisions impose goals and constraints on lower level decision making while the actual decisions are implemented through a number of execution functions. The hierarchical relation between operating tasks such as scheduling, supervisory control, fault diagnosis, monitoring and so on is commonly represented schematically in an 'integration pyramid'. Macchietto [52] states somewhat ironically that every paper on process integrations should have its own 'integration pyramid', stressing the diversity of such schematics and exposing the lack of a common language in addressing such issues. For example there exists disagreement as to the division of the planning and scheduling layers, a discussion which is even further complicated through the use of terms such as short-term scheduling, long term scheduling, strategic planning, capacity planning, operational planning and so on. Adding to that, the fact that people working in the field of process control come from many different areas (control engineering, systems engineering, chemical engineering) it is really no surprise that the number of different integration pyramids is almost equal to the number of authors defining them. We will not break with this tradition, so please find our fabrication in Figure 4.1.

The name 'integration pyramid' suggests a high degree of integration of the tasks that constitute this pyramid. Yet, probably the opposite is true. The process operations hierarchy of today is the result of a long going tradition of adding different pieces of functionality on top of each other. The introduction of MPC as an add-on to existing basic control systems is a good example of this. The introduction of RTPO systems to squeeze more economic performance out of the plant by manipulation of the MPC setpoints is another example. Adding layers with different functionality really has nothing to do with integration, unless the interaction between these layers is carefully accounted for. In the integration



	look ahead	execution rate	scope
scheduling	weeks	[0.1-10]/day	plant/site
plant optimization	days	[0.1-2]/hrs.	plant
advanced control	hrs.	[0.1-1]/min	process unit
basic control	[-]	[1-100]/s	local loop

Figure 4.1: 'Integration pyramid' for process control and optimization.

pyramid that can be drawn for the current state of the art operating strategy (see Section 1.1.3) this is often not carefully done. The example of model inconsistency between RTPO and MPC with potentially severe consequences was explained in Chapter 2. Model inconsistency between scheduling and control models may be just as tedious, making computed 'optimal' production schedules either infeasible in practice or too conservative. A safe way out of such inconsistency problems is to add sufficient conservatism to the solutions, however this will generally conflict with the high-performance operational demands that we envision.

Related to the problem of model inconsistency is the problem of *incompatibility*. In a compatible hierarchy, the interaction between the different layers is well-defined. This enables that each layer can be modified or substituted without having to redefine the hierarchical interaction. For the process control hierarchy this appears not to be the case. First, as stated previously, there is no consensus regarding the process control hierarchy. Second, the assumptions underlying the division in the different layers are often disputable. This means that the modification or substitution of a single layer is in many cases not possible unless the hierarchy is altered as well.

4.3 Model-based integration strategies

From the previous we may conclude that the current process control hierarchy is not the right framework to consider as a basis for our research on supply-chain conscious operation. This means that **we will largely redefine the process operations hierarchy and its different elements to satisfy the specific demands supply-chain-conscious operation puts**]*. According to Bassett et al. [5] "...the preferred approach for achieving integration of application levels is through the formulation and solution of appropriately structured mathematical models", and we largely support this vision. There are several reasons why the use of mathematical models is the key step in the integration of process operations. First, the models provide a consistent, compact representation of the underlying systems, which is accessible for all the different layers in the hierarchy. Second, by the use of the models in appropriate MP tools, the decision making or decision support can be automated. An important downside to the extensive use of and reliance on mathematical models is the difficulty and the costs of modeling. Bassett [5] distinguishes three types of model-based integration, *single-level control*, *multi-level control* and *conceptual decomposition*.

Single-level control

Integration by means of a single-level control strategy is theoretically optimal. In the single-level strategy all decisions are computed by a monolithic application. Since all aspects of the process operations problem are integrated in a single controller, model inconsistency will not appear. A *single-level control strategy* to the problem of supply-chain-conscious process operations implies the design of a process operations system which controls the process while supporting the purchasing and sales decision making. This necessitates to include all relevant time scales of the operations problem (i.e. weeks/months to capture market changes, and seconds/minutes to describe fast dynamics which should be controlled) into one control problem. This will generally lead to combinatorial control problems which are of enormous dimension and hence computationally infeasible. Further, from an implementation point of view the development of such a strategy seems at least over-optimistic and probably unrealistic in light of the current status of the process operations. Still, this approach symbolizes the ultimate goal in the integration and automation of process operations and is worthwhile to study for this reason only. The single level control strategy will be further elaborated on in Section 4.4.

Multi-level control

This approach comprises the mathematical decomposition of a single-level control problem into a set of lower-level control problems which are coordinated by the top-level. The main idea is that a single, highly complicated control problem falls apart in a set of simpler control problems and a coordination problem, the sum of which is of lower complexity than the original problem and with the primary goal to reduce computation time. The important contributions in this field were by Wismer, Findeisen and Mesarovic in the 1970's, see e.g. [92, 21, 57]. With the multi-level control approach generally only small computational advantages can be attained relative to the single level control approach which rules it out for practical implementation. Further investigation of this method is omitted.

Conceptual decomposition

The conceptual decomposition approach is most often applied in practice. In this approach, a large control problem is decomposed in a set of simpler, hierarchically interconnected control problems on the basis of insight in the problem structure. The motivation for conceptual decomposition is often intuitive and based on rather vague notions, which distinguishes this approach from the mathematical decomposition applied in the multi-level approach. Actually, the current process operations hierarchy can be seen to be the result of a not so carefully done conceptual decomposition. Using this approach, optimality can no longer be guaranteed; in the best case, the loss of performance can be characterized quantitatively. Through the pragmatic decomposition of the operations problem into a set of smaller ones a trade-off can be made between optimality and computational and implementational feasibility. Bassett et al. [5] discuss a few characteristics of many real-life decision making problems which he defines to be the basic motivations for conceptual decomposition. The most obvious ones are the *diversity of time scales*, and *uncertainty.* It is the diversity of time scales in many real-life problems that enables to consider different aspects of the problem at different sampling rates. Uncertainty (about the process behavior, the market etc.) obviously makes it useless to compute future decision strategies in detail. Since this research aims to deliver solutions which can be implemented in real life, a conceptual decomposition approach may be the best attainable one. It will be further discussed in Section 4.5.

4.4 A single-level approach to production management

The systematic investigation of the supply-chain-conscious production in the previous sections suggests that it should be possible to design a single level process operations system which controls the process while supporting the decision making of purchase and sales managers. Although the practical feasibility of such a method is questioned a priori, it is still interesting to investigate its main ingredients. A possible decision structure is given in Figure 4.2. The single decision authority is represented by the oval shaped block "decision feedback/process control". The decision block has access to information from the plant (measurements, status reports, etc.) and from the sales and purchasing departments. The latter is in the form of an *ord./opp.* database as discussed in Section 3.3.3. Information on storage levels is made available as well. The

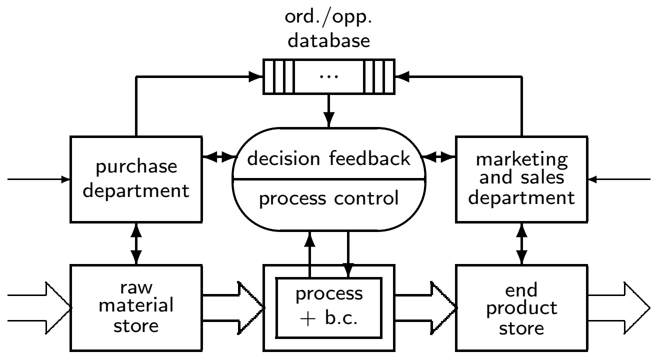


Figure 4.2: A single level approach to supply-chain-conscious production management and process control.

process operations system has two main tasks: 1. to control and optimize the process in compliance with the market conditions, 2. to provide feedback to the purchasing and sales managers regarding which opportunities are indeed opportune and which are not. To avoid the rigor and length a general description would entail, we choose to examine the design of such a controller by means of an example.

4.4.1 Application to case I: the blending process

As an example of the implementation of a single level supply-chain controller we study the operation of a very simple processing unit: a blender. A process flowsheet is given in Figure 4.3. Raw material types A and B which are bought from the market are stored in two storage tanks. Different product grades are produced, where the grade is determined by the concentration of component A. The end product market for the two blends is assumed to be heavily in motion, resulting in large, daily fluctuations in demand (and hence price). The aim of the process control system is to control the plant in such a way that the better sales deals are made possible, while guaranteeing 'in time' delivery of product orders. The control system will depend on and utilize mathematical models representing the main supply chain mechanisms. The derivation of these will be treated next. The presented modeling approach is far from unambiguous. Besides attempting to capture a bit of realism in the description we foremost aimed for *simplicity*, and also *linearity*. The reason for this is that even for a simple processing plant like a blender, detailed, nonlinear modeling would render the computations intractable.

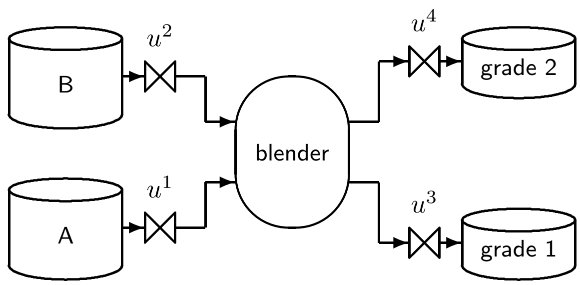


Figure 4.3: Flowsheet of the blending process and the raw material and end product storage.

Supply chain modeling for the blending process

Production subsystem If perfect blending is assumed, the process dynamics are given by the two component balances

$$\frac{dx^1}{dt} = u^1 - (u^3 + u^4)\frac{x^1}{x^1 + x^2};$$
$$\frac{dx^2}{dt} = u^2 - (u^3 + u^4)\frac{x^2}{x^1 + x^2},$$

where x^1 and x^2 are the mass holdups of respectively component A and B. u^1 and u^2 are the mass flows of respectively component A and B into the blender. u^3 and u^4 are the production flows of respectively product grade 1 and product grade 2. The product quality depends on the ratio x^1/x^2. Both product grades 1 and 2 are defined accordingly by an upper and lower bound on the quality:

$$q_l^g < \frac{x^1}{x^2} \leq q_u^g, \quad g = 1, 2.$$

Variables G^g take a value 1 if the quality of the content of the blender corresponds to grade g and 0 otherwise:

$$G^g = \begin{cases} 1, & \text{if } q_l^g < \frac{x^1}{x^2} \leq q_u^g, \\ 0, & \text{otherwise.} \end{cases}$$

The production flows are constrained from above by a maximum and can only take a non-zero value if the blender content has the corresponding quality:

$$u^3 < G^1 u_u^3, \quad u^4 < G^2 u_u^4.$$

No off-spec production is allowed. Assuming the upper and lower bound on the quality to be sufficiently tight we can approximate the original *nonlinear* differential equations by the following *linear* ones

$$
\begin{aligned}
\frac{dx^1}{dt} &= u^1 - \frac{q_u^1}{1+q_u^1}u_3 - \frac{q_u^2}{1+q_u^2}u_4,\\
\frac{dx^2}{dt} &= u^2 - \frac{1}{1+q_u^1}u_3 - \frac{1}{1+\$q_u^2}u_4.
\end{aligned}
$$

which leads to the following discrete time, linear representation of the process model

$$
\begin{aligned}
&x_{k+1}^1 = x_k^1 + \tau u_k^1 - \tau\frac{q_u^1}{1+q_u^1}u_k^3 - \tau\frac{q_u^2}{1+q_u^2}u_k^4,\\
&x_{k+1}^2 = x_k^2 + \tau u_k^2 - \tau\frac{1}{1+q_u^1}u_k^3 - \tau\frac{1}{1+q_u^2}u_k^4,\\
&u_k^3 < G_k^1 u_u^3, \quad u_k^4 < G_k^2 u_u^4,
\end{aligned} \tag{4.1}
$$

where $\cdot_k = \cdot(k\tau)$. Remains the challenge to relate G^g to the process states in a linear fashion. This is done by introducing the following constraints:

$$
\begin{aligned}
&q_l^g x_k^2 - x_k^1 - (1-G_k^g)Q_l^g < 0,\\
&x_k^1 - q_u^g x_k^2 - (1-G_k^g)Q_u^g < 0,
\end{aligned} \tag{4.2}
$$

with $G_k^g \in \{0,1\}$. The definition of these constraints is quite similar to the general formulation of mixed logic, dynamics phenomena in the Mixed Logic Dynamics by Bemporad and Morari [7]. Constraints are added on the total holdup in the blender and all material flows:

$$
\begin{aligned}
&M_l < x_k^1 + x_k^2 < M_u,\\
&u_l^j < u_k^j < u_u^j, \;\; j = 1,2,\ldots,4.
\end{aligned} \tag{4.3}
$$

In accordance with the minimum and maximum levels for the holdup as given above, we require $Q_l^g > q_l^g M_u$ and $Q_u^g > M_u$ to guarantee feasibility of the product quality constraints.

Market subsystems For this example, we will only model the end product market. Raw material supply is supposed to be continuous and unlimited. In correspondence with Section 3.3 the state of the *sales market* is described by the introduction of a set of sales orders and opportunities $S_k^{e,s} \in \{0,1\}$ with $s \in \{1,2,\ldots,n_{S,e}\}$ and $e \in \{0,1\}$. $S_k^{e,s}$ is one if the s^{th} sales ord./opp. for end product e is executed at time $k\tau$ and zero otherwise. Each ord./opp. has several attributes. The amount of material $SA^{e,s}$ and the unit price $S\$^{e,s}$ are defined. Further, for every ord./opp. the validity time span is defined by a set of samples $\Omega^{e,s} \subset \mathbb{N}^+$. The parameter $SO^{e,s}$ determines whether ord./opp. $S^{e,s}$ is an order ($SO^{e,s} = 1$) or an opportunity ($SO^{e,s} = 0$).

Each sales opportunity *can* be executed once in the validity time span, each sales order *must* be met during its validity time span which leads to the following constraints

$$SO^{e,s} \leq \sum_{k \in \Omega^{e,s}} S_k^{e,s} \leq 1, \tag{4.4}$$

$$S_k^{e,s} = 0, \ \ \forall t \notin \Omega^{e,s}. \tag{4.5}$$

Storage subsystems The end product stores are modeled by writing down the corresponding mass balances

$$ES_{k+1}^1 = ES_k^1 - \sum_{s=1}^{n_{S,1}} S_k^{1,s} SA^{1,s} + \tau u_k^3, \tag{4.6}$$

$$ES_{k+1}^2 = ES_k^2 - \sum_{s=1}^{n_{S,2}} S_k^{2,s} SA^{2,s} + \tau u_k^4. \tag{4.7}$$

Storage capacity is limited:

$$ES_l^e \leq ES_k^e \leq ES_u^e, \ \ e = 1, 2. \tag{4.8}$$

The objective In agreement with Section 3.3 the company-wide objective is defined as the CAV. We include raw material costs, sales revenues and interest on the capital balance. Because no raw material market is modeled, the cost price for the raw material is assumed constant over the horizon. Let $P\$^r$ be the price of raw material r and γ the fractional interest rate. Then, the cumulative added value is given by the following recursion

$$V_{k+1} = (1+\gamma)V_k - \sum_{r=\{1,2\}} P\$^r \tau u_k^r + \sum_e \sum_s S_k^{e,s} SA^{e,s} S\$^{e,s}. \tag{4.9}$$

The net added value recursion of (4.9) can be computed over the whole lifespan of the manufacturing site. However, if we would attempt to optimize the expected economic performance of a manufacturing site over its entire lifespan we would run in severe problems of different nature. First, the number of optimization parameters would grow unacceptably, taking away even the smallest hope that we would be able to solve such an optimization problem. Second, we would demand an unrealistic effort of the sales people, namely to predict the changes in the end product market over an horizon of many years.

Taking these arguments into account, we will continue to consider a much shorter horizon length H, typically covering several weeks, in the definition of the objective. A consequence of this is that the effects *outside* the horizon of the decisions made *within* the horizon are not accounted for in a natural fashion. This problem is not uniquely related to the control problem under consideration here, actually it is inherent to every receding horizon control problem with a finite prediction horizon. In MPC for example, the use of only a finite horizon can cause an unstable closed loop system, even when the open loop optimizations made in every iteration look reasonable. In reaction to this observation several MPC schemes were proposed with guaranteed closed loop performance. The most straightforward proposal is to include an end-point constraint in the optimization. Other solutions comprise the selection of appropriate final state weights.

We can copy either one of these approaches to improve the consistency of our objective formulation. The formulation of an end point constraint seems reasonable to capture the final state of the process, however highly undesirable in relation to the storage levels, simply because the desired status of the storage at the end of the horizon is not known. Therefore, we propose the use of a final state-weighting on the storage levels in combination with an end-point constraint on the process states. If we assume linear weights $E\$^e$ on the final storage levels of the end products then the final objective can be defined as

$$J = V_H + \sum_e ES_H^e E\$^e. \tag{4.10}$$

Optimal control solution

The set of factual decision variables is the union of the manipulated variables of the process (u_1, u_2, u_3, and u_4) and the sales decisions $S_k^{e,s}$. The manipulated process variables are continuous decision parameters, the sales and purchase decisions are discrete (binary) decision variables. The control problem is to choose the decision parameters in such a way that the economic objective is maximized:

<u>maximize</u> the objective (4.10) <u>subject to</u> the added value recursion (4.9), the process dynamics (4.1,4.2), the process constraint (4.3), the storage recursion (4.6,4.7), the storage constraints (4.8), and finally the sales constraints (4.4,4.5).

Because all constraints are linear and the set of decision parameters contains continuous as well as discrete parameters this optimization problem is a Mixed Integer Linear Programming (MILP) problem, which we can solve using e.g. BB techniques, see e.g. [22] or the brief introduction to BB techniques in the product specifications

grade (g)	q_l^g	q_u^g
1	0.995	1.005
2	1.395	1.405

process constraints

flow (i)	u_l^i	u_u^i
1	0	0.2
2	0	0.2
3	0	1
4	0	1

M_l=5
M_u=12

Table 4.1: Product specifications and process constraints for the blending example.

appendix of this thesis (Appendix B). The solution of such problems is typically very time-consuming, especially for large numbers of integer decision parameters. This would not be catastrophic if we could do with a single computation every week or month and an open loop implementation of the solution. Unfortunately, an open loop control solution is of little use. First, the market situation changes continuously and so will the market predictions (and hence the ord./opp. database). Also, due to disturbances and inaccuracy of the process model the actual plant behavior will deviate from the predictions. Although disturbances and model uncertainty were not considered in the formulation of the optimal control problem, these aspects are inherent to any practical situation and there must be a mechanism to handle them. The elementary way of dealing with disturbances and the time-varying states of the market is through *feedback control*, which can be achieved via a repeated computation and implementation of the optimal control strategy, i.e. receding horizon control. For the blending process example, receding horizon control comprises the following steps:

1. measure the status of the plant and the storage levels and scan the modifications in the ord./opp. database,

2. formulate and solve the economic optimization problem,

3. implement the controls u_k^i, $i = 1, \ldots, 4$, set $k = k + 1$ and go back to 1.

Results

We solve the blending optimization problem for a specific realization of the ord./opp. database. Sampling time is chosen 1 hr.[1] and the horizon length 120 samples i.e. 5 days. The relevant process parameters are given in Table 4.1. All parameters are dimensionless.

The end product market database is given Table 4.2. Raw material prices are chosen $P\$^1 = 1$, $P\$^2 = 1.2$. End-storage appreciation is chosen $E\$^1 = 1.7$,

[1]A sampling time of 1 hr. is unrealistically long for real-life applications, however smaller sampling times wouldn't add much realism yet a significant increase of computational complexity to this example.

Sales of grade 1

s	$SA^{1,s}$	$S\$^{1,s}$	$\Omega_{1,s}$	$SO^{1,s}$
1	7	1	{5,10}	0
2	6	1.8	{5,10,15,20}	0
3	3	1.3	{15,20,25,30}	1
4	7	1.4	{35,40,45,50}	0
5	8	2.5	{55,60,65}	1
6	7	1.6	{60,65,70,75}	0
7	8	1.5	{80,85}	0
8	3	1.3	{90,95}	0
9	5	1.7	{100,105,110}	0
10	8	2.5	{105,110}	0

Sales of grade 2

s	$SA^{2,s}$	$S\$^{2,s}$	$\Omega_{2,s}$	$SO^{2,s}$
1	7	1	{5,10,15}	0
2	4	2	{15,20,25}	1
3	8	1.8	{20,25,30,35}	0
4	4	1.3	{35,40,45,50}	0
5	5	1.7	{55,60}	1
6	8	1	{60,65,70}	0
7	5	2	{75,80,85}	1
8	6	1.8	{80,85}	0
9	4	1.3	{95,100,105}	0
10	7	1.7	{105,110}	1

Table 4.2: Sales order and opportunity database for the blending example.

$E\$^2 = 1.5$ and the fractional interest is 0.0001 per hour. The problem was implemented in the mathematical modeling system GAMS. We used the MILP solver CPLEX to solve it. The solution of MILP's is an intricate task in general. CPLEX enables the user to set a few solver-options to steer the BB solution process in a direction which is deemed efficient for the particular problem or problem instant. For the blending problem however, the standard settings appeared satisfactory. The problem was not solved to *guaranteed* optimality because that would require unacceptable computation times. A useful indication of the quality of an integer solution is its distance from the best relaxation amongst all open nodes. We interrupted the solution processes at a relative gap smaller than 0.02, which took about 30 minutes on a Pentium II personal computer (PC). The optimum found was 62.423. The resulting optimal control strategy is plotted in Figure 4.4. Note that the optimal strategy is to continue production of grade 1 for another 25 hours, then make a transition to grade 2 and produce grade 2 for about 40 hours. Finally switch back to grade 1 and produce grade 1 for the last 40 hours. The storage levels of product 1 and 2 are plotted in Figure 4.5. Sales actions are indicated by their corresponding number. Observe that for product 2 only the production orders are met, the sales opportunities are ignored. Instead, the attractive sales opportunities 2 and 10 for product 1 are selected.

Based on the solution of this instant of the optimal control problem the following actions can be taken:

1. u_0^1 and u_0^2 are implemented on the plant, i.e. the feed conditions are retained such that production of grade 1 can be continued,

2. sales managers are notified on the attractiveness and feasibility of sales opportunities 2 and 10. Based on this information they may decide to negotiate with their customers on possibilities to turn the sales opportunities into orders.

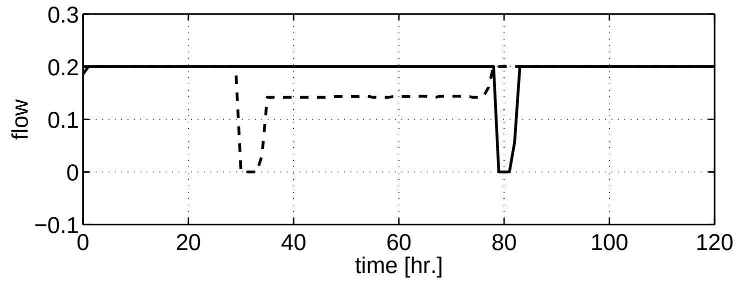


Figure 4.4: Optimal raw material flow for blending system. Solid: u^1, dashed: u^2.

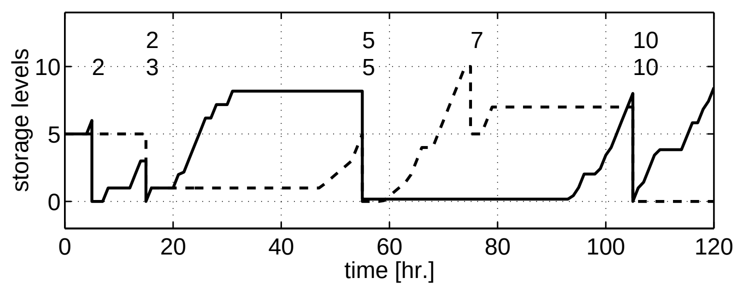


Figure 4.5: Storage levels of product 1 (solid) and product 2 (dashed) for the optimal control strategy. Sales ord./opp. numbers are indicated: the bottom row for product 1 and the top row for product 2.

Meanwhile additional sales orders or opportunities are added to the database and redundant ones are removed. After one hour the optimal control problem is solved again based on the most recent information on the state of the plant, the storage levels and the sales ord./opp. database.

4.4.2 Discussion

Clearly, the single level supply-chain conscious control approach will lead to unmanageable optimization problems when applied to a real-life situation. The combination of short sampling times (for satisfactory control) with long look-aheads (to account for changes in the market) inevitably leads to an explosion of the number of decision variables.

The poor computational tractability is not the only drawback of the single level approach. First, it is at least questionable whether such a controller can satisfy the safety and reliability requirements that *any* process control system must primarily meet. Even *nominal* stability analysis of the resulting closed loop system is no trivial task; to investigate stability properties in the presence of disturbances and plant-model mismatch seems completely out of reach. A related question is whether safe and reliable behavior can be achieved *at all* through the minimization of an *economic objective* only. The economic objective may leave certain crucial modes 'unobservable' which would necessitate the definition of additional 'control-type' objectives. For example, in case of the blending control problem the objective is insensitive to variations in the level of the blending tank. This may lead to level swings that may be undesirable for other than economic reasons.

Another problem with the single level approach is the effect of disturbances on the actual closed loop performance. The most practical approach to dealing with disturbances is to neglect the effect of disturbances in the prediction which leads to solving a deterministic optimization problem. For Linear Quadratic Gaussian problems, this deterministic control problem will even lead to the optimal control when combined with an optimal state estimator (Kalman Filter), see e.g. [40]. Unfortunately the separation principle does not hold here; in the problem that we consider the ignorance of the effect of disturbances in the optimization may easily incur infeasibility of the process constraints, the sales orders and the storage limitations. An *engineering* approach to avoiding these infeasibilities is by introducing a *back-off* from the actual constraints. The choice of the back-off from the process constraints can be done on the basis of statistical analysis, see for example [48, 34], and is relatively straightforward; for the storage constraints this is somewhat more cumbersome and the "back-off from sales orders" is not even a notion that is well-defined.

The most rigorous approach to avoiding infeasibility is to include the effect of unknown disturbances in the control problem formulation. This would lead to worst-case finite horizon optimization problems. Solutions to *open loop* worst case problems are known to be extremely conservative because they ignore the effect of feedback in the prediction. Thereby, the tractability of such problems is low in general. The alternative, *closed loop* worst case optimization (see e.g. [42] for such a formulation for linear quadratic MPC) is more elegant however even less tractable.

It may be concluded that the single level control approach is of academic interest only, its practical implications are too hard to handle. Fortunately, the results from the blending example indicate the existence of effective, practical alternatives to the single level approach. Namely, observe that the solution of the blending example clearly exhibits two different time scales. At the fastest, control moves change from hour to hour to maintain the desired quality. At the slowest, it is decided *which* product is produced *when*. Observe from Figure 4.4 that at this slowest time scale only two or three decisions are being taken in a period of 5 days. The presence of different time scales opens possibilities for the most appealing alternative to the single level approach: the *conceptual decomposition approach*. How this approach can be applied to define a practically feasible solution shall be discussed in the next section.

4.5 Hierarchical production scheduling and process control

This section discusses the definition of a hierarchical control strategy for supply-chain-conscious operation of chemical plant. Bassett [5] discusses different reasons for conceptual decomposition, a few of which were mentioned in the previous section as well. One of the most elementary reasons for a decomposition is *time scale* separation. It is clear by intuition and it has also been demonstrated in the blending example that the relevant time scale on which the scheduling problem needs to be considered is significantly different from the time scale relevant to the actual real-time control of the plant. Modifications to the production schedule will be made in response to changes in the market situation, which may occur daily, weekly or monthly, depending on the market nature. In contrast, process disturbances occur on a second-to-second time frame and in order to deal with them, the control system should operate on a sufficiently fast sample/execution rate. **The main decomposition that we propose is hence to deal separately with the two questions 1: what products/feedstocks will be produced/processed when? and 2: how will the production be realized?**]*. The first question will in the remainder be denoted the *scheduling* problem. The second question refers to the *plant-control* problem and will be dealt with in Chapter 6. The decomposition into a scheduling problem and a control problem is intuitive and complies with many existing hierarchical structures. The proposed hierarchical control system is depicted in Figure 4.6.

The control and decision support system now consists of two separate blocks. The first, represented by the oval box "decision feedback/production scheduler" has two main tasks. First, it should compute a production *schedule* in compliance with the market conditions and the current and future status of the plant. To this end it has access to the ord./opp. database and to the status of the plant. The second task is to provide relevant feedback regarding sales and purchasing opportunities to the sales and purchasing managers. The production schedule is communicated to the second layer of the control hierarchy, the "process control and optimization" block. The production schedule will act upon this block as a boundary condition, a constraint. Feasibility of this boundary condition can be guaranteed through a consistent model use in both layers as will become clear from the next chapter. The role of the process operators (the

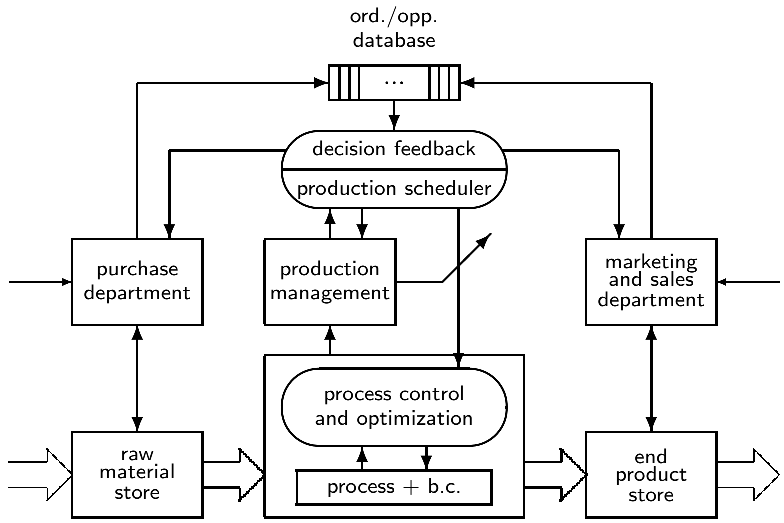


Figure 4.6: A decomposition approach to supply-chain-conscious production management and process control.

block “production management”) shifts to supervision, monitoring and information supply. Clearly, any technical defect or modification to the plant should be communicated to the scheduler so that plant models can be updated likewise.

4.6 Contributions of this chapter

The main aim of this chapter is to analyze the demands supply-chain-conscious operation puts on the process control hierarchy. To this end, we describe the current process operations hierarchy consisting of a basic control layer, a MPC layer, a RTPO layer and a production scheduling layer.

We explain why this framework is not fit for market-driven operation, the main limitation being the restriction of economic optimization to the steady state behavior. Recall from Chapter 2 that a market-focused operating strategy leads to an *intentional dynamic* operation of the plant.

Besides being inadequate for the purpose of market-drive operation we believe that the current process operations hierarchy impels inconsistency and incompatibility of the different layer’s functionality. Serious model-inconsistency is present between the RTPO and the MPC layer as well as between the RTPO and the scheduling layer. Therefore, instead of making modifications to the individual layers we choose to redefine the process operations hierarchy largely in accordance with our view on market-focused operation.

Underlying the definition of a new process operations hierarchy for continuous processes is the notion of 'model-based' integration. Fully in agreement with the suggestions of Bassett et al. [5] we believe that the consistent use of dedicated mathematical models representing the essential behavior of the production plants leads the way to a market-focused automation of production control and process operations.

Two interesting model-based integration strategies were discussed. The first, a single level approach, tries to integrate in the functionality of the scheduler as a decision support tool the actual process control decision making. Though theoretically nice and successfully applied to the small blending case, this approach entails infeasible computational demands for problems of realistic size. The main problem with the single level approach is that the resolution of the action taking should be very high in order to incorporate the process control decisions whereas the horizon should be long in order to include the effect of the long term market behavior on the action taking. Fortunately we (and the results from the simple blending example confirm this suspicion) can distinguish two different time scales regarding the production management and decompose the decision making problem accordingly. At the longer time scale decisions regarding "*what* product grades are produced *when*" are considered and at the shorter one decisions regarding "how the production of the relative grade is realized". Decisions associated with the longest time scale will in the sequel be denoted "scheduling decisions" and are supported by the scheduler. This scheduler was in the previous chapter introduced as a decision support tool that advises the three main players (purchasing,production and sales managers) in the internal supply chain. Its implementation will be discussed in Chapter 5. Decisions associated with the shortest time scale will be denoted "control decisions" in the remainder and we will define automated control solutions that implement those. The design of these control solutions is the subject of Chapter 6.

Chapter 5

Supply chain-conscious production scheduling

This chapter presents the design of a production scheduler for continuous multi-grade processes. First, the need for flexible production scheduling for these processes is emphasized (5.1). Next, it is shown how the behavior of continuous chemical processes can be characterized in an efficient and consistent manner such as to arrive at a computationally feasible and realistic formulation of the scheduling problem (5.2). Finally the actual formulation is given (5.3) and illustrated by means of an example (5.4).

5.1 Introduction - flexible scheduling

The decomposition proposed in Section 4.5 aims to arrive at a feasible operating strategy by splitting up the production management problem in a *production scheduling problem* and a *production control problem*. This decomposition complies with current practice, however our design of the scheduling layer differs significantly from the current situation which we believe is not fit to meet the requirements of *intentional dynamics*-plant operation.

First, the scheduling approaches available nowadays use very poor representations of *process dynamics*. In some cases transition dynamics (and hence time, cost, material usage) is neglected at all, in the best case fixed transition times are incorporated. This may be a satisfactory description in case of the slate scheduling approach (for example used in HDPE production) described in Chapter 1 where only small process transitions are implemented. However is not be the case if the plant is operated according to the more flexible intentional dynamics approach where possibly large transitions may occur depending on the economic attractiveness. The latter can only be assessed if an accurate representation of the process dynamics is used in the scheduling layer. How this can be done is one of the main topics of this chapter.

Second, the current scheduling approaches do not support short term purchasing and sales decision making. Instead, fixed production requirements are set that the scheduler has to meet. For example, the HDPE slate scheduling is solely oriented towards maintaining average storage levels. Short term purchasing and sales decisions are not considered and flexibility to changes in the market can only be achieved by keeping end products on stock. In the intentional dynamics approach flexibility to changes in the market is to be obtained from flexible operation of the plant itself so that storage levels can be reduced. A consequence of this is that purchasing and sales management starts to interfere with production and has to be integrated in the short term production scheduling. This chapter describes how this can be done.

For case III, HPDE production, the integration of short term production scheduling and sales management is believed to yield strongly increased economic performance of the manufacturing site. On one hand due to decreased capital costs tide into end product storage and on the other hand due to the possibility to respond to attractive sales opportunities which leads to an overall increase in revenues. A quantification of the economic potential of our flexible, market-oriented scheduling approach for a typical HDPE production site is given in Chapter 8.

5.2 Production modeling - a task description

To solve the production scheduling problem, we do not need to consider all degrees of freedom in the behavior of the plant at a high level of detail (see the discussion on page 4.4.2). Instead, **we will resort to a description of the plant in terms of operating tasks with accompanying precedence rules**]★. A *task* can be interpreted as a compact characterization of the behavior of the plant over a certain time interval. The time interval on which the execution of a task is considered is either fixed in advance or left as a degree of freedom, however in general the length of this interval is substantially longer than would be required in the single level control approach of Section 4.4. This makes it possible to describe the behavior of the plant over a large time horizon using a preferably small number of tasks, which is the key to making the scheduling problem computationally tractable. The description of the plant behavior in terms of tasks can be seen as a *parametrization* of the behavior of the plant, which has important consequences. If the parametrization is not done properly, the scheduling problem may yield solutions which are not feasible. This will happen for example when transition dynamics are neglected and the behavior

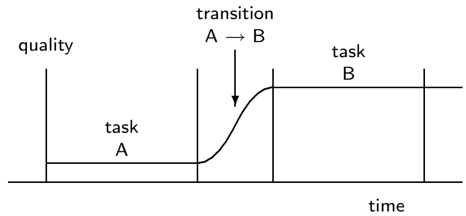


Figure 5.1: Representation of the behavior of a multi-grade process using static production tasks and transition tasks.

of the plant is parameterized in terms of steady state operating tasks only. Also, a poor parametrization may yield scheduling solutions which are far from the optimum. This happens if the chosen parametrization reflects the potentials of the process behavior poorly. Ideally, we would like to parameterize the behavior of the plant in such a way that the achieved performance is close to the fictional performance that were achieved if a single level approach would be used.

5.2.1 Task selection

While thinking of suitable parametrizations of the plant behavior in the scope of production scheduling problems it appears useful to first distinguish two classes of tasks which are inherently different: dynamic tasks and quasi-static state tasks. Dynamic tasks refer to the behavior of the process during transitions, or while dealing with the effect of load changes. Quasi-static tasks refer to the operation of the process in or at least in the vicinity of a distinct operating point. Using the notions of dynamic and quasi-static tasks the complete behavior of the plant is characterized by all feasible interconnections of the quasi-static and the dynamic tasks. Feasible interconnections are those for which the end-conditions of the first task match the initial conditions of the second. The use of quasi-static and dynamic tasks in modeling the behavior of a continuous multi-grade plant is illustrated in Figure 5.1.

The selection of tasks proceeds via a systematic determination of the sets of operating conditions and transitions that represent the practical operation of the plant. **We will in the remainder focus on multi-*grade* processes only**]*. For multi-*feedstock* plants a similar description can be given. Let a model of the plant, *including the basic control system*, be given by the following set of DAE's

$$\dot{x} = f(x, u, y), \tag{5.1}$$
$$0 = g(x, u, y), \tag{5.2}$$
$$z = C_x x + C_u u, \tag{5.3}$$

where $x(t) \in \mathbb{R}^{n_x}$, $u(t) \in \mathbb{R}^{n_u}$, and $y(t) \in \mathbb{R}^{n_y}$ are respectively the state, input and algebraic variables of the model. For ease of notation, the dependency of these variables on time will be omitted in the remainder. $z \in \mathbb{R}^{n_z}$ contains the so-called performance channels, i.e. all variables that are required for the performance evaluation of the plant. The performance evaluation typically comprises the computation of a so-called objective function as well the violation of constraints. These operating constraints are expressed as follows,

$$h(z) < 0. \tag{5.4}$$

All feasible steady state operating conditions are given by the set

$$\mathcal{F} = \{x, u \mid \exists y,\ z \text{ s.t. } f(x,u,y) = 0,\ g(x,u,y) = 0,\ z = C_x x + C_u u,\ h(z) < 0\}. \tag{5.5}$$

In general we are only interested in a limited number of interesting scenarios, e.g. a finite number of product grades or feedstock conditions. The production grade conditions $\mathcal{G}_g$ are by definition given by specific sets of conditions (z) that obey the corresponding constraints:

$$\mathcal{G}_g = \{(x,u) \in \mathcal{F} \mid \exists z = C_x x + C_u u,\ \text{s.t. } g_g(z) < 0\}. \tag{5.6}$$

where g_g defines the quality bounds of grade g. For example, in a distillation plant, these would be lower and upper limits on the purity.

The different production grades are connected via process transitions. We define a transition T_g^h from an element $(x^g, u^g) \in \mathcal{G}_g$ to an element $(x^h, u^h) \in \mathcal{G}_h$ as a quadruple (x, u, y, z) satisfying

$$\begin{array}{llll} \text{plant} & \text{init. cond.} & \text{end cond.} & \text{path constraints} \\ \dot{x} = f(x,u,y) & x(0) = x^g, & x(T) = x^h, & h(z) < 0 \\ 0 = g(x,u,y) & u(0) = u^g & u(T) = u^h & \\ z = C_x x + C_u u & & & \end{array} \tag{5.7}$$

for some $T > 0$. Let $\mathcal{T}_g^h$ be the set of all these transitions. The sets $\mathcal{G}_g$ and $\mathcal{G}_h$ are said to be compatible if there exists a transition T_g^h from any $(x^g, u^g) \in \mathcal{G}_g$ to any $(x^h, u^h) \in \mathcal{G}_h$. Finally, all sequences of transitions are feasible if all pairs $[g, h]$ are compatible. The verification of such conditions is not straightforward, only for specific cases there may exist a computationally feasible approach. Further, although the description of the behavior of the plant in terms of tasks is a reduced representation in comparison with the behavior rendered by (5.1,5.2,5.3) it is still of no use in a scheduling formulation, because it leaves too many degrees of freedom. It appears that we need to specify further how the different tasks are established or, in other words, how the control system is implemented.

5.2.2 Assumption on the control system

To derive a parametrization of the plant behavior that is non-conservative as well as feasible, we need to make realistic assumptions about the *controlled* behavior of the plant, and hence about the performance of the process control layer. This is a typical and very logical requirement of the decomposition we propose and it demonstrates the dependency of the scheduling problem on the technology selection and design of the process control layer. For example, if we assume traditional operator control, the grade change flexibility will in general be limited which has severe consequences for the nature and the number of feasible production schedules: in the worst case we will end up with solutions like the inflexible grade slate [77]. This observation complies with the supposition made in Chapter 2 that the benefits of supply-chain oriented production scheduling rely to a large extent on the quality of the process control system. The specific assumptions that we make with respect to the control system will be discussed next.

Static-tasks

We assume that, **during the static production tasks, the operating conditions are determined according to the *maximization* of an economic criterion**]*. As the basic economic criterion we will use the *added value* as discussed in Section 3.3.4. Let C_r and Y_e denote respectively the consumption of raw materials and utilities r and the production of end product e. We assume these are given as functions of the performance variables: $C_r = C_r(z)$, $Y_e = Y_e(z)$. Then, in case of a static production task, the added value rate is given by

$$L(z) := -\sum_r p^{C,r} C_r(z) + \sum_e p^{Y,e} Y_e(z), \tag{5.8}$$

where $p^{C,r}$ and $p^{Y,e}$ are the instantaneous prices of respectively raw material r and the product e. Using this expression for the added value and disregarding the effect of noise and disturbances, the optimal operating conditions for grade g are found by solving the following, static optimization problem

$$(\bar{x}^g, \bar{u}^g) = \text{argmin}\left\{-L(z) \mid \exists z = C_x x + C_u u,\ \text{s.t. } (x, u) \in \mathcal{G}_g\right\}, \tag{5.9}$$

and the corresponding raw material and product flows are given by $C_r^g = C_r(\bar{z}^g)$ and $Y_e^g = Y_e(\bar{z}^g)$, where $\bar{z}^g = C_x \bar{x}^g + C_u \bar{u}^g$. An intricate problem arises: the prices of the raw materials and end products appear in this optimization, which means that the optimal operating conditions depend on the current state of the market. Indeed, in case of a demanding market an optimal production strategy would tend to maximizing the production, whereas in a saturated market the better strategy might be to minimize production costs. An additional problem is how to determine $p^{C,r}$ and $p^{Y,e}$. Of course, these prices are related to the purchase and sales prices. However, because of the storage dynamics and the fact that production and purchase/sales actions are not synchronized, the factual determination of this value is not straightforward. There are several ways to deal with this problem, depending on the actual dependency of $(\bar{x}^g, \bar{u}^g)$ on the market situation.

First, in case the optimal strategy depends weakly on the market situation, we can ignore the dependency at all and use a single set of operating conditions for each production task.

If, instead there is a strong dependency, it may be sufficient to consider a *finite* set of market *scenarios*. Of course, these are chosen to reflect the most common market situations. This description of the market leads us to assign to every plant grade or grade transition a finite number of different production tasks, corresponding to the different market scenarios that we distinguish. The operating attributes of those tasks are computed by solving (5.9) for the corresponding market scenario (reflected in the choice of $p^{C,r}$ and $p^{Y,e}$).

Transition tasks

The parametrization of the quasi-static tasks in terms of steady state optimal production limits the set of transitions that needs consideration and as such leads to a different definition of transition feasibility. Let the operating conditions $(\bar{x}^g, \bar{u}^g)$ and $(\bar{x}^h, \bar{u}^h)$ be the elements of the sets $\mathcal{G}_g$ and $\mathcal{G}_h$ corresponding to the static tasks g and h respectively. Then, existence of a transition T_g^h can be checked by verifying (5.7) for $(x^g, u^g) = (\bar{x}^g, \bar{u}^g)$ and $(x^h, u^h) = (\bar{x}^h, \bar{u}^h)$. The investigation of the feasibility of such transitions with fixed initial conditions and an end-point constraint is in literature referred to as *switchability analysis*. Vu et al. [90] and White et al. [91] propose, indeed for grade transitions, a straightforward optimization approach to compute approximations of T_h^g (the end-point constraint is somewhat relaxed for computational feasibility). The authors use a rather arbitrary objective function which is the integrated square deviation of the outputs and inputs from the new operating point. Nevertheless, they rightly observe the pre-eminent usefulness of dynamic optimization in distinguishing desirable transitions from undesirable ones. We largely support this observation and will assume that **the process control system governing the implementation of process transitions is based on dynamic optimization**]*. Instead of using an arbitrary objective like in the switchability analysis we will consider objective functions that reflect the economics of the transition. A general formulation of the corresponding trajectory optimization problem is given as follows

$$\min_{T,u\in\mathcal{U}}\left\{\int_0^T L^d(z)dt\middle|\exists x,y,z,\text{ s.t. }(x,u,y,z)\in\mathcal{T}_{\bar{g}}^{\bar{h}},\ x(0)=\bar{x}^g,\ x(T)=\bar{x}^h\right\},\tag{5.10}$$

where L^d is chosen so as to represent the economics of the transition. Similar to the static optimization case, different market situations may lead to different optimal transition modes. $\mathcal{U}$ is the set of trajectories over which u is optimized. If the dependency of the optimal transition on the market situation is weak it is sufficient to define one transition mode for each changeover. If this is not the case, we suggest that a number of distinct scenarios be selected for which the corresponding transition characteristics are computed. Possible scenarios are the following.

Strong demand In case of a demanding market, the main incentive is to maximize production. Then transition times should be limited to the minimum. Transition costs are of secondary importance. Minimum time transitions may also be desirable when several subsequent sales orders are to be met on a short term: the penalty on a late delivery will in general be much higher than the supposedly larger transition costs. To enable the scheduler to select the minimum time transition mode, the characteristics of such a mode must be available in the production database.

Low demand In case of low demand and moderately filled order books, there is no incentive to minimize the transition times. Instead, the difference between the transition revenues and the transition costs should be maximized. This leads to a truly economic transition optimization, where $L^d(z)$ is selected to represent the negative added value rate during the transition.

The different transition modes m are characterized by the corresponding transition times $\tau^{g,h,m}$, the raw material consumption $C_r^{g,h,m}$ and the end product yield $Y_e^{g,h,m}$. The raw material consumption is computed as $C_r^{g,h,m} = \int_{t=0}^{\tau^{g,h,m}} C_r(\bar{z}^{g,h,m})dt$, where $\bar{z}^{g,h,m}$ are the optimal trajectories of the performance variables for problem (5.10). The yield of product e is given by $Y_e^{g,h,m} = \int_{t=0}^{\tau^{g,h,m}} Y_e(\bar{z}^{g,h,m})dt$.

Disturbances and uncertainty

In the previous, model-based optimization was introduced as a means to predict optimal production data for the different grades and grade changes. Of course, due to the presence of disturbances and plant-model mismatch, the *true* production will deviate from these predictions even if the on-line control system attempts to optimize the same objective. There are several ways of dealing with this.

The first is to take the disturbances and the model uncertainty explicitly into account in the determination of the production data, for example by computing the worst-case production over a specified time interval. Dimitriadis et al. [18] propose suchlike worst case optimization problem to analyze the flexibility of systems that operate dynamically under the effect of time-varying uncertainty. Despite its elegance this approach has several drawbacks. First, detailed knowledge on the disturbance characteristics is required. Second, we need to make the choice for the control system explicit. Third, the min-max (or max-min-max [18]) dynamic optimization problem such an approach entails is generally too hard to handle computationally. And finally, worst case formulations generally lead to solutions that are overly conservative.

A much simpler and more straightforward approach is to introduce a *safety factor* < 1 in the calculation of the production numbers. One way of determining this *safety factor* is through experience on the actual plant. Detailed information on the deviation between predicted and actual production becomes available continuously. This information can be used to determine a suitable and realistic level of conservatism in the production description.

5.2.3 A general formulation of the grade change problem

It was argued previously that different transition modes need to be considered to reflect the effect of changing market conditions on the most desirable operation of the plant. Several extreme cases were mentioned, among which the time-optimal transition and the minimum-cost transition. These two will be discussed next and a general framework for formulating such grade change optimization problems mathematically shall given.

Time-optimal transition The classical time-optimal control problem formulation of the minimum time changeover problem would amount to choosing $L^d(z) = 1$. By solving the time-optimal control problem we find the controls which drive the plant to the new steady state operating conditions $(\bar{u}^h, \bar{x}^h)$. However, this does not imply in general that the fastest transition between grade g and grade h is achieved, because these are defined by their corresponding sub sets $\mathcal{G}^g$ and $\mathcal{G}^h$. A side-effect of this is that the minimum time formulation does not honor the fact that valuable end-products are produced *during* the transition. So it might happen that the minimum-time transition leads to enormous losses due to off-spec production where a slightly longer transition might lead to valuable production of on-spec material.

It appears that, although the enforcement of an end-point constraint is necessary to guarantee the behavior of the plant outside the optimization horizon, the time optimal control problem does not capture all the aspects of *fast* transitions that we like to include. A better way to enforce a fast transition between the grades g and h may be to maximize the production of grade g or h or a weighted sum between those over a *fixed* time interval and using an end-point constraint to enforce steady state optimal operation by the end of the time interval. Of course, to ensure feasibility of the optimization problem we need to choose the length of the fixed time interval greater than or equal to the minimum possible changeover time. The corresponding objective is given as follows:

$$L^d(z) = -\sum_e \beta^e Y_e(z), \tag{5.11}$$

where β^e is used to express the relative importance of the different end-products. A practical choice of this weighting may be $\beta^e = p_P^e$. $Y_e(z) \in \mathbb{R}^{n_e}$ is the production flow of the end product e. Which product is being made depends on the state of the process satisfying the corresponding grade constraints or not. Therein lies the most complicated aspect of the formulation of the grade change problem.

Let $F(z) \in \mathbb{R}^{n_F}$ be a vector with all material flows coming from the plant. For each grade we need to relate the end product flows to these material flows. To this end we introduce row vectors $M_g^e \in \mathbb{R}^{n_F}$ with zeros everywhere except for a single '1' at at most one location, which assigns the material flows $F(z)$ to the e^{th} end product flow. The flow of end product e in a particular grade g is then given by:

$$Y_e^g(z) = M_g^e F(z), \tag{5.12}$$

so that the total end product flow can be stated as

$$Y_e(z) = \sum_g G^g M_g^e F(z), \tag{5.13}$$

where

$$G^g = \begin{cases} 1, & \text{if } g_g(z) \leq 0, \\ 0, & \text{otherwise.} \end{cases} \tag{5.14}$$

Note that the definition of the grades by (5.14) renders $L^d(z)$ non-smooth.

Economically optimized transition When there is no particular reason for a fast transition, the transition costs should be minimized. This amounts to defining the transition problem as a purely economic optimization. The economic objective is given by the negative of the added value (compare (5.8) for the static optimization problem):

$$L^d(z) = -\left(-\sum_r p_F^r C_r(z) + \sum_e p_P^e Y_e(z)\right), \tag{5.15}$$

where $C_r(z)$ is assumed a smooth, continuously differentiable function representing the consumption of raw materials and $Y_e(z)$ is given by (5.13). The economic transition optimization problem like the minimum-time transition problem is non-smooth. Moreover, it is a generalization of the minimum-time transition problem (the minimum-time transition problem is obtained by setting $p_F^r = 0$ and $p_P^e = \beta^e$ in (5.15)). Methods for solving the grade change problem shall be treated in Chapter 7.

5.3 Mathematical formulation of the scheduling problem

In the first part of this chapter it has been defined how the plant is characterized in quasi-stationary tasks and transition tasks for the sake of production scheduling. In this section a mathematical formulation of the production scheduler shall be given. For clarity, the main aim of the production scheduler (page 55) is summarized below:

> ....it should compute a production *schedule* in compliance with the market conditions and the current and future status of the plant. The second task is to provide relevant feedback regarding sales and purchasing opportunities to the sales and purchasing managers.

The formulation of the supply-chain conscious scheduling problem given in this section is not meant to be the most rigorous and complete formulation we can imagine. The formulation is simple and tractable. Nevertheless, it contains most of the important aspects of the scheduling problem that we want to take into account, and most important, it enables us to demonstrate the feasibility of the proposed hierarchical control approach. We will first briefly motivate our choice for a Mathematical Programming (MP) approach to describing and solving the scheduling problem (5.3.1). Next, the actual mathematical model shall be described (5.3.2). Aspects related to the solution of the corresponding optimization problem are treated in 5.3.3.

5.3.1 Choice of method

Two basic methods for modeling and solving decision problems like the production scheduling problem can be distinguished: Mathematical Programming (MP) methods, and heuristic methods. Some distinguishing characteristics of these two categories are discussed in Appendix A. Below, a short concluding motivation for the MP approach shall be given. For an elaboration on existing scheduling formulations and exact and heuristic solution methods we refer to the appendix.

The primary aim of our scheduling research is to demonstrate the feasibility and the potential of a supply-chain-conscious, and process-compliant scheduling approach. The formulation of such a scheduling problem is part of this research and on the basis thereof, qualitative statements with respect to expected benefits can be made. Also, because we strongly support the persuasiveness of a quantitative assessment we will study the actual application of the scheduling approach to the simple blender problem in Section 5.4 and to a more realistic, exploratory case of scheduling HDPE production in chapter 8. For such a quantitative assessment to be meaningful, we must at least be able to solve the exploratory case to a *guaranteed* level of optimality. This makes the MP approach the preferred candidate. Another attractive property of the MP approach is mentioned by Zentner et al. [95], namely that it provide a means of encoding combinatorial decisions in a way that identifies sources of difficulties in problems and provides a focus for research. Such research may for example address the development of efficient and accurate heuristic solution approaches. Based on the previous we have decided to **formulate the scheduling problem as a MP**]*.

5.3.2 The model

Time discretization

A crucial choice in the formulation of any scheduling problem is how *time* is represented. Terpstra [84] distinguishes three methods of time representation: discrete time uniform slots, continuous time slots, and continuous time with temporal relations. The first two are most commonly used and will be described here, based on Zentner et al. [95] who present a brief and concise discussion on the competing choices. In the *Uniform Discretization of time Modeling* (UDM) framework the horizon is divided into a finite number of time slots of uniform length. Only at the beginning of each interval changes may occur. The UDM framework is very often used, for example in relation to the well known State Task Network description [39] and the Resource Task Network description [63]. The UDM framework generally leads to a vaste number of integer decision variables, especially when a fine discretization is used. To circumvent this, *continuous time slots* may be considered, see e.g. [94]. Each continuous time slot is given by its starting and end times, which are continuous variables. The accuracy of continuous time formulations is hence better in general. Because the duration of tasks depends on the decision variables the continuous time slot representation is more likely to lead to MINLP's. It cannot be made definite a priori which of the two time representations is most suitable (accurate, efficient) for the problem at hand. However, mature and proven optimization codes exist for MILP's, whereas dealing with MINLP's is still in a rather premature phase. Also, most continuous time descriptions available in literature assume that the events which need to be scheduled have been determined a priori, which is not the case in our problem. Letting these be the decisive arguments, **we will resort to the UDM as a basic framework for the modeling of the scheduling problem**]*. The choice of the interval length, denoted τ in the sequel, is a trade-off between solution resolution and computational tractability.

Production tasks

We introduce decision variables G_k^g, $g = 1, \ldots, n_g$ as the *production decision* variables, where $G_k^g = 1$ means that production task g is started at the beginning of the k-th time span and executed during this time span. Only one task can be performed at the same time:

$$\sum_g G_k^g = 1. \tag{5.16}$$

This expression holds for every k. In the remainder this information will be omitted when it is clear from the equation. The static production tasks can be given any desired length through an appropriate choice of τ. The *transition tasks* however have a fixed and known duration and they must be modeled as such. In the UDM framework, a transition takes one or more intervals, depending on the length of the interval and the transition length. The most straightforward formulation results if τ is chosen to be larger than the maximum changeover time. This case will be studied first.

Consider the transition between task g at k and task h at $k+1$. Because the transitions can be executed in a single time interval and the transition times are known only the starting time for each transition remains to be decided. For simplicity we let the end-time of the transition coincide with the end of the transition interval as shown schematically in the left image of Figure 5.2[1]. To model the transitions we introduce variables $T_k^{g,h,m}$ which, if equal to 1, indicate that a transition from grade g to h and of mode[2] m is executed at the end of time span k. $T_k^{g,h,m}$ relates to G_k^g and G_{k+1}^h in the following manner.

$$\sum_g \sum_h \sum_m T_k^{g,h,m} = 1, \;\; \sum_m T_k^{g,h,m} \leq G_k^g, \;\; \sum_m T_k^{g,h,m} \leq G_{k+1}^h. \tag{5.17}$$

Note that this description also includes the trivial transitions $T_k^{g,g,m}$ (i.e. *no* transition). Further, let TM_k^m be one if transition mode m is executed in time

[1] Note that a more flexible formulation can be obtained through definition of a variety of different transition tasks for each transition mode where the starting times are varied between the extreme values.

[2] The transition mode m refers to the market scenario for which the transition characteristics are computed (see Section 5.2.2).

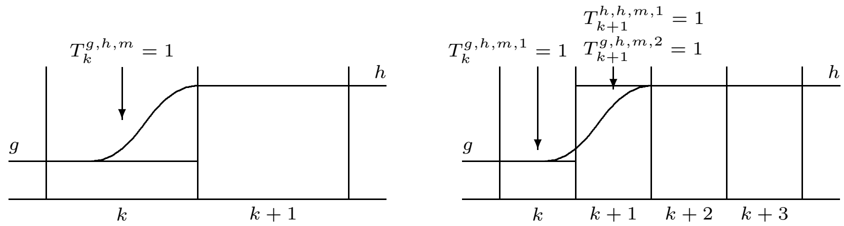


Figure 5.2: Representation of transition tasks in UDM framework in case (left) transition time is smaller than τ, and (right) transition time is smaller than 2τ.

span k and zero otherwise. Then, the following holds:

$$T_k^{g,h,m} < TM_k^m. \tag{5.18}$$

Because all transition times are shorter than τ we need to take the quasi-static production preceding the transition into account to arrive at the appropriate production attributes (raw material consumption and end product yield). Let the transition time for a mode m transition from grade g to grade h be denoted $\tau^{g,h,m}$. Then, the consumption of raw material r and the production of end product e for the corresponding transition are computed as

$$TC_r^{g,h,m} = (\tau - \tau^{g,h,m})C_r^g + C_r^{g,h,m}, \tag{5.19}$$

$$TY_e^{g,h,m} = (\tau - \tau^{g,h,m})Y_e^g + Y_e^{g,h,m}. \tag{5.20}$$

For 'transitions' $T_k^{g,g,m}$ the transition time is zero which yields the corresponding steady state production figures: $TC_r^{g,g,m} = \tau C_r^g$ and $TY_e^{g,g,m} = \tau Y_e^g$. C_r^g, Y_e^g, $C_r^{g,h,m}$, and $Y_e^{g,h,m}$ are the consumption and yield variables as defined in the previous section.

Binary decision variables If only one transition mode is considered for each transition then the set of binary variables is constituted by the grade variables only: $G_k^g \in \{0,1\}$. Equation (5.17) then simplifies to

$$\sum_g \sum_h T_k^{g,h} = 1, \;\; T_k^{g,h} \leq G_k^g, \;\; T_k^{g,h} \leq G_{k+1}^h.$$

Observe that these equations enforce binary *values* of $T_k^{g,h}$ without requiring $T_k^{g,h}$ to be defined a binary variable.

The single-transition mode description leads to a reduction in the number of integer decision variables in comparison with the multiple-transition mode description and is therefore the preferred choice if no large benefits are to be expected from including multiple transition modes. An interesting extension is the case where all possible transitions are parameterized as linear combinations of a finite number (n_T) of transition modes:

$$TC_r^{g,h} = \sum_{m=1}^{n_T} \alpha_m TC_r^{g,h,m}, \;\; TY_e^{g,h} = \sum_{m=1}^{n_T} \alpha_m TY_e^{g,h,m}, \tag{5.21}$$

where $0 \leq \alpha_m \leq 1$ and $\sum_{m=1}^{n_T} \alpha_m = 1$. This transition formulation will in the sequel be denoted 'interpolated transition modeling'. The interpolated transition modeling introduces no additional binary variables.

Multiple-interval transitions The formulation given above can be extended for the case that some transition times exceeds the length of an interval, i.e. in case there exist g, h and m such that $\tau^{g,h,m} > \tau$. We will show here how a transition with a duration $\tau < \tau^{g,h,m} \leq 2\tau$ can be modeled, extensions towards finer grids are straightforward. Consider the transition $g \rightarrow h$, plotted in the right image of Figure 5.2. The transition occupies two intervals: k and $k+1$. To model the transition we introduce new variables $T_k^{g,h,m,2}$ in combination with the following constraints:

$$\sum_m T_k^{g,h,m,2} \leq G_{k+1}^h, \tag{5.22}$$

$$T_k^{g,h,m} = T_{k+1}^{g,h,m,2}. \tag{5.23}$$

Accordingly, raw material consumption and end product yield during the transition are divided over two intervals. The expressions for those are omitted.

Market description

The *transaction-based market description* can be included in the MILP formulation as was already shown in Section 4.4.1 for the blending example. A binary decision variable $S_k^{e,s} \in \{0,1\}$ is used to indicate whether sales ord./opp. s for end product e is executed in time span k (in which case $S_k^{e,s} = 1$) or not ($S_k^{e,s} = 0$). Further, for each ord./opp. we introduce a set of time spans $\Omega^{e,s}$ outside which it may not be executed. This is done for several reasons. First, in practice the orders and opportunities are only valid during a limited time span. Second, it does not seem to make much sense to enable sales and purchase actions every 10 or 12 hours, a more coarse discretization prevents the size of the optimization problem to blow up unnecessarily. Attached to each sales ord./opp. the market database stores the amount of product, $SA^{e,s}$ and the unit price offered, $S\$^{e,s}$. By definition of $\Omega^{e,s}$ we have:

$$S_k^{e,s} = 0, \quad \forall k \notin \Omega^{e,s}. \tag{5.24}$$

Further, each order must be executed exactly once and each opportunity at most once. This gives rise to the following constraints

$$SO^{e,s} \leq \sum_{k \in \Omega^{e,s}} S_k^{e,s} \leq 1, \tag{5.25}$$

where $SO^{e,s}$ is zero if s is an opportunity and one if s is an order. Similar reasoning for purchasing orders and opportunities leads to the introduction of binary decision variables $P_k^{r,p}$ and the constraints

$$P_k^{r,p} = 0, \qquad \forall k \notin \Omega^{r,p}, \tag{5.26}$$

$$PO^{r,p} \leq \sum_{k \in \Omega^{r,p}} P_k^{r,p} \leq 1, \tag{5.27}$$

where $\Omega^{r,p}$ is defined as the set of time spans k outside which purchase ord./opp. p may not be executed and $PO^{r,p}$ is zero if transaction p for raw material r is a purchase opportunity and 1 if it is an order. The purchase attributes are $PA_k^{r,p}$ and $\$P_k^{r,p}$: the amount of feedstock r and its unit price for purchase ord./opp. p.

Inventory description

Let us introduce ES_k^e as the storage level of end-product e at the beginning of time span k and RS_k^r as the storage level of raw material r at the beginning of time span k. The *material balances* for the raw material storage and the end-product storage are defined as follows

$$ES_{k+1}^e = ES_k^e + \sum_g \sum_h \sum_m T_k^{g,h,m} TY_e^{g,h,m} - \sum_s S_{k+1}^{e,s} SA^{e,s}, \tag{5.28}$$

$$RS_{k+1}^r = RS_k^r - \sum_g \sum_h \sum_m T_k^{g,h,m} TC_r^{g,h,m} + \sum_p P_k^{r,p} PA^{p,r}, \tag{5.29}$$

with initial conditions $ES_1^e = ES_{initial}^e$ and $RS_1^r = RS_{initial}^r$. Note that the recursive formulation is conservative in the sense that yield is added at the end of the interval and sales are subtracted at the beginning. This is to prevent possible infeasibilities following from the implicit assumption that the storage levels are constant in each interval. Minimum and maximum constraints on the *storage capacity* can be imposed as follows

$$ES_l^e \leq ES_k^e \leq ES_u^e, \tag{5.30}$$

$$RS_l^r \leq RS_k^r \leq RS_u^r. \tag{5.31}$$

Objective

The objective is defined as the CAV extended by interest on the capital balance (see Section 3.3.4), and can be formulated as follows

$$V_{k+1} = (1+\gamma)V_k + \sum_e \sum_s S_{k+1}^{e,s} SA_S^{e,s} \$^{e,s} - \sum_r \sum_p P_{k+1}^{r,p} PA^{r,p} P\$^{r,p}, \quad (5.32)$$

$$J = V_H + \sum_r RS_{r,H} RV_r + \sum_e ES_{e,H} EV_e, \quad (5.33)$$

where γ is the fractional interest rate and H is the horizon length. The last two terms in (5.33) account for end-storage appreciation which is necessary because we solve a finite horizon approximation of an infinite-horizon problem, see the discussion on this subject in Section 4.4.1.

5.3.3 Solution of the scheduling problem

The number of binary variables changes with the choice of the transition modeling. A formulation with multiple, distinct transition modes leads to the introduction of $H(n+m)$ binary variables *only* for the production modeling. Additional binary variables arise from the modeling of the purchase and sales actions. Their number can be limited through an appropriate choice of the validity sets $\Omega^{e,s}$ and $\Omega^{r,p}$.

Because the objective as well as all constraints are linear and the total set of variables contains binary as well as continuous variables, the scheduling problem is a MILP:

maximize the objective J (5.33) subject to the objective recursion (5.32), the storage constraints (5.30,5.31), the inventory recursion (5.28,5.29), the purchase constraints (5.26,5.27), the sales constraints (5.24,5.25), the transition constraints (5.17,5.18), and the grade constraints (5.16).

This MILP is, like most scheduling problems, NP-hard. This means that no polynomial time algorithm has been found for solving the problem. For NP-hard problems one can in general only hope that an acceptable solution be found in a reasonable time. Although we dare not guarantee reasonable computation times for all instances of the scheduling problem presented above we will, for the interested reader, present two options that may help to achieve this in Appendix C. The first option is, for cases where feasibility of the scheduling problem cannot so easily be checked in advance, to modify the problem so as to avoid infeasibility. The second option is to tune the solvers to specific problem characteristics which may reduce computation time considerably.

g	h	$TC_1^{g,h}$	$TC_2^{g,h}$	$TY_1^{g,h}$	$TY_2^{g,h}$
1	1	1	1	2	0
1	2	1	0	0	1
2	2	1	0.71	0	1.71
2	1	0.167	0.952	0.833	0.285

Table 5.1: Production attributes of the static production tasks and the transition tasks of the blending process.

5.4 Application to case I: the blending process

As an example of the application of the production scheduler we consider the blending plant of Chapter 3.

Problem setup

Only two product grades are considered. Economic optimization of the two tasks does not yield single optimal solutions. For example, for grade 1 all feasible steady state operating tasks that satisfy $x_1/x_2 = 1$, $u^1 = 0.2$, $u^2 = 0.2$, $u^3 = 0.4$ have the same steady state economics. Steady states with minimum inventory will lead to smaller changeover times and are therefore preferred. For the simple blending process no advantage is expected from the definition of multiple transition modes because there is no trade-off between transition costs and transition time. We hence only consider the time-optimal transitions from grade 1 to 2 and vice versa.

To avoid the introduction of a large number of transition variables we choose the length of the discretisation time span such that both transitions can be executed in one time span which leads to the choice $\tau = 5$. The corresponding fractional interest is given by $\gamma = 1.0001^5 - 1 \approx 0.0005$. The choice of the two quasi-static production tasks and the time-optimal transitions leads to the raw material consumption and end product yield data as given in Table 5.1. The storage constraints, the order and opportunity database as well as all initial conditions are adopted from the example in Chapter 3. The problem was implemented in GAMS and solved using CPLEX.

Results

For this problem setting branching priorities proved unnecessary: default solver settings resulted in a sufficiently fast convergence. Solution time was in the order of magnitude of 1 minute for a guaranteed accuracy of 99 %. The optimum found was 62.764 which is even slightly higher than the optimal value for the single

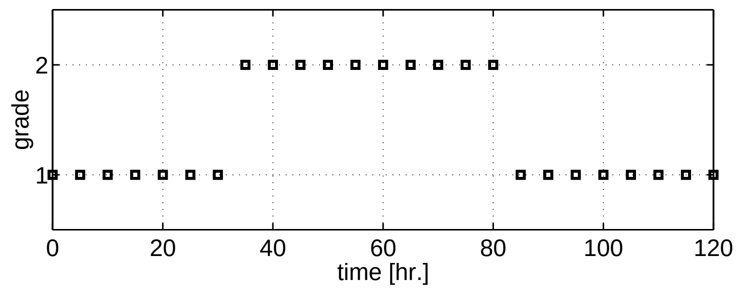


Figure 5.3: Optimal production schedule for the blending process.

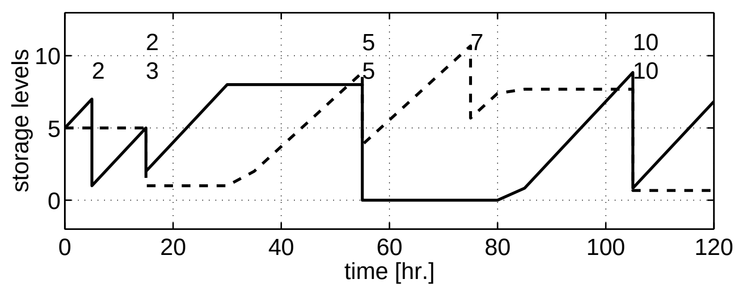


Figure 5.4: Storage levels of product 1 (solid) and product 2 (dashed) for the optimal schedule for the blending process. Sales ord./opp. numbers are indicated: the bottom row for product 1 and the top row for product 2.

level approach to the same example presented in the previous chapter[3]. The resulting schedule is plotted in Figure 5.3. The storage levels for this optimal production schedule are plotted in Figure 5.4. The selected sales transactions are identical to those selected by the single level controller in Chapter 3, compare Figure 4.5. This confirms the supposed adequacy of the parametrization of the plant behavior using quasi-static and dynamic production tasks.

Adding conservatism

It was suggested in Section 5.2.2 that a safety factor should be included in the computation of the production data in order to account for the future effects of

[3]The difference can - apart from an effect of the possibly larger sub-optimality of the optimal control solution in Chapter 3 - be explained from the slight difference in the computation of the cumulative added value.

disturbances and model uncertainty. To illustrate how such a safety factor may affect the scheduling we multiply the end product yield data, $TY_1^{g,h}$ and $TY_2^{g,h}$ by a safety factor of 0.95 and recompute the optimal production schedule and sales strategy. The inclusion of the safety factor in the production modeling leads to a different optimal operating strategy. The optimum found was equal to 57.632 which is significantly lower than the nominal optimum. We cannot conclude from this that the factual supply chain performance will go down by the same amount because in a practical setting the schedule will be recomputed many times based on updated production figures.

The *conservative* optimal production schedule switches to grade 2 already after 20 hours and returns to grade 1 after 92 hours. All orders are still met, however the attractive opportunity 2 for grade 1 is not selected. Instead, opportunity 8 for grade 2 is selected. Observe that the quantity as well as the price for opportunities 2 and 8 are equal. However, opportunity 8 is foreseen at a later date which makes opportunity 2 the preferred one. This example demonstrates the dependency of the 'optimal' operating strategy on the uncertainty about the production and stresses once more *the relevance of a high-quality process control system which renders the process a reliable and well-predictable link in the supply chain.*

Changes in the market

Next we consider the response of the scheduler to changes in the marketplace. Let us consider the supply chain status at a time 5 hours after the computation of the previous schedule. Two units of product A have been added to the end product stores due to 5 hours production. Based on the feedback from the scheduler sales managers have confirmed the feasibility of sales opportunity 2 and the corresponding amount of product 1 is about to be delivered to the client. Further, an increased demand for product 2 is spotted on the market; early negotiations with clients have resulted in the introduction of some attractive sales opportunities for product 2. Accordingly appreciations of the final storage levels for product 1 and 2 have been modified to 1.5 and 1.7 respectively. The updated sales ord./opp. database is given in Table 5.2.

The resulting schedule (computed using a non-conservative description of the production capacity) is plotted in Figure 5.5. The optimal schedule now changes to grade 2 after 25 hours. This complies with the previous schedule, see Figure 5.3. Differently from the previous schedule the production of grade 2 is continued till the end of the prediction horizon. The attractive opportunity 9 for product 2 is selected instead of opportunity 10 for product 1. Clearly the optimal schedule is properly adjusted to the changes in the marketplace.

Sales of grade 1

s	$SA^{1,s}$	$S\$^{1,s}$	$\Omega_{1,s}$	$SO^{1,s}$
1	7	1	{0,5}	0
2	6	1.8	{0,5,10,15}	1
3	3	1.3	{10,15,20,25}	1
4	7	1.4	{30,35,40,45}	0
5	8	2.5	{50,55,60}	1
6	7	1.6	{55,60,65,70}	0
7	8	1.5	{75,80}	0
8	3	1.3	{85,90}	0
9	5	1.7	{95,100,105}	0
10	8	2.3	{100,105}	0

Sales of grade 2

s	$SA^{2,s}$	$S\$^{2,s}$	$\Omega_{2,s}$	$SO^{2,s}$
1	7	1	{0,5,10}	0
2	4	2	{10,15,20}	1
3	8	1.8	{15,20,25,30}	0
4	4	1.3	{30,35,40,45}	0
5	5	1.7	{50,55}	1
6	8	1.9	{55,60,65}	0
7	5	2	{70,75,80}	1
8	6	2.5	{80,85,90}	0
9	4	2.7	{90,95,100}	0
10	7	1.7	{100,105,110}	1

Table 5.2: Modified sales order and opportunity database for the blending example.

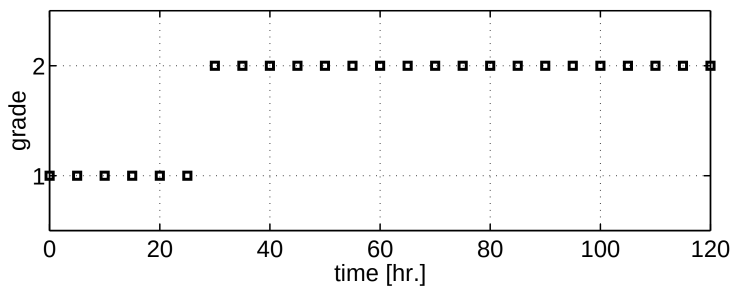


Figure 5.5: Optimal production schedule for the blending example, computed 5 hours after the first schedule with a modified sales ord./opp. database.

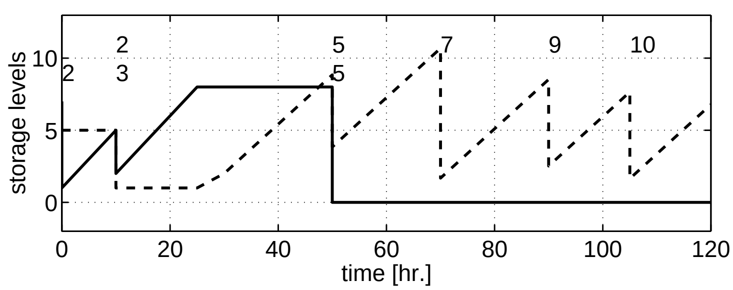


Figure 5.6: Storage levels of product 1 (solid) and product 2 (dashed) for the optimal schedule for the blending process computed 5 hours after the first schedule. Sales ord./opp. numbers are indicated: the bottom row for product 1 and the top row for product 2.

5.5 Implementation issues

Although the formulation of the scheduling problem and its solution may appear straightforward, the actual implementation of the supply-chain-conscious scheduler will be a lengthy and demanding process. There are two important implementation aspects: *information supply*, and the actual *decision making*. These aspects are discussed next. The section will be concluded by a short discussion on the closed loop properties of the interconnection of the internal supply chain and the scheduler.

Information supply

For the scheduler to play its role in the horizontal integration the information supply is required to be frequent, as accurate as possible and complete. For example, if the plant is expected to go through a phase of reduced productivity because of maintenance or a technical problem, the production database should be modified accordingly. Also, sales and purchase managers should provide the scheduler with an unbiased and complete representation of the expected market situation to eventually enable the scheduler to compute which transactions are most favorable instead of making up their own minds lightly. Preferably the information supply should proceed via existing communication systems and using existing databases. This avoids the time-consuming and costly installation of new information technology and will probably contribute to the acceptance of the new decision support system.

Decision making

Production, sales and purchase management will take action (hopefully) on the basis of the feedback from the scheduler.

With respect to the *production management* we first would like to stress that there is no theoretical need for the production managers (operators) to be part of the process operations hierarchy when it comes to the *decision making* part: the proposed decomposition into a scheduling layer and a process control layer is consistent and could, if sufficient guarantee of the quality of the scheduler's solution were obtained by means of some heuristic add-on, lead to a situation with fully automated operation. The scheduler then can be interpreted as a 'internal supply chain controller', few more thoughts regarding this potential role of the scheduler will be given in the final part of this section. Still, we cannot foresee how the end-responsibility for safe and reliable operation can be borne by an automated decision making system alone and we therefore promote the presence of operators. The main tasks of the operator will, apart from plant monitoring and information supply to the scheduler, be to take notice of the computed schedules and decide whether or not to dictate the production tasks to the process control and optimization system. There may be good reasons for deviating from the computed schedule in which case they are allowed to do so, of course not without notifying the scheduler on the modifications so that a new schedule can be computed accordingly. A very important implementation aspect is the institution of a so-called *frozen zone*. A frozen zone is a time zone from the current into the near future for which planned production actions are not allowed to change. Of course, the institution of frozen zones limits the flexibility of the scheduler and will hence lead to suboptimal behavior. Nevertheless, it prevents unexpected and jumpy behavior of the planned production actions and it may hence increase the acceptability of the computed schedules and the scheduler itself.

Purchasing and sales management will use the feedback from the scheduler as background information in their negotiation with customers on orders and contracts. Also, they can use the scheduler to check the sensitivity of the company-wide objective with respect to changes in the order and opportunity attributes, such as prices, quantities, validity time spans. Of course such a use of the scheduler requires that the computations are reasonably fast which may lead in practice to the necessity of including heuristics in the solution process, especially for large-scale problems.

The scheduler as an 'internal supply chain'-controller

Although the presence of process operators and purchasing and sales managers in the actual decision making is in our view imperitave, it is an interesting line of reasoning to suppose for a moment that the scheduler executes full control over the purchasing and production actions and to analyze the interconnection of the internal supply chain and the scheduler in its characteristics as a control system. Such an analysis may provide understanding of the elementary feedforward and feedback mechanisms that may occur in the internal supply chain and it clearly exposes the role of disturbances therein.

To this end, consider the control scheme in Figure 5.5. This control scheme is an abstract representation of the physically structured decision scheme presented in Figure 4.6 where all human decision makers are left out. The dynamics of the internal supply chain are given by the difference equations that represent the evolution of storage levels and the added value, respectively (5.28,5.29) and (5.32) and by a delay that keeps track of the grade in the previous production interval (observe that the computation of end product production and raw material consumption is based on the transition variables which depend on the current *and* the previous grade variable.).

The scheduler has at its disposal the following controls: Purchasing actions (P), production actions (G), and sales actions (S). The states of the internal

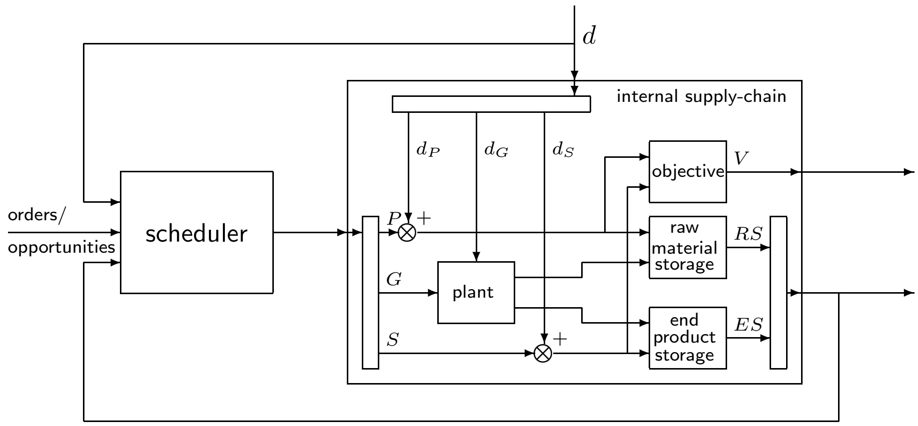


Figure 5.7: The scheduler as an 'internal supply-chain controller'.

supply chain are the storage levels (RS, ES), the accumulated added value (V) and the production grade (G). The scheduler determines the optimal controls for a given order and opportunity database which is provided externally.

External factors disturb the operation of the internal supply chain. We distinguish disturbances in the purchasing strategy (d_P), disturbances in production (d_G) and disturbances in the sales strategy (d_S). Disturbances in the purchasing and sales strategies (e.g. delayed or canceled deliveries) are often known in advance and can hence be forwarded to the scheduler. The effect of disturbances in the production probably is observed before the end of a certain production interval, hence an estimation can be forwarded to the scheduler as well. Measured outputs are the storage levels which are fed back to the scheduler. The control task is to compute the controls in such a fashion that the predicted added value is maximized subject to constraints on the storage levels and given the states of the internal supply chain and a certain realization of the order/opportunity databases. The scheduler performs this task in a deterministic, receding finite horizon fashion. The actual closed loop performance is the result of the interplay of the scheduler's actions and the disturbances and will depend on several design factors such as the horizon length.

In most control systems, *stability of the closed loop behavior* is essential. Because intentional dynamic and thus non-stationary behavior is aimed for and storage levels are physically constrained, stability does not seem to be a very relevant notion here. An issue that is clearly more essential is the *feasibility* of the operation. Disturbances as outlined above may incur infeasibility of the operation. In Section C.1 it is outlined how infeasibility of the MILP can be repaired by relaxation of the orders so as to end up with schedules that are feasible with respect to a modified order database. This does not work for the controls that are actually implemented in each cycle. To avoid unexpected infeasibility of the operation it is thus foremost essential to investigate the one-step-ahead feasibility of the controls. Fortunately, this is almost handled through the way in which we model the storage mass balances. Observe from (5.28) and (5.29) that the sales transactions are subtracted from the end product storage levels at the beginning of the production interval and that purchase transactions are added at the end. So even if the purchased material arrives too late, production can proceed according to plan. Also, if the produced end product levels fall short, sales orders can be delivered anyway. Of course, at the next cycle the effect of these disturbances will be visible and a relaxation of the MILP may be necessary.

Our analysis of the control system that results by viewing the scheduler as an internal supply chain controller is qualitative only and rather intuitive. A *quantitative* assessment of the performance of the internal supply chain control system is an interesting research topic.

5.6 Contributions of this chapter

This chapter presents a mathematical formulation of a production scheduling problem for continuous multi-grade chemical processes.

An extensive description of how the plant's behavior can be characterized using production tasks is given. The proposed characterization in finite-interval stationary tasks and transition tasks seems adequate for a large class of multi-grade (or multi-feedstock) processes. Production attributes for these tasks can be derived via model-based static, respectively dynamic optimization. A general mathematical formulation of the economic grade change problem is given for which dedicated optimization strategies will be presented in Chapter 7.

The mathematical formulation of the scheduling problem utilizes the well-known UDM framework to divide the look ahead of the scheduler in a finite series of time intervals with the same duration. At each interval production, purchasing and sales decisions can take place. Inventory of raw material and end products is modeled by formulating the associated mass balances. A new aspect in this problem formulation is the way the transitions and the associated material flows are modeled. Another contribution is the characterization of the market using orders and opportunities as discussed in Chapter 3. Mathematical modeling of the scheduling problem yields a MILP which can be solved using preferably BB algorithms.

Chapter 6

Economic optimization and control

Chapter 4 motivated and defined a hierarchical decomposition of the plant operations problem in a task scheduling problem and a process control problem. In this chapter, the definition of the latter will be given as well as several approaches towards solving it. First, the ingredients of the control problem shall be outlined (6.2). Next, different approaches to this problem shall be discussed mainly conceptually. Three operating scenarios shall be discussed for which different control strategies are defined. The first two scenarios are chosen so as to highlight different aspects of the plant optimization problem. To this end the first scenario (6.4) ignores the presence of persistent disturbances whereas the second scenario (6.5) considers quasi-static production only. The second scenario resembles the configuration for which current RTPO strategies were developed. A comparison of our approach with the current RTPO solutions shall be given. The third scenario represents the most realistic case with grade changes and the presence of persistent as well as fast disturbances (6.6). All proposed methods are illustrated by means of application on case II, the simulation of a binary distillation column.

6.1 Introduction

In the previous chapter we showed how a chemical plant can be seen and exploited as being a flexible link in the supply chain of which the operation can be scheduled optimally with respect to the market situation. A main prerequisite for this flexible scheduling is that the plants operates in a predictable fashion, both in stationary operation and during transitions. At present this is often not the case: transitions are often operator-controlled and there is a large spread in transition times, even when the same transition is implemented at different instances. Existing advanced Process Control and Real Time Optimization solutions could be used to improve the situation, however as already indicated in Chapter 1, these solutions were developed for the (stationary) optimization of mainly refinery processes and are not suited for optimization and control of nonlinear processes with large transitions. A new, integrated optimization and control strategy which is in line with the *intentional dynamics* approach to plant operation shall be described in this chapter. The approach combines aspects from existing NMPC schemes and model-based dynamic-economic optimization. The latter can be regarded an indispensable ingredient in any large scale nonlinear process control strategy (either off-line or in the famous *receding horizon* implementation) and in fact a major part of our work on advanced process control and optimization is dedicated to the problem-specific definition and solution of dynamic optimization problems. The great potential of dynamic optimization in transition control for a HDPE reactor shall be demonstrated in Chapter 8.

6.2 Problem formulation

A consequence of the decomposition of the plant operation problem into a scheduling problem and a control problem is that the determined schedule acts as a constraint on the solution of the control problem. Hence, the actual controlled behavior of the plant must satisfy the requirements on production, and product quality that are put by the schedule. This is the first essential aspect of the plant control problem that we will discuss (Section 6.2.1).

In the previous chapter it was further argued that sufficient amount of conservatism should be included in the computation of production schedules to avoid infeasibility of the schedules and the bad consequences thereof (in particular customer dissatisfaction). This means that the operating constraints imposed by the scheduler will often be not very stringent and will leave room for economic optimization of the process operation. Several economic goals may be aimed for: cost minimization, production maximization, or combinations thereof (Section 6.2.2).

Of course, economic optimization of the operation is only meaningful if more elementary requirements with respect to the process operation such as safety and stability are met. Various ways to include these aspects in the control strategy shall be mentioned (Section 6.2.3). Finally, the role of process disturbances shall be outlined (Section 6.2.4).

6.2.1 Scheduling constraints

An important factor in the definition of the process control and optimization problem is the implementation of the scheduling solution as a constraint. The success of the hierarchical decomposition proposed in the previous chapters depends to a large extent on the feasibility of the interconnection between the scheduler and the process control system. The necessity of a clear and unambiguous definition of the coupling was observed by [49] who introduced the notion "coordination port" to describe the interconnection of the scheduling layer and the APC layer. No specific definition of the coordination port was proposed, instead it was suggested that a variety of possible interconnections exists.

One choice of the coordination port leads us to impose the selected sales and purchasing transactions as well as minimum and maximum storage levels as constraints on the process control problem. This leaves a maximum amount of freedom for the process control system to *optimize* the plant behavior, while guaranteeing the feasibility of in-time product deliveries. A drawback of this choice is that the process control system should largely recompute the optimal production schedule, which would take us back to the practically impossible optimal control solution of Section 4.4.1. Another choice of the coordination port is to impose the operating conditions that result from connecting the optimal quasi-static production tasks to the optimal transition tasks as constraints or setpoints on the control system. This makes the process control problem relatively easy, namely that of tracking prespecified trajectories. However, this approach leaves no freedom for economic re-optimization of the steady states and the transitions in case of persistent disturbances, which may lead to severe sub-optimality.

As a compromise between these choices, we propose that **minimum production as well as maximum raw material consumption levels be imposed as constraints at discrete time instances**]*. By this choice of the interconnection the sequence of *grades* as well as bounds on the production levels are forced onto the process control system while leaving the control system sufficient amount of freedom in determining the actual controls. The general enforcement of the scheduling constraints for the k-th production interval can be stated mathematically as follows.

$$\int_{t^k}^{t^k+\tau} Y_e(z)dt \geq \sum_g \sum_h \sum_m \bar{T}_k^{g,h,m} TY_e^{g,h,m}, \tag{6.1}$$

$$\int_{t^k}^{t^k+\tau} C_r(z)dt \leq \sum_g \sum_h \sum_m \bar{T}_k^{g,h,m} TC_r^{g,h,m}, \tag{6.2}$$

where $\bar{T}_k^{g,h,m}$ are the optimal transition variables and t^k denotes the start of the $k-th$ production interval. The reader should note that this specific choice of enforcing the scheduling constraint is by no means the "best" in general. Specific cases may require a different approach, for example for computational reasons.

6.2.2 Economic optimization

Economic optimization was mentioned earlier in relation to the task selection for the scheduling problem formulation (5.2). It was discussed that the effect of different market situations on the desired operation of the plant should be reflected in the process database. Further, we proposed that this can be realized by computing the optimal operating conditions/transitions for a few distinct and preferably extreme cases. In case of high-fidelity models and in the absence of disturbances, these *off-line* determined operating conditions will be rather adequate for *on-line* use as well. However, in the presence of disturbances and in case the market conditions deviate from the predicted values, large benefits can be gained from *on-line* optimization.

It is a fundamental question whether the optimization of an *economic* objective alone can yield satisfactory process behavior. We believe that the theoretical answer to the previous question is yes, and the corresponding approach consists of translating all aspects of the plant behavior (amongst which safety, stability and reliability, the primary goals underlying the current process control systems) into economics. This approach is extremely rigorous and probably practically infeasible in most cases. A more practical formulation of the previous question is hence: "what aspects of the process behavior need to be incorporated in the economic objective in order to guarantee satisfactory behavior?". This question is not necessarily easier to answer, however we may get a feel for the answer by elaborating on it a bit further. The first part of the answer consists of a thorough investigation of all the financial aspects of the operation of the plant. For example, we need to consider the plant's life span, production times, maintenance costs, costs of repairs and replacements and so on. The second part of the answer forces us to investigate and model *quantitatively* the most significant dependencies of these costs and revenues on the process variables. For example, the utilization of a valve needs to be translated into the expected time and costs of inspection, repair or replacement.

It is clear that a lot of stochastic factors are involved in such a modeling exercise, which makes the definition of the objective and hence the corresponding decision making problem extremely difficult. Our pragmatic approach to circumvent these problems is to **ignore all economic aspects that cannot *directly* be related to material or utility flows in the definition of the economic objective**]*. Their impact on the long-term economics is captured by translating them into more manageable control-type objectives and constraints which have no direct economical interpretation. Although this approach leaves us with some pragmatic choices to be made in the definition of the eventual control problem and in the evaluation of the performance, we deem it the most practical and we will hence adopt it in our research. Possible ways to enforce the control requirements shall be treated next.

6.2.3 Control requirements

The primary control requirements are safety, reliability and stability of the process. Safety leads to the introduction of bounds on critical process variables such as temperatures and pressures which should not be exceeded. Reliability is a somewhat more vague notion and it is one amongst many other requirements that cannot so easily be translated in a set of constraints or objectives.

Fortunately, in most practical applications plant safety is (from the control perspective) primarily handled by the basic control layer and the associated safety system. The basic control system has several attractive features, the most important one being its *simplicity*. It is because of this limited complexity that the implementation of the basic control system can be made very robust. Critical functions can be implemented redundantly at limited cost and safety and failure analysis can be done relatively easy. Mainly for these reasons **we promote and will assume in the remainder of this thesis the availability of a basic control layer**]*.

Despite the presence of a basic control system, additional control requirements, for example 'smooth' behavior of the controls, may exist in relation to the advanced control implementation. Instead of giving a complete overview of actual control requirements we will outline briefly how these can be incorporated in an optimization setting. We distinguish three different implementations of the control requirements

Minimization of a control objective. This is the most straightforward way of enforcing certain control requirements. A typical control objective is the weighted 2-norm, for example used in Linear Quadratic Control or MPC. Quadratic weights are utterly suitable to enforce variance conditions, with an obvious application in quality control. In combination with the economic objective the institution of a control objective function leads to a multi- or mixed-objective optimization problem.

Process constraints. Some control requirements may be enforced through the introduction of additional constraints, for example the limitation of the rate of change of certain process variables.

Parametrization of controls [1]. It may seem less obvious how we can enforce

[1] Mathematically, control parametrization can also be included in the category of process

control requirements through a parametrization of the controls. However, note that the parametrization of the controls limits the set of possible control signals; choosing the right parametrization obviously makes it possible to exclude undesirable input patterns.

In the remainder, we will assume that the control requirements are incorporated via either one of the mechanisms described above.

6.2.4 Disturbances and plant parameter variations

The operation of most processing plants is subject to external disturbances. Examples of such are ambient temperature, pressure variations in feed and production pipes, variations in feed and utility quality. Mechanisms happening internal to the process can also be interpreted as having a disturbing effect on the process operation. Examples are heat exchanger fouling and catalyst deactivation. Modern control theory distinguishes sharply between disturbances and parameter variation (or parametric uncertainty), consider for example the generalized plant framework for linear models with uncertainty or linear parameter varying (LPV) systems [97]. In relation to process control systems this distinction seems somewhat artificial. Parameter variations can be modeled as disturbances and vice versa, depending primarily on the level of detail in the process description. Consider for example fouling of a heat exchanger. A popular approach to account for this is to consider the UA-factor (the product of the heat transfer coefficient and the heat-passing surface) to be an unmeasurable, time-varying parameter. Alternatively, we can assume that an external disturbance acts on the UA-factor. Even a third option exists: to model the fouling mechanistically. To avoid confusion, we will in the remainder make no distinction between parameter changes and disturbances. Whenever we speak of disturbances the reader may just as well interpret those as being parameter changes.

A more relevant distinction is between measurable versus unmeasurable disturbances. The characteristics of measurable disturbances can be derived directly from the measurements. The presence of unmeasured disturbances needs to be *estimated* on the basis of measurements of the process variables. We stress that for both types of disturbances the characterization by means of *disturbance models* is imperative: good controllers are distinguished from poor ones by their quality to anticipate on future changes; whether or not this can be done succesfully depends amongst others on the possibility to predict the behavior of the disturbances. One may doubt the meaningfulness of disturbance modeling, especially for stochastic disturbances but then note that even the determination of a mean and a covariance can be a valuable characterization of the disturbance.

constraints.

Another distinction is between fast, stochastic disturbances and slow persistent disturbances. The first type of disturbance will cause mainly fast fluctuations of the process variables with no direct economical interpretation, the latter will have a persistent effect on mass and energy flows and thus directly on the added value. Both types of disturbances are looked upon from different angles when it comes to the development of control strategies as will become clear from the next section.

6.3 Exploration of possible approaches

Summarizing the previous section, the ingredients of the process control and optimization setting under consideration are the following: large scale systems, nonlinear dynamics, economic performance objectives, operating constraints, disturbances. At present, there is no 'systems and control' theory for dealing with all these aspects simultaneously. For smaller scale nonlinear control problems the stabilization has been studied extensively, leading to several constructive nonlinear control strategies such as feedback linearization, and passivity designs, see e.g. [75]. However, for these methods performance analysis and synthesis is often lacking, as are disturbance and constraint handling. Amongst the approaches that enable to take constraints into account, MPC strategies (or receding horizon control strategies in general) outnumber alternative approaches by far. Although we know of no systematic approach to analyzing the closed loop performance of MPC systems in the presence of disturbances, the concept of receding horizon control has many nice, intuitive properties which make it well suitable as a basic framework for the control strategies that we will develop. The next sections will discuss control and optimization approaches for different disturbance scenarios. The discussion is inspired by the conceptual contribution to the design of process optimization strategies by [31].

6.3.1 Disturbance-free case

If there weren't any disturbances nor uncertainty in the market prices and if the plant model were to be perfect, then an open loop control would suffice. A good candidate for this open loop control could be determined by solving a finite horizon optimal control problem with an economic objective (5.15) and subject to the process dynamics (5.1,5.3) the process constraints (5.4) and the scheduling constraints (6.1) and (6.2).

For large DAE's this optimal control problem is very hard to solve, let alone solve it sufficiently fast. An approximation of the problem can be obtained by splitting up the horizon in quasi-static tasks and transition tasks and optimizing the individual tasks successively. Observe that the very same decomposition is used in the parametrization of the plant behavior for the scheduling formulation. The solution of this approximate problem proceeds in several steps. First, the optimal steady state operating conditions in all quasi-static production time spans are computed using (5.9) and subject to the additional constraints (6.1,6.2). The resulting static operating conditions are denoted the *nominal static conditions*.

Next, we solve a sequence of nominal transition optimization problems (5.10). The corresponding input and state trajectories are denoted the *nominal transition trajectories*. Strategies for solving these specific dynamic optimization problems are treated in Chapter 7. The resulting sub-optimal control strategy is obtained by adjoining the optimal controls in all time spans and is denoted $\mathbf{u}^R$ in the remainder. The corresponding state trajectory is denoted $\mathbf{x}^R$ remainder.

6.3.2 Dealing with disturbances and parameter variations

Two classes of disturbances were identified: fast, stochastic disturbances and slow drift-like disturbances. Any practical operating strategy must be able to deal with both types of disturbances. The most elementary way of dealing with disturbances is through feedback. Feedback can reduce the sensitivity of essential process variables with respect to disturbances. The traditional control problem seeks to *eliminate* the effect of disturbances, however this is not the appropriate view on disturbances from the perspective of process optimization. Note that even if we *can* suppress the effect of a disturbance on a certain process variable, this can be done only by tolerating a deviation on one or more other process variables (in most cases the manipulated variables). The challenge is to allocate the effect of disturbances such that the overall economic performance is less affected. This motivates the use of *real-time* economic optimization as a basic feedback strategy.

In linear systems and control theory the common approach to taking into account the effect of disturbances and parameter variations is by modeling them. A generic modeling framework for linear plants with parameter uncertainty and disturbances is the standard plant configuration [97] which allows for external influences, performance channels and model uncertainty to be described in a systematic manner. The standard plant configuration may just as well be used as a modeling framework for nonlinear plants, the main difference being that a systematic analysis of system properties and synthesis of optimal controllers is lacking for the nonlinear case. In fact, even the nominal stability and performance analysis is not straightforward. This makes dealing with disturbances in our setting very awkward and motivates us to resort to pragmatic solutions.

The pragmatic solution that we propose is based on [41] and builds on the following elements :]*

- **a linear modeling framework for disturbances and parameter variations,**
- **on-line, 'nonlinear model'-based estimation of unmeasured disturbances and parameters,**
- **a** *deterministic* **'nonlinear model'-based receding horizon control strategy.**

Observe that the approach relies on an unjustly supposed *separation principle* for nonlinear systems. "Unjustly" because no equivalent of the well-known separation principle for linear systems exists for nonlinear systems. Nevertheless, we think it is justifiable and even recommendable to develop nonlinear process control strategies based on insights from linear systems and control theory.

The receding horizon control strategy consists of the repeated solution of an open loop optimal control strategy. Only the first moves are implemented after which the computations are repeated. The computations should be done reasonably fast to enable to control even the fast dynamics. This makes the suboptimal open loop control solution outlined in the beginning of this section no candidate for receding horizon implementation. Approximations to this ultimate optimization strategy need to be made, depending on the requirements that specific disturbance scenarios entail. We distinguish three special cases which we believe capture many situations that arise in practice. The following description concerns mainly the *structural* concepts, the mathematical formulations will follow in subsequent sections.

Scenario 1: Only fast disturbances

The first special scenario that we consider is the scenario where there are no persistent disturbances and only fast, zero-mean, well-damped disturbances. For this class of disturbances, the states of the disturbance models will converge to zero fast. As a consequence, would we implement the nominal optimization in a receding horizon fashion, then successive solutions are expected to lay very close to the nominal optimal controls for large prediction times. In other words, no significant persistent effect of the disturbances on the longer term optimal control solution is expected. An appropriate approximation of the receding horizon optimal control solution may hence be achieved through a re-optimization of *only the leading part* of the nominal control trajectories while retaining the tail of the nominal optimal control. The approximate control problem remains one of optimizing the behavior of the plant only over a short horizon with obvious computational advantages. In the remainder the approximate control problem shall be identified as the Short Horizon Optimal Problem (SHOP). For consistency of the SHOP with the longer term objectives, the end-point of the SHOP

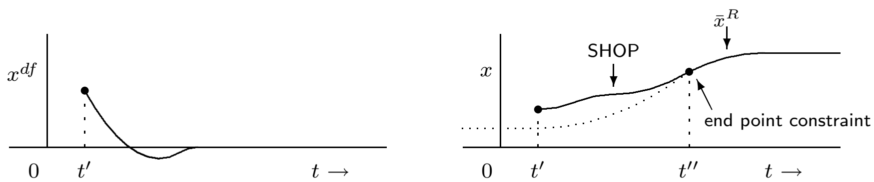


Figure 6.1: The prediction of a fast disturbance on the basis of its state estimate (left) and the modification of the open loop state trajectories through the corresponding solution of the SHOP (right).

is forced to lay on or in the near vicinity of the nominal reference trajectories. If the length of the horizon of the SHOP is chosen too short, obviously infeasibility of this end-point constraint will result. The length of the horizon should hence be chosen such that the end-point constraint is feasible or at least approximately feasible.

This approach is presented schematically in Figure 6.1. In the left picture, the prediction of a typical fast disturbance is plotted, based on the estimate of the state (x^{df}) of the corresponding disturbance model. In the right picture, the dotted line indicates the nominal optimal state trajectory $\bar{x}^R$. The SHOP aims to drive the state back to $\bar{x}^R$ at time t'' with minimum costs. This approach shall be further elaborated on in Section 6.4.

Scenario 2: fast disturbances and slow drifts, no grade changes

The next scenario we consider is a combination of fast, stochastic disturbances and persistent disturbances for quasi static operation only, i.e. in the absence of grade changes. The reason why this is an interesting scenario is that it represents the application area of current Real-Time optimization strategies [1, 47, 4].

In the absence of grade changes and (significant) load changes the nominal optimal operating conditions are given by the optimal solution of a steady state economic optimization problem. Persistent disturbances, such as for example heat exchanger fouling, catalyst deactivation or feedstock impurities will have a significant effect on the optimal operating strategy. We propose that the tail of the modified optimal strategy can be approximated sufficiently well by *steady state* operation. The optimal steady state conditions are computed via a Static Optimization Problem (SOP) based on an estimate of the steady state effect of the persistent disturbances and/or parameter variations. This steady state optimum is then used as an end-point condition for a SHOP. Observe that the long-term effects of the persistent disturbances are handled by the static re-optimization whereas the short term effects as well as the effects of fast, stochastic disturbances are dealt with by a dynamic re-optimization. The

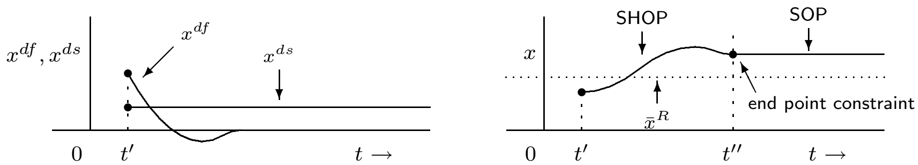


Figure 6.2: The prediction of fast and slow disturbances on the basis of the state estimates (left) and the modification of the open loop state trajectories through the corresponding solution of the SOP and the SHOP (right).

proposed strategy is presented schematically in Figure 6.2. In the left picture, the prediction of a fast (x^{df}) and a slow (x^{ds}) disturbance is plotted. The corresponding effect of these on the computation of the 'optimal' strategy is plotted in the right figure. This figure shows, with the dotted straight line, the nominal optimum steady state value for x. The solid straight line shows the new, static optimum which is computed from the SOP. The SHOP is defined as to drive the state to the new steady state optimum at time t'' and with minimum costs.

Comparison with traditional RTPO The proposed strategy has similarities with the traditional steady state RTPO strategy, but there are some fundamental differences. First, in traditional RTPO the estimation of parameters and persistent disturbances is done only after a steady state detection has been successfully performed. In practice, true steady states hardly occur which often makes a relaxation of the steady state detection criteria necessary. In our setting, the estimates of parameters and persistent disturbances are updated continuously on the basis of a *dynamic* estimation problem. A second difference is in the allocation of tasks to the steady state optimization and the dynamic optimization. In the traditional approach, the RTPO delivers setpoints for the dynamic optimization (MPC). Economics are only dealt with at the level of RTPO, MPC has control-type of objectives, typically penalizing quadratic deviations of some outputs and inputs from their 'ideal' values. In our approach, the static optimization is executed to compute the tail of the new open loop controls. The dynamic optimization computes the leading part, using an economic objective possibly extended by a control objective. Static optimization and dynamic optimization can hence be seen to take care of different parts (in *time*) of an underlying *monolithic* optimization problem.

Scenario 3: Fast and persistent disturbances and grade changes

The last scenario we describe is the one that is most interesting in relation to the supply-chain oriented operation that we foresee. It concerns the combination of grade changes with persistent and fast disturbances.

The effect of the persistent disturbances on the optimal control profiles may be significant and must hence be accounted for. We can still make use of the static re-optimization to compute the tail of the new solution. The leading part of the solution would then be computed via a dynamic optimization. However, due to the presence of grade changes, this leading part can be very long making the corresponding dynamic optimization problem computationally demanding. The computational complexity of the dynamic optimization problem increases even further due to the non-smoothness introduced by the grade transitions (see Section 5.2.3). This motivates the decomposition of the dynamic optimization problem into a SHOP and a Long Horizon Optimization Problem (LHOP). The SOP and the LHOP are computed less frequently than the SHOP and take the long-term effects of the persistent disturbances into account. The SHOP uses a point on the LHOP profile as an end-point constraint and deals with the fast disturbances. The proposed strategy is schematized in Figure 6.3. Like in scenario 2, the SOP, LHOP and SHOP take care of different sections (in time) of an underlying infinite horizon optimization problem. A consistent coupling of these sections is achieved through the institution of end point constraints.

Slow dynamic disturbances. Another situation for which the very same strategy can be used arises when we consider slow, predictable, persistent dynamic disturbances such as drifts or poorly damped periodic disturbances. If modelable, then one would like to take the presence of these disturbances into account in the dynamic optimization. This will generally lead to the necessity of considering very long prediction horizons. A practical solution is the decomposition of the dynamic optimization into a LHOP and a SHOP as described above. Although the remainder of this thesis will not consider these types of disturbances, it is worthwhile to keep in mind the more general applicability of the real-time dynamic optimization method that will be presented in Section 6.6.

6.4 Scenario 1: off-line trajectory optimization

This section discusses the control configuration for scenario 1, i.e. the scenario where only fast, zero mean disturbances occur. In this scenario, nominal reference steady state operating conditions and trajectories are provided through off-line optimization. Disturbances are dealt with by a receding SHOP. This control configuration is depicted in Figure 6.4.

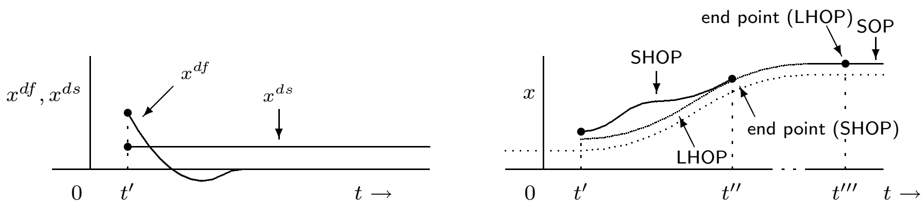


Figure 6.3: The prediction of fast and slow disturbances on the basis of the state estimates (left) and the modification of the open loop state trajectories through the corresponding solution of the SOP, the LHOP and the SOP (right).

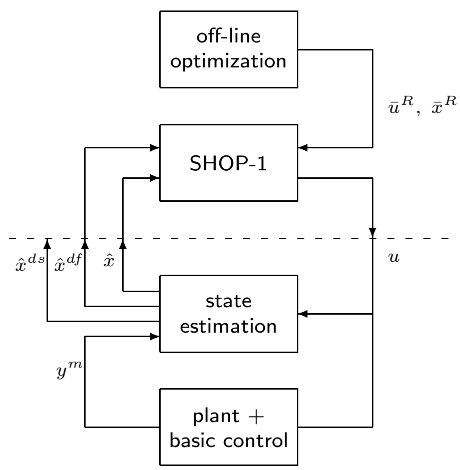


Figure 6.4: Control configuration for the scenario of grade changes with fast disturbances.

6.4.1 Description of the control approach

Off-line optimization

The off-line static optimization problem for a particular grade g is obtained by extending (5.9) by a set of constraints on the production levels in accordance with the schedule. For simplicity, we leave out the possibility of having multiple market scenarios.

$$\min_{x,u}\left\{-L(z)\middle|\exists y,z\text{ s.t. }\begin{array}{lll}\text{plant description} & \text{process constraints} & \text{scheduling constraints}\\ 0=f(x,u,y) & h(z)<0 & \tau Y_e(z)\geq TY_e^{g,g}\\ 0=g(x,u,y) & \text{grade constraints} & \tau C_r(z)\leq TC_r^{g,g}\\ z=C_xx+C_uu & g_g(z)<0 & \end{array}\right\}, \tag{6.3}$$

where $Y_e(z)$ is given by (5.13). The optimal solution of (6.3) for grade g is denoted $(\bar{x}^g,\bar{u}^g)$.

The dynamic optimization problem for a grade change $g\rightarrow h$ is obtained by extending (5.10) by the appropriate scheduling constraints. The horizon length is chosen equal to the length of a production interval, i.e. τ (in case only single-interval transitions are considered, see Section 5.3.2).

$$\min_{u\in\mathcal{U}}\left\{\int_0^\tau L^d(z)dt\middle|\exists x,y,z,\text{ s.t. }\begin{array}{ll}\text{plant} & \text{init./end cond.}\\ \dot{x}=f(x,u,y) & x(0)=\bar{x}^g, x(\tau)=\bar{x}^h\\ 0=g(x,u,y) & \text{path constraints}\\ z=C_xx+C_uu & h(z)<0\end{array}\right. \tag{6.4}$$

$$\left.\begin{array}{l}\text{scheduling constraints}\\ \int_0^\tau Y_e(z)dt\geq TY_e^{g,h,m},\quad \int_0^\tau C_r(z)dt\leq TC_r^{g,h,m}\end{array}\right\},$$

where $\mathcal{U}_S$ is the set of trajectories over which the optimization is performed. We will in the remainder limit ourselves to considering **uniformly discretized, piece wise constant signals**]$^\bigstar$. How this problem can be solved at reasonable computation costs is shown in the next chapter. The optimal trajectories for the grade change $g\rightarrow h$ are denoted $(\bar{x}^{g,h},\bar{u}^{g,h})$. The trajectories of the states, the inputs and the performance variables describing the nominal behavior of the plant over the entire set of production intervals is obtained by adjoining the quasi-static trajectories and the transition trajectories in the correct order and are denoted $(\bar{x}^R,\bar{u}^R,\bar{z}^R)$.

Disturbance modeling

The SHOP is based on a process model that captures the effect of disturbances on the plant. To this end, we extend the plant model (5.1,5.3) to include the effect of the disturbances:

$$\begin{aligned}\dot{x} &= f^f(x, u, y, x^{df}),\\ 0 &= g^f(x, u, y, x^{df}).\end{aligned} \tag{6.5}$$

x^{df} are the states of the fast disturbance model. The fast disturbances are modeled in a linear dynamics stochastic framework:

$$\dot{x}^{df} = A^{df} x^{df} + B^{df} w, \tag{6.6}$$

where $w(t)$ is a Gaussian random variable with covariance R^w. All eigenvalues of A^{df} are in the left half of the complex plane.

SHOP formulation

The definition of the SHOP builds on the formulation of the economic grade change optimization problem. Recall that the objective function used in the reference optimization problem (6.4) leads to a discontinuous optimization because of the grade-dependent production flows. To avoid this in the SHOP it seems reasonable to fix the grade variables G^g (see (5.14)) to their nominal values, denoted $\bar{G}^{g,R}$ in the remainder. Note that this fixes the time instances at which the predicted product quality switches from one grade to another. Although this introduces some conservatism in the formulation (the nominal switching times need not be the optimal ones in the presence of disturbances) a significant decrease of computational complexity is achieved. The corresponding SHOP at time t' is defined as follows:

SHOP-1

$$\min_{u \in \mathcal{U}_S} \left\{ V^S(z) \,\middle|\, \exists x, y, z \text{ s.t. } \begin{array}{lll} \text{plant} & \text{disturbances} & \text{init./end cond.} \\ \dot{x} = f^f(x, u, y, x^{df}) & \dot{x}^{df} = A^{df} x^{df} & x(0) = \hat{x}(t') \\ 0 = g^f(x, u, y, x^{df}) & \text{path constraints} & x(H^S) = \bar{x}^R(t'') \\ z = C_x x + C_u u & h(z) < 0 & x^{df}(0) = \hat{x}^{df}(t') \end{array} \right.$$

$$\left. \begin{array}{ll} \text{sched. constr.} & \\ \int_0^{H^S} Y_e(z)dt \geq \int_{t'}^{t''} Y_e(\bar{z}^R)dt & g_g(z) < \epsilon_g,\ \forall g \text{ s.t. } \bar{G}^{g,R} = 1 \\ \int_0^{H^S} C_r(z)dt \leq \int_{t'}^{t''} C_r(\bar{z}^R)dt & Y_e(z) = \sum_g \bar{G}^{g,R} M_g^e F(z) \end{array} \right\}, \tag{6.7}$$

with H^S the horizon length of the SHOP and with $t'' = t' + H^S$. V^S is the economic integral objective, possibly extended with control-type penalties. ϵ_g is a small positive number, which we introduce to relax the grade quality constraints. $\hat{x}(t')$ is an estimate of the process state, $\hat{x}^{df}(t')$ is an estimate of the disturbance model state.

In order to comply with the scheduling constraints, production and consumption are required to be larger, respectively smaller than the levels computed for the nominal reference trajectories.

Relaxation of the end-point constraint

The end-point constraint ensures the consistent coupling of the SHOP solution to the nominal reference trajectory. Nevertheless, it may be hard to satisfy. First, due to the common presence of input saturations and an often low-dimensional parametrization of the controls, the end-point constraint need not be feasible. The *finite-horizon controllability* of constrained, nonlinear systems can only be assessed after enormous computations, for example by gridding the initial and end-point state space and a solution of a (non-convex!) feasibility problem for each grid-point.

Unfortunately, even if the end-point constraint is feasible in theory, many iterations may be required to satisfy it within the desired tolerance. Several solutions have been proposed for dealing with this problem in relation to the synthesis of stabilizing NMPC laws. The prevailing ideas are summarized in [62]. It must be noted however that most of the research in this field considers the regulatory control problem with quadratic weights on inputs and outputs only.

One suggestion [58] is to substitute the end point constraint by an inequality constraint. The inequality constraint enforces that the state is driven into a neighborhood of the origin where the nonlinear system is stabilized by a linear control law. The scheme is referred to as a "dual-mode" control scheme because the controller switches from an open loop control to a linear feedback law. Though theoretically nice, this approach is of no use in our setting. First, the end point that we would like to enforce is no equilibrium in general, so that the computation of a stabilizing linear control law and an associated region of attraction is not possible. Further, the presence of disturbances makes it very unlikely that the states will actually end up into the specified neighborhood of the origin. Finally, because this dual-mode scheme suggests that from a certain time on the plant is controlled using a linear control law, performance losses will be significant.

Other approaches consist of an extension of the objective function by a terminal penalty on the final state in combination with an end point inequality constraint, see e.g. [15]. The main idea is to choose the penalty term so as to enforce monotonicity of the objective function after which, for nominal stability, it suffices to show that the objective function is a Lyapunov function for the system. Although the resulting stability proof appears of academic interest only (only the nominal case is considered, the presence of disturbances and plant-model mismatch as well as incomplete information on the states are ignored), the idea of substituting the end point equality constraint by a terminal penalty is attractive for various reasons.

First, the institution of a terminal penalty enables to enforce the end point equality constraint in a manner that is computationally appealing. Observe the similarity with penalty methods for equality-constrained nonlinear optimization (we refer to Section F.2 of the Appendix for a brief introduction). Second, infeasibility of the end-point constraint will not imply infeasibility of the SHOP, so that costly computation time will not be wasted on an infeasible optimization problem (observe that infeasibility cannot be concluded in advance). The penalty term will make sure that the final state will at least be in the vicinity of the desired end point.

Linear approximation

Although the optimization problem (6.7) is a reduced-complexity approximation of the off-line reference optimization it may still be too involved to solve it sufficiently fast for real-time implementation (computation time should generally not exceed several minutes). A significant further reduction of the computational complexity can be achieved if the optimization is done subject to *linearized* dynamics. Along the nominal trajectory, a linear description of the dynamics may be sufficiently accurate for the computation of the controls. Of course, this approach is justified only if the solutions of the receding horizon problems remain close to the nominal trajectory. However, note that this will indeed be the case if we assume the mean value of the disturbance to be zero. A straightforward implementation of the linearization approach leads to the substitution of the nonlinear dynamics in (6.7) by

$$\begin{aligned} x &= \bar{x}^R + \Delta x, \\ u &= \bar{u}^R + \Delta u, \\ \Delta \dot{x} &= A(t)\Delta x + B(t)\Delta u, \end{aligned} \tag{6.8}$$

where $A(t)$ and $B(t)$ are computed as follows

$$A(t) = \frac{\partial f}{\partial x} - \frac{\partial f}{\partial y}\left[\frac{\partial g}{\partial y}\right]^{-1}\frac{\partial g}{\partial x}, \tag{6.9}$$

$$B(t) = \frac{\partial f}{\partial u} - \frac{\partial f}{\partial y}\left[\frac{\partial g}{\partial y}\right]^{-1}\frac{\partial g}{\partial u}. \tag{6.10}$$

All Jacobians at time t are evaluated in $(\bar{x}^R(t), \bar{u}^R(t), \bar{y}^R(t))$. If the objective function is approximated using e.g. the trapezoid rule and the constraints are evaluated only at discrete samples, then it suffices to discretize the linearized dynamics to end up with a parametric optimization problem. The discrete

Linear Time Varying (LTV) dynamics are given by

$$\begin{aligned} x_i &= \bar{x}_i^R + \Delta x_i, \\ u_i &= \bar{u}_i^R + \Delta u_i, \\ \Delta x_{i+1} &= \Phi_i \Delta x_i + \Gamma_i \Delta u_i, \end{aligned} \tag{6.11}$$

where Φ_i is the state transition matrix and Γ_i is the input-to-state matrix. Several ways of computing Φ_i and Γ_i shall be treated in Section E.4 of the appendix in which implementation details are discussed. If $V^S(z)$ is chosen to be the economic objective and the $F(z)$ is linear, then the resulting linearized and discretized optimization problem reduces to a Linear Programme (LP). In case of an extension with a quadratic control-type of objective a Quadratic Programme (QP) results. LP's and ((semi-) positive definite) QP's are easily solved using proven and robust convex programming algorithms [60].

Regularization To analyze consistency of the SHOP solutions with the off-line trajectories in the nominal case, we consider the solution of the SHOP at a time t' in the k-th production interval such that $t^k < t'$, and $t'' < t^k + \tau$. Let the k-th production interval contain a grade transition. Further, we assume that the SHOP and the off-line trajectory are solved using the same parametrization of the controls and that $x(0) = \bar{x}^R(t')$. Then by the principle of optimality, the solution of the SHOP (6.7) should coincide with the corresponding section of the solution of the off-line optimization problem (6.4), i.e. $\bar{u}^{shop}(t) = \bar{u}^R(t' + t),\ t = [0, H^S]$. However, consistency of the solutions may be lost due to linearization. To analyze this, we have to check whether the optimality conditions for the nonlinear model-based SHOP coincide with those for the linear-model based SHOP, for the minimizing argument of problem (6.7). For compactness of notation, we study the scalar case. We further omit the path constraints from the consideration.

Let the original optimization problem be represented by the minimization of a function $V_u(u) = V(z(u))$ with $V(z) = lz + qz^2$ a linear quadratic cost function with $q \geq 0$. We assume the existence of a local minimizer $\bar{u}^R$ for the nominal problem. The corresponding optimal performance variable is denoted $\bar{z}^R$. In order for $(\bar{u}^R, \bar{z}^R)$ to be a local minimizer we know that the following first and second order optimality conditions should hold

$$\frac{dV_u}{du} = \frac{dV}{dz}\frac{dz}{du} = (l + 2q\bar{z}^R)\frac{dz}{du} = 0; \tag{6.12}$$

$$\frac{d^2V_u}{du^2} = \frac{d^2V}{dz^2}\left(\frac{dz}{du}\right)^2 + \frac{dV}{dz}\frac{d^2z}{dz^2} = q\left(\frac{dz}{du}\right)^2 + (l + 2q)\frac{d^2z}{du^2} > 0, \tag{6.13}$$

where all Jacobians are derived in $(\bar{u}^R, \bar{z}^R)$. With the linearized dynamics given by $\hat{z}(u) = \bar{z}^R + \frac{dz}{du}\Delta u$, the objective function for the linearized-dynamics problem becomes:

$$\hat{V}_u(u) = V(\hat{z}(u)) = l(\bar{z}^R + \frac{dz}{du}\Delta u) + q(\bar{z}^R + \frac{dz}{du}\Delta u)^2, \tag{6.14}$$

The first order optimality conditions of the approximate problem obviously coincide with those of the original problem. However, the Hessian of the linearized-dynamics problem is different:

$$\frac{d^2\hat{V}_u}{du^2} = q\left(\frac{dz}{du}\right)^2. \tag{6.15}$$

The term that relates to the second order derivative of the dynamics is missing. If q is zero, the Hessian of the linearized dynamics case will be zero so that $\bar{u}^R$ is *not* a unique minimizer of the approximation of the nominal problem. Instead, multiple solutions exist (in this case even infinitely many).

To circumvent this, we propose to regularize the approximate optimization problem. The regularization implies the addition of an extra term to the objective function of the approximate problem that forces the solution to be equal to the solution of the off-line nonlinear-dynamics problem in the nominal case. An obvious candidate for this regularization term is $(z - \bar{z}^R)^T Q_R (z - \bar{z}^R)$ with $Q_R > 0$, since its contribution vanishes in the optimum $\bar{z}^R$.

Another reason why regularization is often applied to optimization problems is robustness. Note that the inclusion of a quadratic weighting on the deviation from the nominally optimal trajectories forces the SHOP solutions to be close to the nominal trajectories. This excludes large excursions of the input and state trajectories from the solution set which seems adequate since the linear dynamics description will only be valid in the neighborhood of the trajectories along which it has been derived.

Handling infeasibilities

The SHOP problem includes a set of path constraints that correspond to the different grade regions that are traversed. In the presence of process disturbances, these path constraints are likely to become infeasible, especially for small values of ϵ_g. A typical way of dealing with infeasibility is constraint relaxation. In case the SHOP returns no answer due to infeasibility, one or more grade constraints are relaxed to ensure that a feasible solution is obtained. A suitable relaxation scheme may be to start to relax the constraints at those instances that are closest to the current time. The relaxation comprises the modification of the grade constraint as follows

$$g_g(z) < \epsilon_g + r, \quad r > 0.$$

The objective is extended to include a penalty on the relaxation parameter: $V^S + \alpha_r r$ for a suitable weighting α_r.

State estimation

The presented strategy assumes that the process states as well as the states of the disturbance model are estimated on-line. Several techniques exist for the estimation of states in nonlinear process models. The most popular approach is the application of an Extended Kalman Filter (EKF) (for an excellent description see [43]). Another well known approach is *receding horizon estimation*, see e.g. [73, 69, 83]. Although the design of state estimators has been studied rather intensively in relation to this research, see e.g. [86], we choose not discuss the issue of state estimation in detail in this thesis. In our examples we will make use of hand-tuned EKF's without further mention. It should be noted however that in practical application of the control technology described in this chapter the design and implementation of a state estimator will typically be the first, very difficult task. A task which will succeed only if a model of reasonable accuracy is available.

6.4.2 Application to case II: binary distillation

As an example of the implementation of the strategy presented in this section we consider the control and optimization of a binary distillation column. The column is represented schematically in Figure 6.5. The feed, containing two different components enters at the middle tray. The lighter component will accumulate in the top of the column whereas the heavier component will tend towards the bottom. The vapor flow leaving the column from the top is condensed and partially fed back into the column. Part of the liquid flow leaving the column from the bottom is vaporized in the reboiler and fed back into the column.

Model

The modeling assumptions are the following

- constant molar holdup,
- theoretical plates,
- constant relative volatility,
- heat balance can be ignored, and
- perfect control of level in reboiler and reflux drum.

We consider a total number of 20 trays with the feed entering the 10^{th} tray. Then, under the above-mentioned assumptions we can write down the following

performance channels		
1	(c^1)	top purity
2	(c^{20})	bottom impurity
3	(D)	distillate flow
4	(W)	bottom outflow
5	(R_r)	reflux ratio
6	(J')	boil-up rate
inputs		
1	(R_r)	reflux ratio
2	(J')	boil-up rate
outputs		
1	$y^{m,1}$	top purity
2	$y^{m,2}$	bottom impurity
3	$y^{m,3}$	distillate flow
4	$y^{m,4}$	bottom outflow
disturbances		
1	$(x^{df,1})$	feed comp. fluctuation
2...5	$(x^{df,2}, \ldots, x^{df,5})$	measurement noise on all sensors

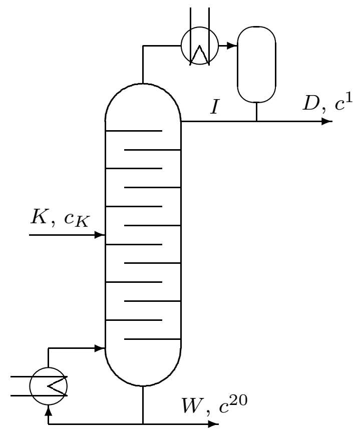


Figure 6.5: Schematic process flow sheet of the binary distillation column.

component balances [36].

$$O\frac{dc^i}{dt} = \begin{cases} I(c^{i-1} - c^i) + J(v^{i+1} - v^i), & i = 2, \ldots, 9, \\ Ic^{i-1} - I'c^i + J'v^{i+1} - Jv^i + K(c_K + x^{df,1}), & i = 10, \\ I'(c^{i-1} - c^i) + J'(v^{i+1} - v^i), & i = 11, \ldots, 19, \end{cases}$$

where the mole fractions of component 1 in the liquid and the vapor phase are given by respectively c and v. The liquid and vapor flow above and below the feed tray are given by respectively (I, J) and (I', J'). K is the feed flow and c_K the feed flow composition. O is the molar holdup at the trays. The liquid and vapor flows above and below the feed tray are related as follows

$$\begin{aligned} I' &= I + q_K K, \\ J' &= J - (1 - q_K)K. \end{aligned}$$

The component balance for the reflux drum is modeled as follows

$$O_d \frac{dc^1}{dt} = Jv^2 - (I + D)c^1,$$

where the distillate flow and the reflux flow are given by respectively

$$D = \frac{1}{R_r + 1}J, \quad I = \frac{R_r}{R_r + 1}J,$$

with R_r the reflux ratio. The reboiler component balance is given by

$$O_R \frac{dc^{20}}{dt} = I'c^{19} - J'v^{20} - Wc^{20},$$

parameter	description	value
α_v	relative volatility	1.89
q_K	feed condition	1
O_d	Holdup in reflux drum	200 Kmol
O_R	Holdup in reboiler	400 Kmol
O	Holdup on plates	50 Kmol

Table 6.1: Process parameters for the binary distillation column.

where W is the bottom product flow given by

$$W = I' - J'.$$

At each tray the vapor-liquid equilibrium is computed as follows

$$v^i = \frac{\alpha_v c^i}{1 + (\alpha_v - 1)c^i}.$$

The feed composition disturbance is assumed to be generated by the following dynamic disturbance model

$$\dot{x}^{df,1} = -10x^{df,1} + w^{df,1}.$$

The measurement noise disturbances are given by $x^{df,i} = w^{df,i}$, $i = 2, \ldots, 5$. The measured outputs are modeled as follows

$$\begin{aligned} y^{m,1} &= c^1 + w^{df,2}, \\ y^{m,2} &= c^{20} + w^{df,3}, \\ y^{m,3} &= D + w^{df,4}, \\ y^{m,4} &= W + w^{df,5}. \end{aligned}$$

$w^{df,1} \ldots w^{df,5}$ are random sequences with covariances equal to respectively $\{0.5, 10^{-4}, 10^{-4}, 10^{-4}, 10^{-4}\}$. The parameters used in the simulations are given in Table 6.1. We assume that three different grades for the top product are specified and two different grades for the bottom product. The specifications on respectively the purity of the top product and the impurity of the bottom product are given in Table 6.2. We can distinguish a total of 6 production grades. The different production grades for the column are given in Table 6.3. The operation of the column is subject to process constraints. The constraints we used in this study are given in Table 6.4

Problem formulation

We consider the operation of the distillation column during the transition from grade 3 to grade 5 (see Table 6.3).The operation of the plant is scheduled in

top product			bottom product		
e	${x_l^g}^T$	${x_u^g}^T$	e	${x_l^g}^B$	${x_u^g}^B$
1	0.00	0.98	4	0.00	0.05
2	0.98	0.99	5	0.05	1.00
3	0.99	1.00	-	-	-

Table 6.2: Grade specifications for top and bottom product in binary distillation column.

g	constraints ($g_g(z)$)	
1	$0.00 < z^1 < 0.98$	$0.00 < z^2 < 0.05$
2	$0.00 < z^1 < 0.98$	$0.05 < z^2 < 1.00$
3	$0.98 < z^1 < 0.99$	$0.00 < z^2 < 0.05$
4	$0.98 < z^1 < 0.99$	$0.05 < z^2 < 1.00$
5	$0.99 < z^1 < 1.00$	$0.00 < z^2 < 0.05$
6	$0.99 < z^1 < 1.00$	$0.05 < z^2 < 1.00$

Table 6.3: The six production grades for the binary distillation column.

constraints		
0.97	$< z^1 <$	1
0	$< z^2 <$	0.2
100	$< z^3 <$	900
100	$< z^4 <$	900
1.4	$< z^5 <$	9
900	$< z^6 <$	4500

Table 6.4: Process constraints for the binary distillation column.

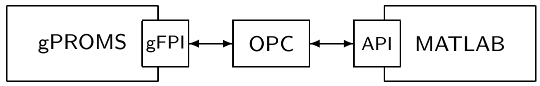


Figure 6.6: Simulation configuration with gPROMS, MATLAB and an OPC server connecting those.

production intervals of 6 hours. The sequence of tasks that we consider in this simulation is [3,3,5] such that the grade change is preceded by a quasi-static production interval corresponding to grade 3 and succeeded by a quasi-static production interval corresponding to grade 5. By off-line dynamic optimization (see Section 7.3), reference trajectories for inputs and states have been determined along which the linearized models used in the SHOP are derived. All grade variables are fixed to their optimal values, so that the economic objective becomes a LTV weighting on the performance variables. The grade constraints are slightly relaxed through a choice of $\epsilon_g = 0.002, \; g = 1, \ldots 6$. End point constraints on the production levels are included to make the on-line solution comply with the production schedule. We use the trapezoid rule to approximate the integral objective. The economic objective is extended with a penalty term corresponding to the end-point constraint as was motivated previously. Also, we include a quadratic weighting on the deviation of the inputs from the reference trajectories for regularization purposes. The SHOP problem hence becomes a QP. Details of the SHOP formulation are given in E.1

Software implementation

The software setup that is used in our simulations is shortly described here. There exists a variety of modeling and simulation packages for large chemical processes. AspenTech's Aspen Dynamic Modeler, and PSE's gPROMS are amongst the most popular ones. We used gPROMS for modeling and simulation of DAE systems. To facilitate the use of gPROMS models in control and optimization studies we developed a TCP-IP based communication link to the computational package MATLAB in which all control and optimization codes were programmed. The interface uses the *Foreign Process* facility from gPROMS as well as the *Application Program Interface* and the corresponding mex-functions from MATLAB. The TCP-IP based communication interface was in a later stage professionalized and robustified by IPCOS Technology (Boxtel, The Netherlands) and ISMC (Leuven, Belgium). In the final version of the communication software, data exchange between gPROMS and Matlab was managed by an OPC-server (OPC stands for "OLE for Process Control"). A schematic lay-out of the simulation setup is given in Figure 6.6.

Results

The closed loop simulation results of the system outputs are plotted in Figure 6.7. The dashed lines indicate the reference trajectories z^R. The thin lines represent the open loop simulations with only the nominal trajectory as control input. The thick lines are the simulation results with the SHOP-1. Apparently, this control configuration manages to maintain the performance variables close to the nominal trajectories. The scheduled production levels are met.

An interesting observation can be derived from the trajectories of the control variables in Figure 6.8. The closed loop controls hardly deviate from the nominal trajectories except at certain specific locations in time. The reason for this mild control action is that only *harmful* deviations of the states from their nominal values are responded to, where 'harmful' should be interpreted as either being undesirable for the process economics or as being likely to incur violation of process or grade constraints.

For example in the interval from 8 to 12 hours significant deviations of the states from the nominal trajectories can be observed whereas the control actions are almost similar to the nominal ones. Apparently the state deviations neither have an economic impact nor are likely to cause violation of relevant process or grade constraints so that the control actions remain limited. This behavior is typical for economics-based control and is rather different from the behavior that would be obtained if general quadratic penalties on deviations from setpoints were used.

6.5 Scenario 2: static re-optimization

Next we study the scenario where in addition to fast, zero-mean disturbances slow, persistent disturbances occur. For now, we neglect the presence of grade changes. This scenario represents the configuration that is typically being studied in most research on RTPO and it is therefore worthwhile to consider. It was suggested in Section 6.3 that the real-time control and optimization problem be decomposed into a *static* optimization problem (SOP) which computes the infinitely long tail of the solution and a short-horizon *dynamic* optimization (SHOP-2) which computes the leading part. This control strategy is represented schematically in Figure 6.9 and will be described in this section.

6.5.1 Description of the control approach

Disturbance modeling

First, to account for the presence of slow, persistent disturbances in the plant model, we consider in addition to the fast disturbance model, a random walk

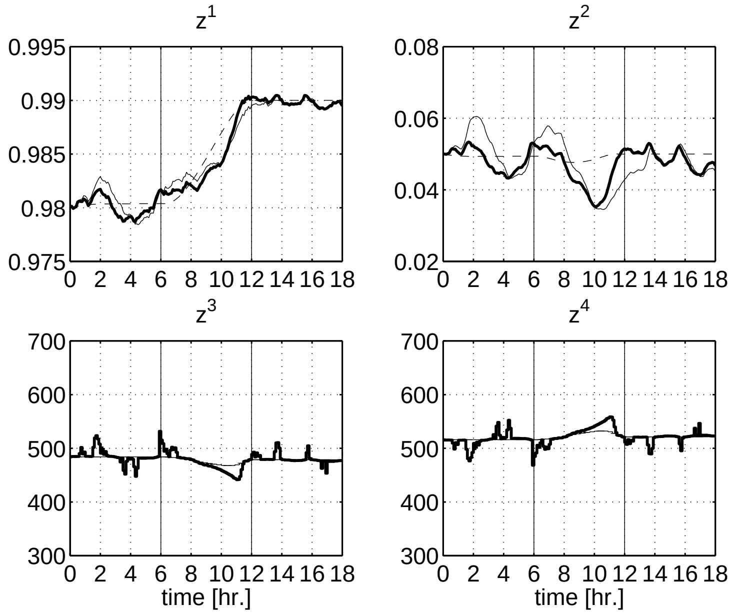


Figure 6.7: Top purity (z^1), bottom impurity (z^2), distillate flow (z^3), and bottom outflow (z^4), for a task sequence $[3, 3, 5]$ with fluctuations in the feed composition and SHOP-1 control (dashed line: nominal, thin lines: open loop, thick lines: closed loop).

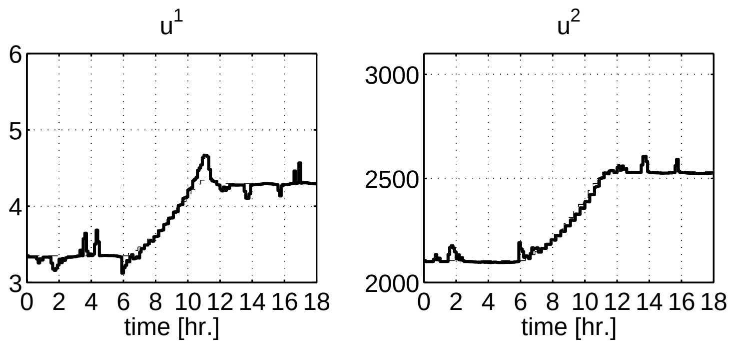


Figure 6.8: Manipulation of the reflux ratio (u^1) and the boil-up rate (u^2) for a task sequence $[3, 3, 5]$ with fluctuations in the feed composition and SHOP-1 control (dashed line: nominal, thick lines: closed loop).

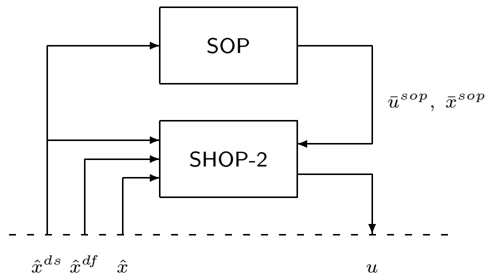


Figure 6.9: Control configuration for the scenario of persistent disturbances and in the absence of grade changes.

disturbance model given as follows

$$\dot{x}^{ds} = B^{ds} w^{ds}, \tag{6.16}$$

with w^{ds} a Gaussian white noise process. An estimate of x^{ds} is updated only before the execution of the static optimization problem (SOP). In between two subsequent executions of the SOP, x^{ds} is held constant. This is done to ensure that the computed optimal steady state will be a feasible end point of the SHOP.

Implementation of scheduling constraints

Persistent disturbances may have a significant effect on the actual production rates. The steady state end-point conditions should be computed in such a way that the production rates that are imposed by the schedule are met whenever possible. Of course, in case of very large persistent disturbances some of the production constraints will become infeasible, in which case infeasibility should be communicated to the scheduler. More on handling infeasibility will follow later. Here, we first analyze how the scheduling constraints can be imposed.

Let t^k be the start of the k-th production interval. At any time t' for which $t^k < t' < t^k + \tau$ the predicted production and consumption rates should satisfy

$$(t^k + \tau - t')Y_e(z) + P_e^k(t') \geq \sum_g \sum_h \bar{T}_k^{g,h} T Y_e^{g,h}, \tag{6.17}$$

$$(t^k + \tau - t')C_r(z) + U_r^k(t') \leq \sum_g \sum_h \bar{T}_k^{g,h} T C_r^{g,h}, \tag{6.18}$$

where $\bar{T}_k^{g,h}$ are the optimal values of the transition variables computed by the scheduler and $P_e^k(t')$ and $U_r^k(t')$ are the real production and consumption of respectively end product e and raw material r up to time t' for production interval k. If the accumulated production and consumption are reset at the beginning of each production interval, then the following holds.

$$P_e^k(t') = \int_{t^k}^{t'} Y_e(z(t))dt, \;\; U_r^k(t') = \int_{t^k}^{t'} C_r(z(t))dt. \tag{6.19}$$

In some cases it may be more practical to transfer excess or shortage of production/consumption in one production interval to the beginning of the next, leading to non-zero initial conditions for the accumulated production and consumption.

SOP formulation

The static optimization problem at a time t', $t^k < t' < t^k + \tau$, is defined as follows.

SOP

$$\min_{x,u} \left\{ -L(z) \middle| \exists y, z \text{ s.t. } \begin{array}{ll} \text{plant description} & \text{process constraints} \\ 0 = f^s(x,u,y,\hat{x}^{ds}) & h(z) < 0 \\ 0 = g^s(x,u,y,\hat{x}^{ds}) & \text{grade constraints} \\ z = C_x x + C_u u & g_g(z) < 0 \end{array} \right. \\ \left. \begin{array}{l} \text{scheduling constraints} \\ (t^k + \tau - t')Y_e(z) + P_e^k(t') \geq \sum_g \sum_h \bar{T}_k^{g,h} TY_e^{g,h} \\ (t^k + \tau - t')C_r(z) + U_r^k(t') \leq \sum_g \sum_h \bar{T}_k^{g,h} TC_r^{g,h} \end{array} \right\}, \tag{6.20}$$

where $\hat{x}^{ds}$ is the current estimate of the persistent disturbance. (6.20) is a (generally non-convex) NLP which can be solved to a local minimum using e.g. gradient-based optimization techniques. Optimal steady state values of the input, state and performance variables are denoted $(\bar{x}^{sop}, \bar{u}^{sop}, \bar{z}^{sop})$.

SHOP formulation

The formulation of the SHOP is obtained by extending the formulation of the SHOP in the previous section by a description of the slow, persistent disturbances. The following formulation results.

SHOP-2

$$
\min_{u\in\mathcal{U}_S}\left\{V^S(z)\middle|\exists x,y,z \text{ s.t. }
\begin{array}{lll}
\text{plant} & \text{disturbances} & \text{path constraints}\\
\dot{x}=f^{f,s}(x,u,y,x^{df},x^{ds}) & \dot{x}^{df}=A^{df}x^{df} & h(z)<0\\
0=g^{f,s}(x,u,y,x^{df},x^{ds}) & \dot{x}^{ds}=0 & \\
z=C_x x+C_u u & &
\end{array}
\right.
$$
$$
\left.
\begin{array}{lll}
\text{init./end cond.} & & \text{sched. constr.}\\
x(0)=\hat{x} & x^{df}(0)=\hat{x}^{df}(t') & \int_0^{H^S} Y_e(z)dt \geq \int_{t'}^{t''} Y_e(\bar{z}^{sop})dt\\
x(H^S)=\bar{x}^{sop} & x^{ds}(0)=\hat{x}^{ds}(t') & \int_0^{H^S} C_r(z)dt \leq \int_{t'}^{t''} C_r(\bar{z}^{sop})dt
\end{array}
\right\},
\tag{6.21}
$$

As in the SHOP problem treated in the previous section, it seems opportune to relax the end point constraint in order to improve the computational feasibility. A further, major decrease in computational complexity can be achieved if we use a linear approximation of the dynamics. How this can be done in the presence of the static re-optimization will be treated next.

Linear approximation

Like in the derivation of the SHOP problem in the previous section, we propose the use of a LTV model instead of the nonlinear dynamics. However, due to the absence of a reference trajectory in the case of the static re-optimization, the choice of a trajectory along which this linearization should be derived is not straightforward.

A rather useful and intuitive solution that was proposed in literature [61] for a class of discrete-time nonlinear systems is to derive the linear approximation along the trajectory that results if we apply the controls from the previous iteration to the nonlinear dynamics, choosing the initial state equal to the current state estimate. Because the persistent disturbance is assumed to vary in time only slowly no large deviations of the optimal solutions from the previous ones are to be expected which justifies the use of this linear approximation.

We let the SHOP solution from the previous time step be denoted $\bar{u}^{shop,l-1}$, where $l-1$ is the previous instant. Based on this solution, a prediction for the solution of the SHOP at the l-th time instant is given as follows

$$
u^{p,l}(t)=\begin{cases} \bar{u}^{shop,l-1}(t+\Delta T_{shop}), & 0<t<H^S-\Delta T_{shop},\\ \bar{u}^{sop}, & H^S-\Delta T_{shop}<t<H^S, \end{cases} \tag{6.22}
$$

where ΔT_{shop} is the sampling time of the SHOP. The trajectories along which the linearization is derived are given by

$$\left\{ x^{p,l}, y^{p,l}, x^{df,p,l}, x^{ds,p,l} \;\middle|\; \begin{array}{l} \text{plant} \\ \dot{x}^{p,l} = f(x^{p,l}, u^{p,l}, y^{p,l}, x^{df,p,l}, x^{ds,p,l}) \\ 0 = g(x^{p,l}, u^{p,l}, y^{p,l}, x^{df,p,l}, x^{ds,p,l}) \\ \\ \text{init. cond.} \\ x^{p,l}(0) = \hat{x}(t'),\; x^{ds,p,l}(0) = \hat{x}^{ds}(t'),\; x^{df,p,l}(0) = \hat{x}^{df}(t') \end{array} \right\}. \tag{6.23}$$

The trajectories associated to the LTV dynamics are then given by

$$\begin{aligned} x &= x^{p,l} + \Delta x, \\ u &= u^{p,l} + \Delta u, \end{aligned}$$

where Δx and Δu are constrained by the LTV dynamics as in (6.8). The computational complexity of this LTV formulation of the SHOP is somewhat bigger than that of the SHOP treated in the previous section. At each time instant the model equations need to be solved over the horizon of the SHOP and a new LTV description of the dynamics needs to be derived. Still, for not too large problems, these computations will be feasible in real time. Most important, after discretization, the optimization problem reduces to solving a LP or QP (depending on the objective function that is used) compared to a NLP for the nonlinear dynamics case.

Handling infeasibilities

Large disturbances may cause the scheduled production to be infeasible. A consequence of the enforcement of the production schedule onto the process control problem is that we must provide for a way to handle such infeasibilities. Infeasibility of the scheduling constraints is revealed by the fact that the SOP returns no feasible solution. As soon as infeasibility is concluded, one or more production constraints should be relaxed until a feasible solution is obtained. The resulting production levels should be communicated to the scheduler so that the prediction of the production level can be adjusted accordingly.

Several relaxation strategies can be defined. In some cases it may be wise to utilize a fixed relaxation strategy, where the sequence of constraints that is relaxed is fixed in advance. A downside of this is that in the worst case many iterations are required to end up with a feasible optimization problem. In other cases, physical insight in the process combined with knowledge on the estimated disturbance levels may provide suitable relaxation rules. For example in the distillation column example a low fraction of the light component in the feed is likely to incur infeasibility of the top production constraints; vice versa infeasibility of the bottom production rates may occur in case of a high fraction of the light component.

6.5.2 Application to case II: binary distillation

As an example of the implementation of the SOP/SHOP-2 strategy we consider again the operation of the continuous binary distillation column treated in the previous section. We will consider the operation of the plant during a series of three quasi-static production intervals corresponding to grade 3. In addition to the fast stochastic disturbance a slow deterministic disturbance in the feed composition is present. The composition is first gradually decreased from 0.5 to 0.49 after which it is held constant at this value. To account for the presence of the deterministic feed disturbance we add to the process model the following persistent disturbance model:

$$\dot{x}^{ds} = w^{ds},$$

and we modify the component balance for the feed tray accordingly:

$$O\frac{dc^{10}}{dt} = Ic^{9} - I'c^{10} + J'v^{11} - Jv^{10} + K(c_K + x^{df,1} + x^{ds})$$

The changes in the estimates of the deterministic disturbance will cause the static re-optimization to compute new, optimal end-points for the SHOP-2. The sampling time of the static re-optimization (ΔT_{sop}) is chosen to be 36 minutes. In the simulations, we include a computation time for the static re-optimization of 6 minutes (1 sample of the SHOP-2). The true computation time is much smaller, however computation times in the range from several minutes to an hour can be expected for real-life problem sizes. It may be argued that the sampling time should be chosen equal to the computation time. However, because of the very slow variation in the feed composition no large benefit was gained by sampling faster. Simulation times would have increased though. Implementation details are given in E.2.

Results

The closed loop simulation results are plotted in Figures 6.10 and 6.11. The configuration with the SOP and the SHOP-2 manages to maintain the quality variables within the specifications of grade 3 at any time. Interestingly, the bottom impurity is decreased to values in the range 0.03-0.04. At first sight, there is no economic benefit to be gained from this decrease in impurity. The contrary is even true: boil-up and reflux rates are increased by a significant amount in order to establish the decrease. However, a closer analysis of the static process characteristics learns that this is the only way to meet the production constraints for the top product despite the change in the feed composition. Indeed, to guarantee that the nominal (or almost nominal) amount of the lighter component leaves the column at the top for a smaller concentration of this lighter component in the feed we need to decrease its presence at the bottom.

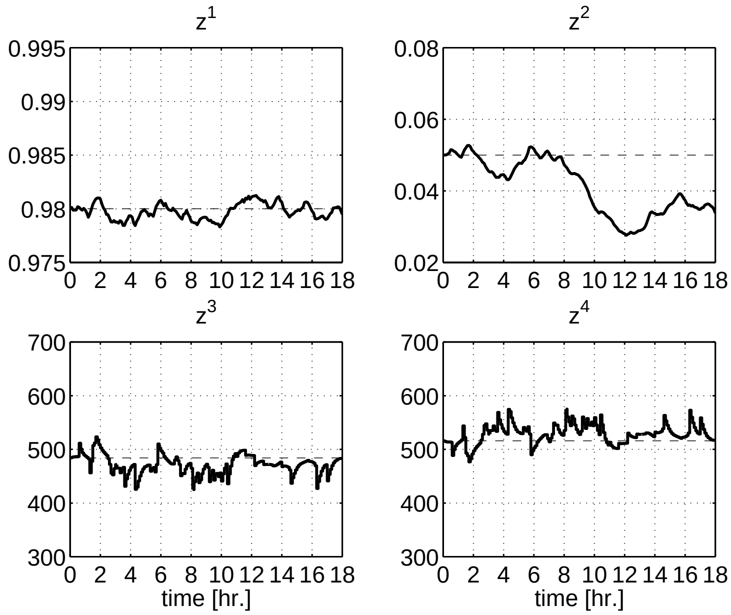


Figure 6.10: Top purity (z^1), bottom impurity (z^2), distillate flow (z^3), and bottom outflow (z^4) for a task sequence [3,3,3] with persistent fluctuations in the feed composition and the control configuration consisting of the SOP and the SHOP-2 (dashed lines: nominal, thick lines: closed loop).

The behavior of the feed composition estimate can be denoted from Figure 6.12. Observe that the estimate of the feed composition lags the true value by about 2 hours which is due to the slow dynamics that map the feed composition to the top and bottom compositions. Despite the estimation error, acceptable control performance is achieved though.

6.6 Scenario 3: dynamic re-optimization

Next we consider the situation where grade changes are to be executed in the presence of persistent disturbances. Obviously, the presence of persistent disturbances cause the optimal changeover strategy to shift to different trajectories. In theory, we could use the configuration discussed in the previous section, consisting of a static reoptimization (SOP) and a dynamic optimization (SHOP), where the latter computes in a receding horizon fashion the optimal changeover strategy for which the end-point is continuously updated by the SOP. How-

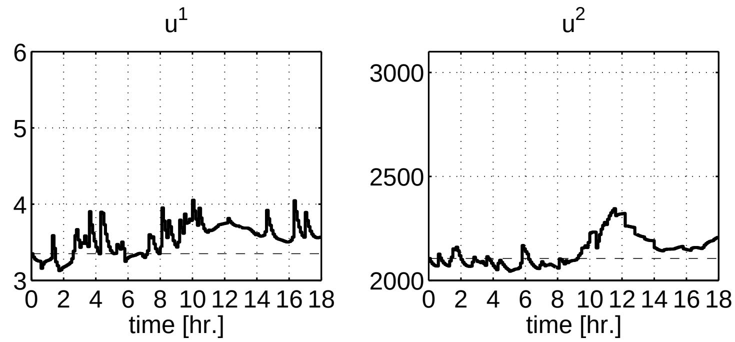


Figure 6.11: Manipulation of the reflux ratio u^1 and the boil-up rate u^2 for a task sequence [3,3,3] with persistent fluctuations in the feed composition and the control configuration consisting of the SOP and the SHOP-2 (dashed lines: nominal, thick lines: closed loop).

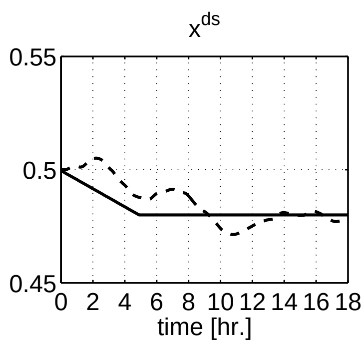


Figure 6.12: Trajectory of the deterministic component in the feed composition (solid) and the estimate thereof (dashed).

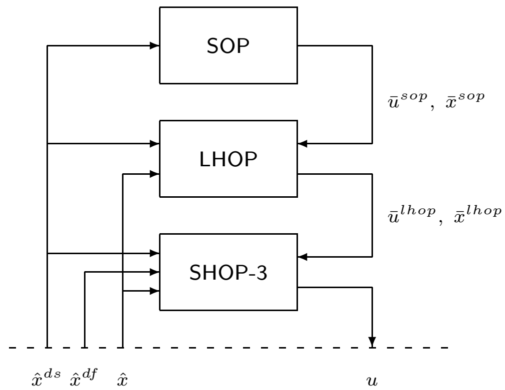


Figure 6.13: Control configuration for the scenario of persistent disturbances and in the presence of grade changes.

ever observe that, in order to assess the full effect of the persistent disturbance on the changeover, the SHOP would typically be required to have a very long look ahead (horizon), which may make the problem computationally intractable. Linearization of the dynamics, as proposed in the previous section, may make the problem computationally tractable, however the validity of such a linear approximation may be doubted, because the persistent disturbances may cause the optimal changeover strategies to deviate significantly from the nominal solutions. Also, it does not seem realistic to suppose that the grade variables, i.e. the times at which transitions from one grade region to another take place, remain unaltered in the presence of persistent disturbances. To prevent severe sub-optimality we should recompute the grade variables as well.

The suggested control strategy comprises a decomposition of the dynamic optimization problem into a long and a short horizon optimization problem (respectively LHOP and SHOP) where the SHOP includes an end-point constraint to connect its solution to the trailing part of the LHOP. The LHOP is computed and implemented at a slow sampling frequency and takes care of the scheduling constraints and the transitions between different grade regions. The SHOP runs at a sampling frequency that is comparable to that of the SHOP discussed in the previous section and has a more modest task, namely to control the state back to a specified point on the LHOP trajectories while guaranteeing that the production quality as well as the process variables remain within their bounds. The desired end-point of the LHOP is given by the solution of the SOP as in the previous section. This control configuration is depicted in Figure 6.13.

6.6.1 Description of the control approach

Implementation of scheduling constraints

The scheduling constraints are primarily enforced at the SOP/LHOP-level. The SOP is solved subject to a nominal production constraint which can be derived as follows. Let t''' be located within the k-th production interval such that $t^k < t''' < t^k + \tau$. Naturally, through the choice of the horizon of the LHOP, a quasi-static production task is allocated to this production interval. Then, the nominal production rate constraint that has to be included in the SOP is as follows:

$$\tau Y_e(z) \geq \sum_g \sum_h \bar{T}_k^{g,h} TY_e^{g,h}, \tag{6.24}$$

$$\tau C_r(z) \leq \sum_g \sum_h \bar{T}_k^{g,h} TC_r^{g,h}. \tag{6.25}$$

To enforce the scheduling constraints on the LHOP we first define $PI_{t'}$ to be the set containing the indices of the production intervals for which the production constraint needs to be enforced in the solution of the LHOP at time t':

$$PI_{t'} = \{k = 1, \dots \mid t' \leq t^k + \tau \leq t'''\}. \tag{6.26}$$

Then for the first index k in this set the production constraints are given by

$$\int_{t'}^{t^k+\tau} Y_e(z(t))dt + P_e^k(t') \geq \sum_g \sum_h \bar{T}_k^{g,h} TY_e^{g,h}, \tag{6.27}$$

$$\int_{t'}^{t^k+\tau} C_r(z(t))dt + U_r^k(t') \leq \sum_g \sum_h \bar{T}_k^{g,h} TC_r^{g,h}, \tag{6.28}$$

and for the remaining indices k in this set, the production constraints are given as follows

$$\int_{t^k}^{t^k+\tau} Y_e(z(t))dt \geq \sum_g \sum_h \bar{T}_k^{g,h} TY_e^{g,h}, \tag{6.29}$$

$$\int_{t^k}^{t^k+\tau} C_r(z(t))dt \leq \sum_g \sum_h \bar{T}_k^{g,h} TC_r^{g,h}. \tag{6.30}$$

Further, let the end point of the LHOP, t''', be located within the j-th production interval. Then, additional production constraints are imposed at the final time in order to guarantee feasibility of the production constraints at the end of the

j-th interval.

$$\int_{t^j}^{t'''} Y_e(z(t))dt \geq \sum_g \sum_h \bar{T}_j^{g,h} TY_e^{g,h} - (\tau - (t''' - t^j))Y_e(\bar{z}^{sop}), \tag{6.31}$$

$$\int_{t^j}^{t'''} C_r(z(t))dt \leq \sum_g \sum_h \bar{T}_j^{g,h} TC_r^{g,h} - (\tau - (t''' - t^j))C_r(\bar{z}^{sop}). \tag{6.32}$$

LHOP formulation

Apart from the scheduling constraints, the definition of the LHOP is basically the receding horizon version of the economic grade change optimization problem introduced in Section 5.2.3. Let the solution of the LHOP in the previous $(l-1)-th$ cycle be denoted $\bar{u}^{lhop,l-1}$. Then, the mathematical formulation of the LHOP in the l-th cycle is as follows.

LHOP

$$\min_{u \in \mathcal{U}_S} \left\{ V^L(z) \middle| \exists x, y, z \text{ s.t. } \begin{array}{lll} \text{plant} & \text{disturbances} & \text{init./end cond.} \\ \dot{x} = f^s(x,u,y,x^{ds}) & \dot{x}^{ds} = 0 & x(0) = \hat{x}(t') \\ 0 = g^s(x,u,y,x^{ds}) & & x^{ds}(0) = \hat{x}^{ds}(t') \\ z = C_x x + C_u u & & x(H^L) = \bar{x}^{sop} \end{array} \right.$$

$$\left. \begin{array}{ll} \text{path constraints} & \text{sched. constr.} \\ h(z) < 0 & (6.27,\ldots,6.32) \\ u(t) = \bar{u}^{lhop,l-1}(t + \Delta T_{lhop}),\ t \in [0, T_{L,calc}] & \end{array} \right\}, \tag{6.33}$$

where V^L is the economic objective function, possibly extended by some control-type penalties. H^L is the horizon length of the LHOP, the selection of which will be discussed in the sequel. ΔT_{lhop} is the sampling time of the LHOP. $T_{L,calc}$ is an estimate of the calculation time required to solve the LHOP. The input is not allowed to deviate from the previous solution during the first $T_{L,calc}$ seconds because the LHOP solution will not be available until after $T_{L,calc}$ seconds anyway. If the input were allowed to change also during this first time span then this would unintentionally contribute to the deviation of the predicted state at time $t' + T_{L,calc}$ from the real state.

Selection of the prediction horizon (LHOP)

In case there are no slow, dynamic drift disturbances but only grade changes, the horizon length of the LHOP is predominantly determined by the length of a grade change. In fact, because the end-point of the LHOP is by definition located in a quasi-stationary task interval the horizon length becomes a dynamic variable. The first call to the LHOP is made presumably several hours in advance of the actual grade change. The look-ahead of the LHOP should then be sufficiently long to reach the steady state operating conditions corresponding to the target grade. As the grade change proceeds, the horizon length of the LHOP is allowed to shrink, presumably up to a minimum allowed horizon length. In case slow, dynamic drift disturbances are present, there is a clear incentive to run the LHOP continuously. In that case, during stationary operation (no grade changes), a fixed horizon length would be used, while the horizon length would be determined according to the decision scheme outlined above when grade changes come in the picture. The time-varying character of the horizon length is clearly illustrated in the example that is treated next.

6.6.2 Application to case II: binary distillation

We consider again the operation of the binary distillation column. The real-time dynamic optimization strategy is shown for the case where a grade change between grade 3 and 5 is to be established in the presence of a deterministic disturbance in the feed composition as in the previous section. The LHOP will, together with the SOP be executed every 36 minutes. The solution of the LHOP is implemented with a 6 minute delay as for the SOP in the previous section. Implementation details are given in E.3.

Results

The closed loop simulation results are plotted in Figures 6.14 and 6.15. Several interesting observations can be made. First, observe that, despite the significant disturbance in the feed composition, the top composition is close to the nominal value for most of the time. In the evaluation of the real production we relaxed the bounds on the quality by 0.002. Top and bottom purities lay within these relaxed quality specifications during the quasi-static production tasks. The transition is established in the nominal transition time.

The real production levels are plotted in Figure 6.16 together with the production targets for the three intervals of 6 hours. All production levels are according to the production schedule. Sufficient production of the top product is guaranteed through a decrease of the bottom impurity as in the example shown in the previous section.

Finally, the length of the horizon of the LHOP at the different time instances at which it is executed are plotted in Figure 6.17. Initially, a minimum horizon length of 7 samples is used. Then, as the end of the first production interval is approached, the horizon length is extended abruptly to a value 16 so as to oversee the entire second interval in which the transition is to take place. Thereafter the horizon length is gradually decreased until the minimum of 7

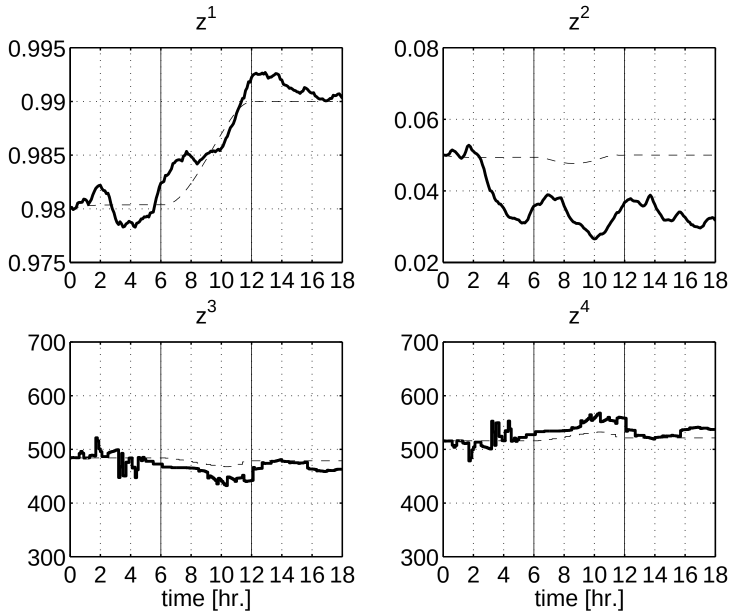


Figure 6.14: Top purity (z^1), bottom impurity (z^2), distillate flow (z^3), and bottom outflow (z^4) for a task sequence [3,3,5] with persistent and fast fluctuations in the feed composition and the control configuration consisting of the SOP, LHOP and SHOP (dashed lines: nominal, thick lines: closed loop).

samples is reached again, which is maintained until the end.

6.7 Discussion - spatial decomposition

In this chapter, the plant-wide control and optimization problem has been treated as were it a *process unit* control problem. No attention was paid to the aspect of *spatial decomposition*. This is a logical consequence of our choice to consider *single-machine plants* only (see Section 3.3.1), however the relevance of spatial decomposition in most practical applications makes a short discussion on this topic imperative. First, let us state that there is no theoretical basis for a spatial decomposition of the process control and optimization system. Theoretically optimal performance is achieved if the plant is treated as a single, multi-input multi-output system on which the control strategies presented in this chapter are applied.

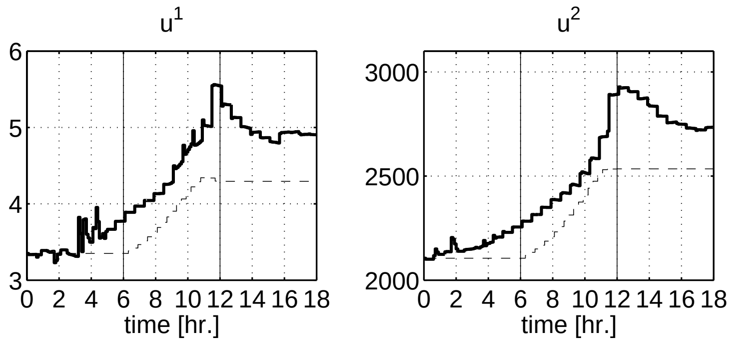


Figure 6.15: Manipulation of the reflux ratio u^1 and the boil-up rate u^2 for a task sequence [3,3,5] with persistent and fast fluctuations in the feed composition and the control configuration consisting of the SOP, LHOP and SHOP (dashed lines: nominal, thick lines: closed loop).

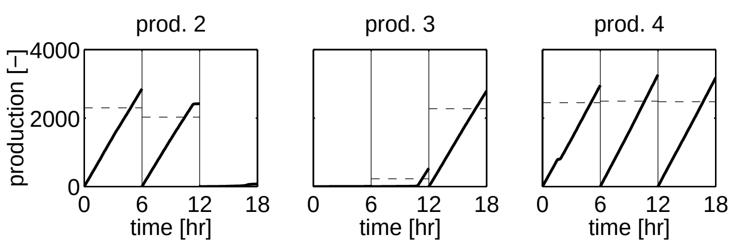


Figure 6.16: Production levels of product 2, 3 and 4 during the execution of a task sequence [3,3,5]. Dashed lines indicate the production targets corresponding to the scheduling constraints.

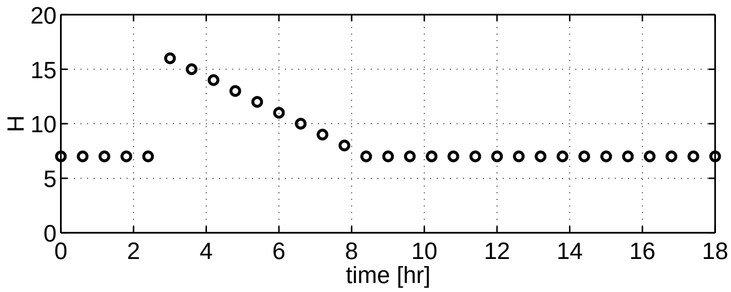


Figure 6.17: Horizon length (in number of samples) of the LHOP at the different time instances during the execution of a task sequence [3,3,5].

Unfortunately, this integrated control approach is seldom feasible in practice. The first reason why most practical plant-wide control problems are decomposed into several smaller process-unit control problems is the *computational infeasibility* of a fully-integrated control approach. A typical plant-wide control problem may involve several hundreds of inputs (mv's) and 'performance variables' (cv's). It appears impossible, even with tomorrow's computing power to compute on a sufficiently fast execution rate the controls in a centralized fashion. This is already the case for current linear model-based MPC algorithms. Extensions towards dealing with nonlinear plants as proposed in this chapter will make the computations even more involved. The second reason is *maintainability*: a set of smaller process controllers is more easily maintained (tested, monitored, updated, debugged) than a single process controller of extremely large dimension. Related to this issue, the robustness (regarding software and hardware, *not* in the 'robust control'-sense) of a distributed controller implementation will generally be higher than that of a single controller.

Accepting spatial decomposition to be inevitable for the various reasons mentioned above we will next briefly discuss possible decomposition strategies for the control strategies treated in this chapter. To this end we will first review how spatial decomposition is implemented in present-day plant-wide control strategies.

Spatial decomposition in the traditional plant-wide control hierarchy
In the state-of-the-art plant-wide control and optimization approach, see Figure 1.3, spatial decomposition is applied to the *dynamic optimization* (linear MPC) only. The RTPO generally overlooks the behavior of the entire plant. Different MPC's are installed on single process units or clusters of several process units. Setpoints for the MPC's are generated by the RTPO. If we interpret

the task of the RTPO as to coordinate the actions of the different MPC's it is obvious that this coordination is only *static*. Dynamic interaction between the different process units and their control is ignored which may cause severe problems. As an example we consider a refinery application consisting of a furnace section and a distillation section. Suppose the RTPO predicts that there is room for a slight increase in throughput. The dynamics of the furnaces are generally comparatively fast, so that the desired change in throughput will be realized quickly. However, this causes an abrupt off-set in the conditions of the flows entering the distillation columns which may make the quality of the distillation products traverse beyond specifications or, even worse, cause flooding of the columns. This situation would not have appeared if the (slow) dynamics of the distillation columns had been taken into account properly while increasing the throughput. Obviously, the spatial decomposition as being practiced in present-day plant-wide control systems has a serious shortcoming when it comes to dealing with the dynamic interaction between different process units.

Possibilities for spatial decomposition in our approach Our approach to plant-optimization and control builds essentially on the decomposition of a single-level, infinite (or very long) horizon optimization problem into a SOP, a LHOP and a SHOP. The SOP and LHOP consider the effect of persistent disturbances on the optimal steady state operating conditions and the transients towards this steady state, respectively. The SHOP deals with fast, zero mean disturbances on a short horizon.

Slow persistent disturbances and grade changes are likely to have a *plant-wide* impact. Thus it seems desirable to let the SOP and the LHOP consider the behavior of the entire plant. Fortunately, sampling times for the SOP and the LHOP are allowed to be reasonably large, which may make a plant-wide optimization feasible, even with today's computers. The fast zero-mean disturbances are unlikely to cause large conflicts in the interaction of process units and can hence be dealt with locally by different SHOP's. This suggest a spatial decomposition only at the SHOP level, pretty much in compliance with the decomposition applied in today's plant-wide control systems. However, the *plant-wide* scope of the dynamic optimization (in the LHOP) avoids the problems with conflicting unit dynamics that occur in the traditional setting.

6.8 Contributions of this chapter

The hierarchical operating strategy proposed in Chapter 4, consisting of a production scheduling layer and a process optimization and control layer, puts specific demands on the process control design.

The production scheduler dictates how the plant should be utilized so as to flexibly meet market demands regarding quantity and quality of delivered goods. To realize the right quantity and quality of these goods in time and with attractive plant economics is the task of the process control system. Regarding the interconnection of the scheduling layer and the process control layer this chapter proposes to enforce the scheduling constraints (desired quantities and qualities of the end products) at discrete time instances. Infeasibility of these constraints may occur due to process disturbances in which case the expected effect on the production data must be communicated to the scheduler so that the production schedule can be adapted accordingly.

The scheduling constraints in combination with the process constraints restrict the operation of the plant, however room for economic optimization may exist. Therefore, the basic function of the process control systems that we propose is to optimize the process economics subject to the above-mentioned constraints. To deal with disturbances the implementation of this basic function is done in combination with a state estimator and according to the so-called receding horizon principle, leading to a control scheme that is comparable to existing NMPC schemes. The main difference with existing NMPC schemes is that existing NMPC schemes perform set point tracking whereas our control performs on-line economic optimization.

To cope with the scheduling constraints as well as the effect of fast disturbances, the controller should typically have a long horizon in combination with fast sampling. This is computationally not feasible, therefore this chapter presents several approximate, decomposition-based control configurations for specific disturbance situations. The most complicated scenario that is considered is the scenario where persistent, and fast stochastics occur during the operation of a multi-grade plant. For this scenario, a decomposition of the original NMPC problem in three layers is proposed: a Static Optimizer (SOP) computes optimal steady state conditions for the production task that marks the horizon of the dynamic optimization. The solution of the SOP is used as the target end point of a Long Horizon dynamic Optimizer (LHOP) which computes at a low sampling frequency the trajectory of the states and the inputs such that the scheduling constraints are met and an economic objective is optimized. The LHOP, due to its low sampling frequency naturally restricted to dealing with slowly varying disturbances, considers only the persistent disturbances. Fast disturbances are dealt with by a Short Horizon Optimizer (SHOP) which is executed at a high sampling frequency. The target for the end-point of the SHOP is located at the LHOP trajectory. To make real-time implementation of the SHOP possible the use of linear approximations of the nonlinear model is suggested. These can be derived along the trajectory that is computed by the LHOP.

The proposed methodology is described with a main focus on constructive aspects. Stability and closed-loop performance analysis or synthesis aspects are deemed too hard to handle at this stage and hence omitted. Instead, the characteristic behavior of the economic control strategy is shown for the operation of a binary distillation column. The results demonstrate that the enforcement of the scheduling constraints in combination with the institution of economic control objectives make the closed loop control system respond to feed disturbances in an non-traditional but intuitively correct manner. Conventional control systems would attempt to remove the effect of the disturbance from the cv's where the trade-off is made based on the chosen quadratic weights. When using true economic objectives, the trade-off is made based on economic motifs.

Chapter 7

Dynamic optimization strategies

Dynamic optimization plays an essential role in the scheduling and control strategy described in the previous chapters. In the formulation of the production scheduling problem (Chapter 5), dynamic optimization is used to distinguish economically attractive process transitions from less attractive ones. The kernel of the real-time control system (Chapter 6) is a receding horizon model-based optimization. To make an efficient implementation of the real-time control approach possible we must put effort in limiting the computation time of these optimizations. This chapter describes the development of tailor-made optimization algorithms for the dynamic optimization problems that have been formulated in previous chapters. Specific attention will be paid to the grade change optimization problem and its particular, non-smooth characteristics. First, dynamic optimization approaches for large-scale problems shall be reviewed (7.1). Next, two approaches to solving the grade change optimization problem efficiently will be outlined. The first introduces a smooth, approximate description of the grade region and exploits the structure of the problem in the definition of a NLP based inner loop optimization to compute accurate search directions (7.3). The second approach uses integer variables to describe the grade regions and solves a sequence of MILP's to converge to a solution (7.4). Finally we will show how the real-time, receding horizon implementation of the dynamic optimization algorithms can be exploited to enhance computation speed even further (7.5).

7.1 Introduction

Dynamic optimization aims to determine control and state trajectories for a dynamic system over a finite horizon such that a certain performance index is minimized. Dynamic optimization has its roots in the Calculus of Variations [13]. The application of the Calculus of Variations to the continuous time optimal control problem with no constraints on inputs or outputs leads to a set of necessary conditions which can be guaranteed through the solution of a Two Point Boundary Value problem. Although various methods exist for the solution of these problems, see e.g. [12], they are generally hard to solve. For the constrained-input problem, Pontryagin [66] showed that the set of necessary conditions can be modified in accordance with *Pontryagin's minimum principle*. Computational methods for solving the constrained-input problem are available for specific cases only. Dealing with state constraints in the context of the classical approach to dynamic optimization is even more difficult. An interesting recent development in this respect is the contribution by [6] who use barrier functions to incorporate inequality constraints in the problem formulation, leading to an unconstrained optimal control problem which they solve by the classical forward-backward integration scheme (see e.g. [12]).

An alternative to the variational approach to optimal control is *dynamic programming*. Dynamic programming is based on Bellman's principle of optimality, which states that (we quote from [44])

> An optimal policy has the property that no matter what the previous decisions have been, the remaining decisions must constitute an optimal policy with regard to the state resulting from those previous decisions.

Dynamic programming determines an optimal control strategy by working backward in time from the final stage. For continuous optimal control problem the optimal strategy is defined by the solution of a corresponding partial-differential equation, the Hamilton-Jacobi-Bellman equation. This equation is generally difficult to solve, even numerically. When it can be solved it provides an optimal control in state feedback (closed loop!) form.

The two point boundary value problem and the Hamilton-Jacobi-Bellman equation are generally too hard to solve directly, especially for large scale problems encountered in process systems engineering. This has motivated the development of several NLP approaches to dynamic optimization. The general idea of these is to discretize the optimal control problem to convert it into a finite-dimensional NLP. In these, constraints on inputs and states can be incorporated in a rather straightforward manner.

Two basic NLP approaches to large-scale dynamic optimization of process systems can be distinguished: the sequential (or control parametrization) approach and the simultaneous approach. The *sequential* approach utilizes parametrization of the controls to discretize the problem (see e.g. Vassiliadis, 1993). An integration tool is used to evaluate the model equations and hence the objective function, the constraints and the gradients. Successive search directions towards the local optimum are determined by an outer loop optimizer, which is generally a Sequential Quadratic Programming tool (SQP). In the *simultaneous* approach, both the controls and the states are parametrized [45] to transform, mostly via collocation on finite elements, the dynamic optimization problem into a NLP which can be solved using a Nonlinear Programming tool (e.g. SQP or the Generalized Reduced Gradient method (GRG)). The big advantage of the simultaneous approach is that the objective function and the process model equations converge simultaneously (infeasible path method), while the process model equations are necessarily satisfied in every iteration in the sequential approach. The simultaneous approach can handle open loop unstable processes and enables to include information about the approximate behaviour of the state trajectory into the initial guess [10]. However, the sequential approach is simpler in implementation and especially for stiff systems, it may actually be an advantage instead of a disadvantage that the model equations are satisfied every iteration. Another advantage of the sequential approach for on-line application is that intermediate solutions are feasible (with respect to the model equations) and therefore implementable. For these reasons, in our research we focus on the sequential approach.

7.2 The sequential approach for dynamic optimization

In this description of the sequential approach for dynamic optimization we consider the following problem formulation

$$\min_{u \in \mathcal{U}} \left\{ \int_0^T L^d(z)dt \,\middle|\, \exists x, y, z \text{ s.t. } \begin{array}{ll} \text{plant} & \text{init./end cond.} \\ \dot{x} = f(x,u,y) & x(0) = \bar{x}^g, x(T) = \bar{x}^h \\ 0 = g(x,u,y) & \text{path constraints} \\ z = C_x x + C_u u & h(z) < 0 \end{array} \right\}, \tag{7.1}$$

where L is at least twice continuously differentiable. The conventional sequential solution approach is based on the parametrization of the controls, $u = u(p,t)$, introducing parameters p, together with a discretization of the path constraints $h(z(i\tau)) < 0$, $i = 1, \ldots, m$ to yield a finite dimensional problem (τ is the discretization interval). Common parametrizations make use of splines, polynomials or wavelets.

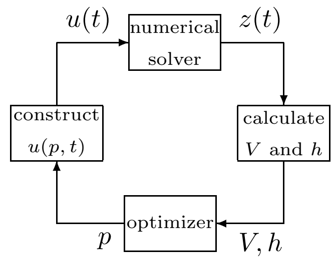


Figure 7.1: Basic schematic of the sequential solution strategy for large scale dynamic optimization.

The solution strategy based on this parametrized problem, which is of sequential nature, is indicated in Figure 7.1 [79]. An initial parameter vector is chosen. With the according input trajectories, the model is integrated using a numerical solver to obtain values for the objective function V, the constraints h and the gradients dV/dp and dh/dp. The gradients can be quite efficiently obtained by integrating, along with the model equations, the so-called *sensitivity equations*[1] [79]. These can be derived by taking the derivatives of the extended model equations with respect to the parameters p:

$$\begin{aligned} \frac{\partial}{\partial t}\left(\frac{\partial x'}{\partial p}\right) = \frac{\partial}{\partial p}\left(\frac{\partial x'}{\partial t}\right) &= \frac{\partial f'}{\partial x'}\frac{\partial x'}{\partial p} + \frac{\partial f'}{\partial u}\frac{\partial u}{\partial p} + \frac{\partial f'}{\partial y'}\frac{\partial y'}{\partial p}, \\ 0 &= \frac{\partial g'}{\partial x'}\frac{\partial x'}{\partial p} + \frac{\partial g'}{\partial u}\frac{\partial u}{\partial p} + \frac{\partial g'}{\partial y'}\frac{\partial y'}{\partial p}. \end{aligned} \tag{7.2}$$

where f' includes an additional differential equation to represent the integral term of the objective $f' = [f(x,u,y)^T, L^d(z)]^T$, $x' = [x^T, v]^T$, g' combines the algebraic equations with the performance allocation $g' = [g(x,u,y)^T, [z - C_x x - C_u u]^T]^T$, and $y' = [y^T, z^T]^T$. The integration of the sensitivity equations can be done quite efficiently since the Jacobian matrices that are required can be taken from the integration of the model equations. Based on the state sensitivities, dV/dp and dh/dp are calculated in a straightforward manner. The function and gradient evaluations are called by the so-called outer loop optimization routine which is in most cases a general purpose NLP solver. Popular methods are the Generalized Reduced Gradient (GRG) method, the Sequential Quadratic Programming method (SQP) and penalty and barrier methods. We will make extensive use of the SQP method which is described in Appendix F. Some of the solutions we propose are inspired by penalty and barrier methods. The main ideas behind those methods are also briefly outlined in Appendix F.

[1] Alternative approaches use finite differences or the solution of the adjoint equations.

7.3 A modified sequential approach to the grade change problem

The *grade change* problem is extensively discussed in this thesis. For the reader's convenience, we repeat the general definition of the grade change problem. L^d is chosen as the negative added value:

$$L^d(z) = \sum_r p_F^r C_r(z) - \sum_e p_P^e Y_e(z), \tag{7.3}$$

with the production rates given by

$$Y_e(z) = \sum_g G^g M_g^e F(z), \tag{7.4}$$

where

$$G^g = \begin{cases} 1, & \text{if } g_g(z) \leq 0, \\ 0, & \text{otherwise.} \end{cases} \tag{7.5}$$

and M_g^e as defined in 5.2.3. Through the definition of the grade variables G^g the grade change optimization problem becomes non-smooth. The approach discussed in this section comprises a smooth approximation of the grade definition (7.5) in combination with a tailor-made control parametrization method. The main idea shall be described next.

7.3.1 Main idea

A smooth approximation of G^g can be obtained for example using the arctan or the tanh function:

$$\tilde{G}^g = \prod_{i=1}^{n_g} \left(\frac{1}{\pi} \arctan(\gamma g_g^i(z)) + \frac{1}{2} \right), \text{ or} \tag{7.6}$$

$$\tilde{G}^g = \prod_{i=1}^{n_g} \left(\frac{1}{2} \tanh(\gamma g_g^i(z)) + \frac{1}{2} \right), \tag{7.7}$$

with $\gamma \gg 1$ and where g_g^i are the scalar components of the vector function g_g. Smooth approximation of the grade equations renders the objective function twice (in fact, infinitely many times) continuously differentiable, which makes the conventional sequential approach with an SQP or GRG outer loop optimizer a candidate for solving it. However, the smooth approximation of the grade change problem is still strongly nonlinear and the SQP or GRG-based optimization may turn out to be extremely ineffective for solving it. This will be elaborated on further next.

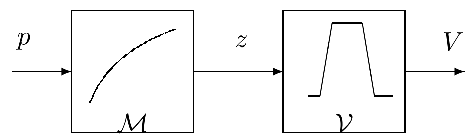


Figure 7.2: Nonlinearity characteristic of the process model and the economic objective function.

Drawback of SQP method for grade change optimization

The conventional sequential approach computes search directions on the basis of (at best) quadratic approximations of the parameters-to-objective map. Considering the strong nonlinearity of the specific grade change objective function these approximations will be of poor quality in general. The consequence of this is that probably many iterations will be needed to converge, and hence many costly evaluations of the functions and the gradients will be required. In typical applications of control parametrization methods over 90 percent of the computation time is spent on the integration of the model and the sensitivities.

To restrain the computation time we need to search for ways to minimize the number of iterations and the best way to do so is by improving the quality of the approximation that is used in each iteration. This is the main idea behind the development of a new optimization approach for grade change problems in particular which we presented first in [88]. How the specific structure of the grade change problem can be exploited to compute search directions more effectively will be analyzed next.

Structure of the grade change problem

The development of this new approach was motivated by the following insight in the structure of the grade change problem. Note that on a finite time span and for a fixed initial condition we can interpret the model as a map $\mathcal{M} : \mathbb{R}^{n_p} \to L_\infty^{n_z}[0,T)$. The objective results from the map of the performance variable trajectories to a scalar $\mathcal{L} : L_\infty^{n_z}[0,T) \to \mathbb{R}$. The functional V is the composition of $\mathcal{M}$ and $\mathcal{L}$, $\mathcal{V} = \mathcal{L} \circ \mathcal{M}$. The map $\mathcal{M}$ is generally smoothly nonlinear, the map $\mathcal{V}$ is strongly nonlinear for the typical grade change problem. This is represented schematically in Figure 7.2. Another essential difference between $\mathcal{M}$ and $\mathcal{L}$ is that the evaluation of $\mathcal{M}$ is extremely time-consuming whereas the evaluation of $\mathcal{L}$ can be done very fast and by straightforward computation once the trajectories of the performance variables have been determined.

This suggest that, in each iteration of the top level optimization a suitable approximation of $\mathcal{V}$ can be obtained by linearizing *only* $\mathcal{M}$. Let us denote this linearization $\bar{\mathcal{M}}(p)$. Then the corresponding sub problem considers the composite map $\bar{V} = \mathcal{L} \circ \bar{\mathcal{M}}$. Note that this choice of approximating the nonlinear problem renders the sub-problem non-convexly nonlinear in contrast to e.g. the SQP approach which solves a convex (quadratic) programme to compute search directions. If the SQP approach is used to solve the sub-problem then the overall dynamic optimization problem becomes a Sequential SQP, or SSQP. Fortunately, because the evaluation of applying $\bar{\mathcal{M}}$ and $\mathcal{L}$ can be done very fast, the inner loop SQP can be solved in a fraction of the total optimization time. Even attempts to solve the inner loop problem globally, for example by selecting several different initial guesses, may be feasible. More essential than the slight increase in the computation time needed for the inner loop problem is the supposition that the search directions resulting from the inner loop optimization will be a lot more accurate than in the case of first or second order approximations, so that fewer iterations are required to converge.

7.3.2 Implementation

The SSQP method relies on the fast evaluation of the map $\mathcal{L}$. The inclusion of the integral objective in the LTV model equations and the integration of the composite model is no option. Due to the strong nonlinearity in the objective function, e.g. (7.6), large gradients will occur leading to very small step sizes. This will slow down the integration of the model significantly. One way to avoid this is through the numerical approximation of the integral using the Riemann sum or the trapezoid rule and a discretization of the LTV dynamics accordingly. This introduces approximation errors, however then note that the smooth objective function was an approximation itself of the original non-smooth objective. Errors due to the approximation of the integral seem acceptable as long as they are of the same order of magnitude as the errors introduced by the smooth approximation of the objective. A more thorough analysis of these approximation errors is beyond the scope of this thesis.

Objective approximation

The Riemann sum approximation of the integral objective is given by:

$$V^{d,0}(Z) = \tau \sum_{i=0}^{N-1} L^d(z_i), \tag{7.8}$$

where $N = T/\tau$, $z_i = z(i\tau)$, and $Z = [z_0^T, z_1^T, \ldots, z_N^T]^T$. The application of the trapezoid rule leads to

$$V^{d,1}(Z) = \tau \left(\frac{1}{2} L^d(z_0) + \sum_{i=1}^{N-1} L^d(z_i) + \frac{1}{2} L^d(z_N) \right). \tag{7.9}$$

Approximations (7.8) and (7.9) can be computed efficiently for arbitrarily complex choices of the objective function, however the approximation may be inaccurate for large τ's. More elaborate approximations of the integral objective may be used whenever deemed appropriate. For an example of this we refer to the distillation column optimization which is treated in the end of this section.

Linearization of dynamics

The dynamics are linearized and discretized in each iteration along the state-input trajectory from the previous optimization cycle. The corresponding linear system is given as follows (for the j-th iteration):

$$Z = Z^{j-1} + \Delta Z, \qquad \Delta Z = T_u \Delta p, \tag{7.10}$$

$$x_N = x_N^{j-1} + \Delta x_N, \qquad \Delta x_N = T_{N_x} \Delta p, \tag{7.11}$$

where T_u is a matrix containing the impulse response coefficients of the LTV system given by the sensitivity equations of the original nonlinear plant (7.2):

$$T_u = \begin{pmatrix} G_{01} & G_{02} & \cdots & G_{0n_p} \\ G_{11} & G_{12} & \cdots & \cdot \\ \vdots & \vdots & \ddots & \vdots \\ G_{N1} & G_{N2} & \cdots & G_{Nn_p} \end{pmatrix}, \tag{7.12}$$

where $G_{ij} = \frac{\partial z_i}{\partial p_j}$ and n_p is the total number of parameters. T_{N_x} is the sensitivity of the final state with respect to the parameters,

$$T_{N_x} = \begin{pmatrix} H_{N1} & H_{N2} & \ldots & H_{Nn_p} \end{pmatrix}, \tag{7.13}$$

with $H_{Nj} = \frac{\partial x_N}{\partial p_j}$.

In accordance with the discretization of the linear dynamics, path constraints are evaluated at a finite number of samples only: $h(z_i) < 0$.

Line search

We confront the search directions coming from the inner loop SQP with the nonlinear dynamics in a one-dimensional line search. The merit function that we apply is of the following form:

$$\mathcal{M} = V^{d,1}(Z) + \sum_{\{i,j\} \in A^C} \rho_1 (h^j(z_i))^2 + \sum_j \rho_{2,j} (x_N^j)^2, \tag{7.14}$$

where A^C is a set defining the {time,constraint}-pairs for which the path constraints are violated. This set is update in each iteration. ρ_1 and $\rho_{2,j}$, $j = 1, \ldots, n_x$ are scalar weighting factors.

Complete procedure

The complete optimization approach comprises a 5 step-procedure, as described below :

Step 1: initialization
j is set to 1 (first iteration). An initial parameter vector of length n_p, $p^j = p_0$, is chosen to initialize the dynamic optimization.

Step 2: objective and constraint evaluation
The model equations are integrated with input $u^j(t) = u(p^j, t)$. The solutions are denoted $x^j(t)$, $y^j(t)$ and $z^j(t)$. The objective $V^{d,1}$ and the constraints h are computed.

Step 3: gradient evaluation
T_u and T_{N_x} are constructed on the basis of the solution of the sensitivity equations of the plant model.

Step 4: determination of search step
A search step is calculated by solving the following NLP:

$$\min_{\Delta p}\left\{ V^{d,1}(Z) \mid \exists Z, \Delta Z, x_N, \Delta x_N \text{ s.t. } \begin{array}{ll} \text{plant} & \\ Z = Z^{j-1} + \Delta Z & x_N = x_N^{j-1} + \Delta x_N \\ \Delta Z = T_u \Delta p & \Delta x_N = T_{N_x} \Delta p \end{array} \right.$$
$$\left. \begin{array}{lll} \text{init./end cond.} & & \text{path constraints} \\ x_0 = \bar{x}^g, & x_N = \bar{x}^h & h(z_i) < 0 \end{array} \right\}, \tag{7.15}$$

using for example SQP optimization. All Jacobians can be calculated analytically, so the coding of the optimization can be done efficiently.

Step 5: evaluation of progress
The new solution $p^\star = p^{j-1} + \alpha \Delta p^j$ is implemented on the nonlinear model as in **step 2**, with $\alpha = 1$. The objective and the constraints are evaluated and the progress is measured in terms of a merit function. In a one-dimensional line search (e.g. by means of bi-section) the step size α is determined such that $\mathcal{M}(p^\star) < \mathcal{M}(p^{j-1})$. Then we set $p^j = p^{j-1} + \alpha \Delta p^j$ and and proceed with **step 3** ($j = j + 1$).

Many minor modifications to this standard procedure may help convergence to a desirable local minimum. For example, it may pay out to solve the inner loop NLP for different initial choices of Δp in order to ensure a better quality of the inner loop solution. This modification is particularly attractive if the solution time for solving the NLP is small in comparison with the time needed for a function and gradient evaluation. Alternatively, we can perturb the initial choice of Δp in subsequent calls of the inner loop optimization to avoid ending up in poor local minima of the inner loop optimization problem. Other possible modifications involve the institution of a trust region and the gradual augmentation of γ (see (7.6) and (7.7)).

The latter modification is motivated from the fact that for large values of γ the inner loop will be typically hard to solve. Choosing γ large initially makes the inner loop problem resemble the original, discontinuous formulation, thus leading to very large gradients and changes therein. The same behavior occurs in the application of barrier methods in case the barrier parameter μ is chosen too small initially. As explained in Appendix F, to resolve this, barrier methods solve a sequence of problems for decreasing values of μ. Similarly, the SSQP method can be implemented such that it solves a sequence of problems for increasing values of γ.

A final modification that we would like to mention is the extension of the inner loop objective function with a quadratic term representing an approximation of the second derivative of the dynamics to the original objective. How such an approximation can be found using standard Broyden, Fletcher, Goldfarb, and Shanno (BFGS) update techniques is treated in [85].

7.3.3 Application to case II: binary distillation

As an example we consider the grade change problem in a binary distillation column, the same process that was studied in Chapter 6. For a schematic diagram of such a process unit and the model description we refer to that chapter.

The controls that are consider in the optimization study are the reflux ratio (u^1) and the boil up rate (u^2). The states are the liquid phase mole fractions on the 20 trays ($c^1, \ldots, c^{20}$). The performance channels are the top purity (z^1), the bottom impurity (z^2), the top outflow (z^3), the bottom outflow (z^4), the reflux ratio (z^5), and boil up rate (z^6). The model contains 20 differential equations and 27 algebraic equations.

Problem formulation

We consider a transition from grade 3 to grade 5. Feed conditions are assumed constant (because determined by up stream unit operations). The operation of the distillation column is subject to an economic cost function given as follows

$$V_{ec} = \int_0^T L^d(z)dt,$$

scenario 1				scenario 2			
top product		bottom product		top product		bottom product	
e	p_P^e	e	p_P^e	e	p_P^e	e	p_P^e
1	1	4	1.5	1	1	4	1.5
2	2	5	0.5	2	2	5	0.5
3	2	-	-	3	4	-	-

Table 7.1: Prices for the different end products of the binary distillation column for two different market scenarios.

where

$$L^d(z) = p_F z^6 - \sum_e p_P^e Y_e(z),$$

where p_F is the unit boil up cost, chosen equal to 0.2. Prices for the different end products are constant and given in Table 7.1 for two different market scenarios. The production rates are given as follows

$$\begin{aligned} Y_1 &= (G^1 + G^2) z^3, & Y_4 &= (G^1 + G^3 + G^5) z^4, \\ Y_2 &= (G^2 + G^3) z^3, & Y_5 &= (G^2 + G^4 + G^6) z^4, \\ Y_3 &= (G^4 + G^5) z^3. \end{aligned}$$

For this specific case where the product quality of the top and the bottom product depend linearly on a single variable only, we can derive the following smooth approximation of the production rates:

$$\begin{aligned} Y_1 &= \hat{G}^1 z^3, & Y_4 &= \hat{G}^4 z^4, \\ Y_2 &= \hat{G}^2 z^3, & Y_5 &= \hat{G}^5 z^4, \\ Y_3 &= \hat{G}^3 z^3, \end{aligned}$$

where

$$\begin{aligned} \hat{G}^1 &= \frac{1}{\pi}(\arctan(\gamma(0.978 - z^1)) + 1/2), \\ \hat{G}^2 &= \frac{1}{\pi}(\arctan(\gamma(z^1 - 0.978)) + \arctan(\gamma(0.988 - z^1))), \\ \hat{G}^3 &= \frac{1}{\pi}(\arctan(\gamma(z^1 - 0.988)) + 1/2), \\ \hat{G}^4 &= \frac{1}{\pi}(\arctan(\gamma(0.052 - z^2)) + 1/2), \\ \hat{G}^5 &= \frac{1}{\pi}(\arctan(\gamma(z^2 - 0.052)) + 1/2), \end{aligned}$$

and where the constraints are slightly relaxed in order to ensure that the computed steady states target is indeed *inside* the specifications of grade 5 and not at the boundary. γ is chosen equal 2000.

We fix the optimization horizon to a length of 6 hours. We use a piece wise constant parametrization of the controls with a discretization time of 0.3 hour, yielding a total number of 40 optimization parameters. In addition to the economic objective function a control objective function is defined. The control objective contains a quadratic weighting on the change in the inputs in combination with a quadratic weighting on the deviation of the final state from the desired end-point:

$$V_{co} = \begin{pmatrix} z_0^5 \\ z_0^6 \end{pmatrix}^T R_\Delta \begin{pmatrix} z_0^5 \\ z_0^6 \end{pmatrix} + \sum_{i=1}^{20} \begin{pmatrix} z_i^5 - z_{i-1}^5 \\ z_i^6 - z_{i-1}^6 \end{pmatrix}^T R_\Delta \begin{pmatrix} z_i^5 - z_{i-1}^5 \\ z_i^6 - z_{i-1}^6 \end{pmatrix} + (x_N - \bar{x}^5)^T Q_N (x_N - \bar{x}^5),$$

where $Q_N = \frac{1}{2}\rho I$ with I a unit matrix of the appropriate dimensions and ρ equal to 10^7. R_Δ is chosen to be a diagonal matrix with diagonal $[1000, 0.01]$. The inclusion of the end-point constraint as a penalty term is inspired by the penalty methods. Unlike the penalty method, we will only solve a single optimization problem for a fixed value of ρ. A consequence of this is that the end point constraint is no longer enforced (this would require ρ to be increased up to ∞ or, in practice, very large values). The overall objective is given as follows

$$V = V_{ec} + V_{co}.$$

$\bar{x}^3$, the supposed initial state, and $\bar{x}^5$, the desired final state are computed through a static optimization of the economic objective function subject to the constraints as described in Section 5.2.2.

Implementation

For a fast evaluation of the objective and the gradients, we can use the Riemann sum or the first order approximation of the objective function. However, a more accurate approximation can be obtained if we just apply a first order hold to the states and inputs and compute the integral exactly. This may not be possible in general, however for the specific choice of $\hat{G}^1, \ldots, \hat{G}^5$ as given above, an expression of the primitive can be obtained analytically. In order to arrive at this expression we use the fact that z^3 as well as z^4 are constant on the control intervals. Then L^d can be seen to consist of a sum of 'arctan' functions for which an analytical primitive exists. The approximation of the integral objective is given as follows

$$\hat{V}_{ec} = \sum_{i=1}^{N} \hat{L}^d(z_i, z_{i-1}),$$

where $\hat{L}^d(z_i, z_{i-1})$ evaluates the integral objective on the interval $[(i-1)\tau, i\tau]$ for the performance signal $z(t) = z_i + (t/\tau)(z_i - z_{i-1}),\ \ t \in [0, \tau]$.

For the solution of the inner loop optimization we use the SQP solver constr.m from the MATLAB optimization toolbox, which we modified to enable use of an initial guess of the Hessian. This makes it possible to 'warm-start' successive inner loop optimization which reduces computation time significantly. Initial trajectories for the inputs are determined by ramping the inputs from the initial steady state to the final steady state values in 6 hours.

The implementation of the model equations is done in the DAE modeling package gPROMS. Integration of the model and the computation of the Jacobians were done within gPROMS. The state trajectories were sampled at the discretization intervals and communicated to MATLAB via an OPC server.

Results

To verify the supposition that a conventional SQP approach is indeed not suited for the solution of the grade change problem we first apply a standard SQP method (constr.m) to the transition problem for market scenario 1.

It took 158 iterations for the SQP algorithm to converge to an optimum of -7176.62. Illustrative for the poor quality of the search directions that were computed from the QP was the fact that the step size did not exceed 0.05 for most of the first 40 iterations (the *Newton* step is equal to 1!), leading to a total number of 394 function evaluations (integrations of the model). Next, the SSQP solver was used to solve the same transition problem. **Only 3 SSQP iterations** (4 function evaluations including the first one) were required to converge to exactly the same optimum value of the objective. The fast convergence of the SSQP method in comparison to the SQP approach is illustrated in Figure 7.3 where the objective value in the successive iterations is plotted for both methods (only the first 100 iterations of the SQP are shown).

Besides the nonlinearity of the economic objective, another reason for the slow convergence of the SQP approach is the dominant presence of the quadratic end-point penalty. Many BFGS Hessian updates are needed to obtain a good estimate of the quadratic curvature of the objective function. To dampen the effect of the quadratic penalty on the convergence speed we next consider the case where the Hessian is initialized based on a computation of the second-order contribution of the end-point penalty and the input-move penalty. We presented this idea, of computing the low-cost[2] part of the Hessian in relation to dynamic optimization for NMPC in [85] and demonstrated the increased performance of the SQP method using the enhanced Hessian information. Here we use the same concept, only for initialization of the Hessian. As an estimate of the initial

[2] 'low cost' in terms of computing power.

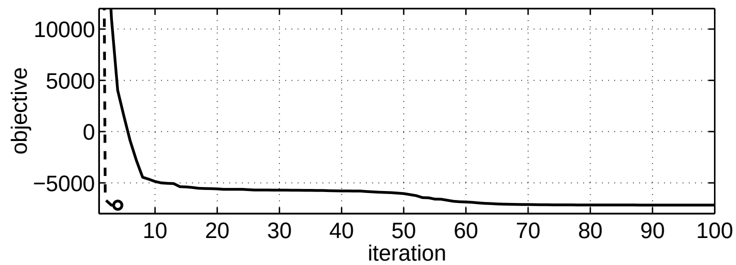


Figure 7.3: Convergence of the objective value to the optimum for the SQP method (solid) and the SSQP method (dashed).

Hessian we will use the following expression

$$H^{p,0} = \Delta_u^T \mathbf{R}_\Delta \Delta_u + T_{Nx}^T Q_N T_{Nx},$$

where

$$\mathbf{R}_\Delta = \begin{bmatrix} R_\Delta & \cdot & \dots & \cdot \\ \cdot & R_\Delta & \dots & \cdot \\ \vdots & \vdots & \ddots & \vdots \\ \cdot & \cdot & \dots & R_\Delta \end{bmatrix}, \; \Delta_u = \begin{bmatrix} 1 & \cdot & \dots & \cdot \\ -1 & 1 & \dots & \cdot \\ \vdots & \vdots & \ddots & \vdots \\ \cdot & \cdot & -1 & 1 \end{bmatrix},$$

and T_{Nx} is the sensitivity matrix that maps the parameters to the final state. This sensitivity matrix can be constructed from the sensitivity equations in a straightforward manner.

Using this initialization of the Hessian, the performance of the SQP approach improves rather significantly. Only 57 iterations are required in order to converge to the same optimum. However, still over 100 function evaluations are done. The SSQP approach still converges in 3 main iterations. The only difference for the SSQP is that the first inner loop SQP is solved in considerably fewer iterations because of the improved adequacy of the initial Hessian. The contribution of the final state weighting to the optimum objective value was as low as 1.65 indicating the small deviation of the final state from the desired end point.

The optimal input and output trajectories for the corresponding transition are plotted in Figures 7.4 and 7.5, respectively. The plotted simulation results were obtained after extension of the optimal control trajectories with a leading part corresponding to 0.9 hour steady state production in grade 3 and a trailing part corresponding to 0.9 hour steady state production in grade 5. The actual optimized trajectories are in between the two vertical rulers. Because

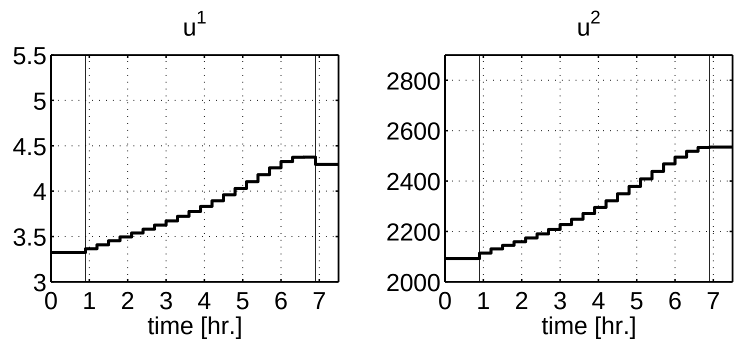


Figure 7.4: (SSQP) Optimal trajectories of the 2 input variables (reflux ratio u^1, and vapor boil up rate u^2) for a transition from grade 3 to grade 5 with market scenario 1.

for market scenario 1 there is no economic incentive for a fast grade transition, controls are very calm. The control objective clearly dictates the outcome of the optimization problem. Note that the penalty on the deviation of the final state from the steady state corresponding to grade 5 is sufficient to guarantee that indeed the desired steady state is attained.

To demonstrate the impact of changes in the economics on the optimal trajectories we next consider the optimization of the transition from grade 3 to grade 5 for market scenario 2. The optimal controls are given in Figure 7.6 and the corresponding trajectories of the first four performance variables in Figure 7.7. Because the price for the high-purity (> 0.99) top product is significantly higher than for the low-purity top product (> 0.98) there is an economic incentive to establish the grade change quickly in scenario 2.

7.4 A successive MILP approach to the grade change problem

The SSQP method described in the previous section may, when combined with a smart strategy for generating randomized initial conditions avoid getting stuck in poor local minima. However, since the eventual optimization is still gradient-based, no guarantees can be obtained on the quality of the optimum and, because the inner loop problem constitutes a NLP as well, on the quality of the search direction. Another approach which may help to overcome the limitations of gradient-based methods is described in this section and proceeds via the introduction of binary variables and the solution of successive MILP's.

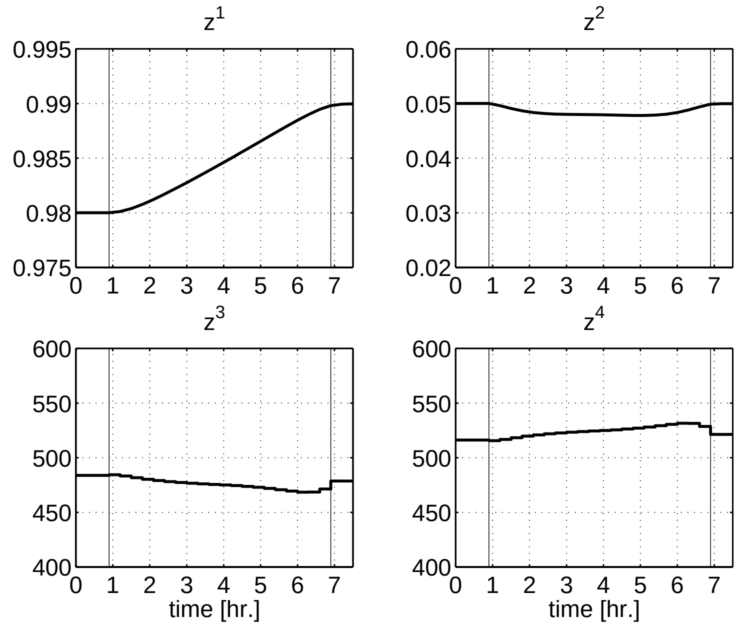


Figure 7.5: (SSQP) Optimal trajectories of the first 4 performance variables (top purity z^1, bottom purity z^2, distillate flow z^3, bottom flow z^4) for a transition from grade 3 to grade 5 with market scenario 1.

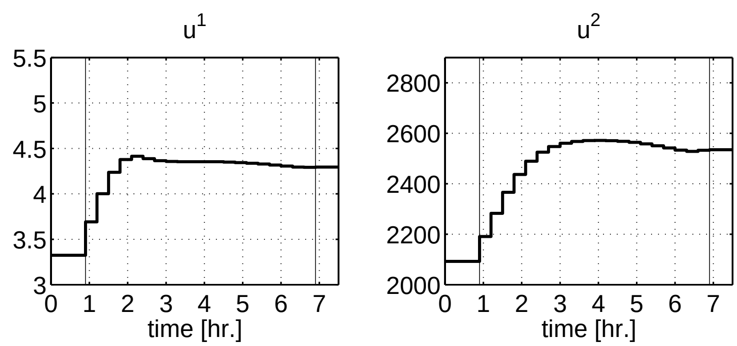


Figure 7.6: (SSQP) Optimal trajectories of the 2 input variables (reflux ratio u^1, and vapor boil up rate u^2) for a transition from grade 3 to grade 5 with market scenario 2.

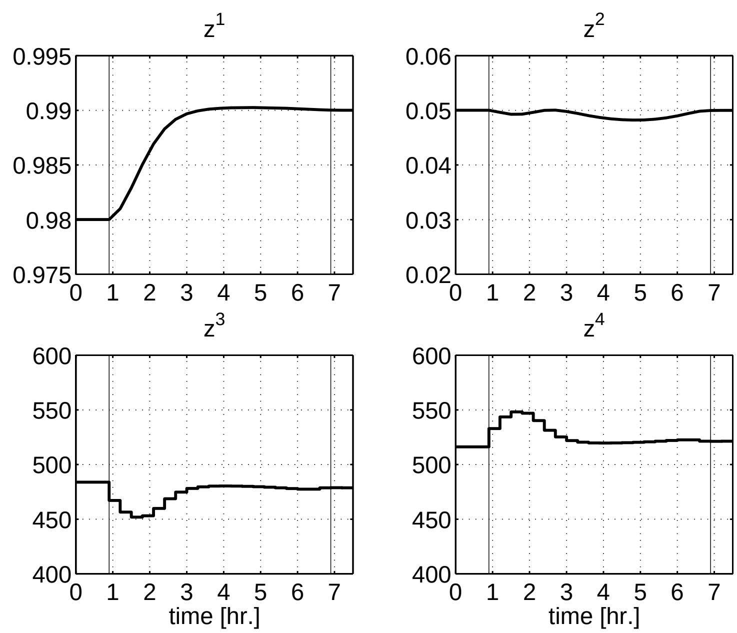


Figure 7.7: (SSQP) Optimal trajectories of the first 4 performance variables (top purity z^1, bottom purity z^2, distillate flow z^3, bottom flow z^4) for a transition from grade 3 to grade 5 with market scenario 2.

7.4.1 Outline of the approach

The crucial step in this approach is the introduction of binary variables $G_i^g \in \{0,1\}$ related to the grade regions:

$$G_i^g = \begin{cases} 1, & \text{if } g_g(z_i) \leq 0, \\ 0, & \text{otherwise.} \end{cases} \tag{7.16}$$

An alternative expression for G_i^g is the following

$$g_g(z_i) - (1 - G_i^g)Q^g < 0, \ \sum_g G_i^g = 1. \tag{7.17}$$

Note that G_i^g enters these equations linearly. For feasibility of (7.17) we require that Q^g be sufficiently large (larger than the maximum that is attained by $g_g(z_i)$ on the feasible set in which z_i lives.) and that the grade regions $\mathcal{G}^g$ are adjacent.

Next, we introduce new continuous decision variables $Y_{e,i}^g$ which represent the flow of end product e during operation of the plant in grade g and at time instant $i\tau$. By the definition of the binary grade variables we require

$$0 \leq Y_{e,i}^g \leq G_i^g Y_{e,u}^g, \tag{7.18}$$

where $Y_{e,u}^g$ is an upper bound on the end product flow. $Y_{e,i}^g$ relates to the material flow $F(z_i)$ as follows

$$\sum_g \sum_e N_e^g Y_{e,i}^g = F(z_i), \tag{7.19}$$

where N_g^e maps the end product flow to the material flow for every end product and in any grade. Finally, the total end product yield at time $i\Delta t$ is given by $Y_{e,i} = \sum_g Y_{e,i}^g$. Using the integer description of the grade regions and after discretization of the objective using e.g. (7.8), an alternative Mixed-Integer Nonlinear Programme (MINLP) formulation of the transition problem can be derived:

$$\min_p \left\{ V^{d,1} \middle| \exists x, y, G_i^g, Y_{e,i}^g, Y_{e,i} \text{ s.t. } \begin{array}{ll} \text{plant} & \text{init./end cond.} \\ \dot{x} = f(x, u(p,t), y) & x(0) = \bar{x}^g, \ x(T) = \bar{x}^h \\ 0 = g(x, u(p,t), y) & \text{path constraints} \\ z = C_x x + C_u u(p,t) & h(z_i) < 0 \end{array} \right.$$
$$\left. \begin{array}{ll} \text{grade defenition} & \text{product flows} \\ g_g(z_i) - (1 - G_i^g)Q < 0 & 0 \leq Y_{e,i}^g \leq G_i^g Y_{e,u}^g, \ Y_{e,i} = \sum_g Y_{e,i}^g \\ \sum_g G_i^g = 1 & \sum_g \sum_e N_e^g Y_{e,i}^g = F(z_i) \end{array} \right\}. \tag{7.20}$$

Several approaches towards solving MINLP's exist; most popular methods are BB and cutting plane methods, see e.g. [22] for an overview. We propose a *successive linearization approach* for the problem at hand. For most problems, h, g_g and F will be linear functions, leaving the process model f, g the only remaining nonlinearity. A linearization of the MINLP can in that case be obtained by substituting the nonlinear dynamics by the linearized dynamics (7.10). The linearized (inner loop) problem is a MILP which is solved in each iteration of the outer loop.

Choice of merit function

There exist two alternative ways to confront the search directions obtained from the inner-loop optimization with the nonlinear dynamics: the trust region approach and the line search approach. To apply a line search we first need to select a merit function. The choice of a merit function for problem (7.20) is not straightforward due to the discontinuous nature of the problem. For example consider the situation where in a particular iteration a certain quality variable is almost brought within the specifications of a very attractive (means: worthy) production grade. If we construct the merit function on the basis of the objective function of (7.20), then the 'closeness to the specifications' will not be rewarded. Instead, the price of the off-spec production will be accounted, such that eventually the search step may even be rejected. One way to avoid this is by using a smooth approximation of the economic objective in the merit function as in the SSQP approach. Observe that such a smooth approximation naturally favours those trajectories of the quality variables that are close to the specifications of attractive grades. The objective-function-related part of the merit function can be complemented by a part representing the violation of the path and end-point constraints as in the previous section.

In few cases it may be more beneficial to use a trust region approach. For example if the solution of the MILP inner loop problem changes a lot in each iteration it may be meaningful to restrain the solution to a region along the previous solution where the LTV description of the dynamics is assumed valid. Because the institution of trust regions is generally highly case-specific we will not pay more attention to the subject here.

Analysis of the MILP inner loop problem

Although the successive MILP approach to grade change optimization provides an interesting alternative to the SSQP method discussed in the previous section, the success of this method will strongly depend on how fast the MILP inner loop problem can be solved. An analysis of the properties of the MILP is given in Appendix D.

7.4.2 Application to case II: binary distillation

As an example of the application of the Successive MILP approach to grade change optimization we consider the grade change problem in a binary distillation column, similar to the previous section. For details on the problem formulation we refer to the previous section.

Implementation

The grade constraints g^g were defined to be the upper and lower bounds on the top and bottom quality as in Table 6.3. A slight modification to the procedure described above is that we introduce two different types of grade variables: g^T and g^B for the top and bottom product, respectively. This reduces the number of variables and constraints. The corresponding grade constraints are

$$g_{g^T}(z_i) - (1 - G_i^{g^T}) < 0, \;\; \sum_{g^T} G_i^{g^T} = 1, \;\; g^T \in \{1, 2, 3\}, \tag{7.21}$$

$$g_{g^B}(z_i) - (1 - G_i^{g^B}) < 0, \;\; \sum_{g^B} G_i^{g^B} = 1, \;\; g^B \in \{4, 5\}, \tag{7.22}$$

with g_{g^T} and g_{g^B} given as follows

$$g_1 = \begin{pmatrix} 0.00 - z^1 \\ z^1 - 0.98 \end{pmatrix}, \; g_2 = \begin{pmatrix} 0.98 - z^1 \\ z^1 - 0.99 \end{pmatrix}, \; g_3 = \begin{pmatrix} 0.99 - z^1 \\ z^1 - 1.00 \end{pmatrix},$$
$$g_4 = \begin{pmatrix} 0.00 - z^2 \\ z^2 - 0.02 \end{pmatrix}, \; g_5 = \begin{pmatrix} 0.02 - z^2 \\ z^2 - 1.00 \end{pmatrix}.$$

The production flow variables are subject to the following constraints

$$\begin{aligned} Y_{e,i}^{g^T} &\le 1000 G_i^{g^T}, \text{ if } e = g^T, & Y_{2,i}^{g^B} &\le 1000 G_i^{g^B}, \text{ if } e = g^B, \\ Y_{e,i}^{g^T} &\le 0, \text{ if } e \neq g^T, & Y_{2,i}^{g^B} &\le 0, \text{ if } e \neq g^B, \\ \sum_{e \in \{1,2,3\}} \sum_{g^T} Y_{e,i}^{g^T} &= z_i^3, & \sum_{e \in \{4,5\}} \sum_{g^B} Y_{e,i}^{g^B} &= z_i^4, \end{aligned}$$

The total production of end products 1 and 2 is given by

$$Y_{e,i} = \sum_{g^T} Y_{e,i}^{g^T}, \text{ if } e \in \{1, 2, 3\}, \tag{7.23}$$

$$Y_{e,i} = \sum_{g^B} Y_{e,i}^{g^B}, \text{ if } e \in \{4, 5\} \tag{7.24}$$

A Riemann sum approximation of the objective is used (7.8) with $L^d(z_i)$ given as in the example in 7.3. The discretization length was chosen equal to 0.3 as in the previous section. To prevent excessive control moves (observe that we did not include any control-type of objective in the formulation so far) we add upper and lower bounds on the rate of change of the two inputs. The upper and lower bounds are given by

$$-0.25 < z_i^5 - z_{i-1}^5 < 0.25, \;\; -200 < z_i^6 - z_{i-1}^6 < 200.$$

Further, to avoid infeasibility of the MILP inner loop problem, the end point constraint is relaxed:

$$\bar{x}^5 - 1e^{-3} < x_N < \bar{x}^5 + 1e^{-3}.$$

The MILP that is solved in each iteration is of moderate size. The number of binary variables is 105. The total number of continuous decision variables is 296 after reduction.

The integration of the model and the generation of the required Jacobians is done in gPROMS. The solution of the MILP inner loop problem is done with GAMS-CPLEX. The packages are interfaced via MATLAB and an OPC server as described in Section 6.4.

Results

We consider a transition from grade 3 to 5 for the second market scenario (higher price for high-purity product). Only 7 iterations are required to converge to a minimum of -11446.1. The solution of the successive MILP's proceeds very fast, total optimization time is in the same order of magnitude as for the SSQP. The optimization results are plotted in Figures 7.8 (inputs) and 7.9 (outputs). The transition is established in 1.5 hours. To realize such a fast transition both the reflux ratio and the boil-up rate are first increased up to a value that is larger than the final steady state values after which they are decreased gradually. The reflux ratio increases at a maximum rate initially so obviously the rate constraint is the bounding one with respect to the transition time.

7.5 Real-time optimization

So far, we discussed the development of optimization routines for off-line purposes. In Chapter 6 various real-time optimization strategies were discussed. In real-time optimization, due to the receding horizon mechanism, succeeding optimization problems are typically rather similar. Solution methods employed in Real-time optimization should benefit from this. Obvious tricks are the re-utilization of optimization results, such as an initial guess or the Hessian. The following discussion concerns the SSQP optimization only.

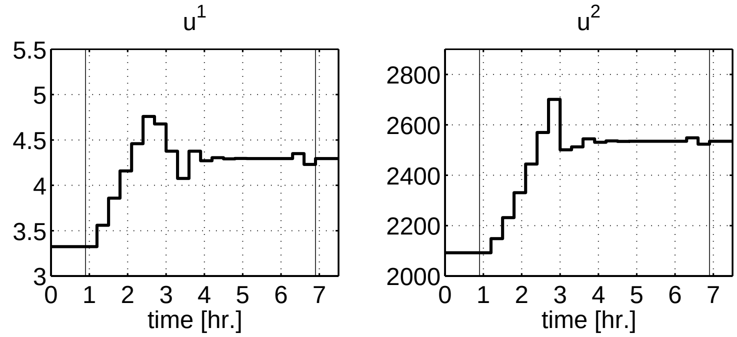


Figure 7.8: (successive MILP) Optimal trajectories of the 2 input variables (reflux ratio u^1, and vapor boil up rate u^2) for a transition from grade 3 to grade 5 with market scenario 2.

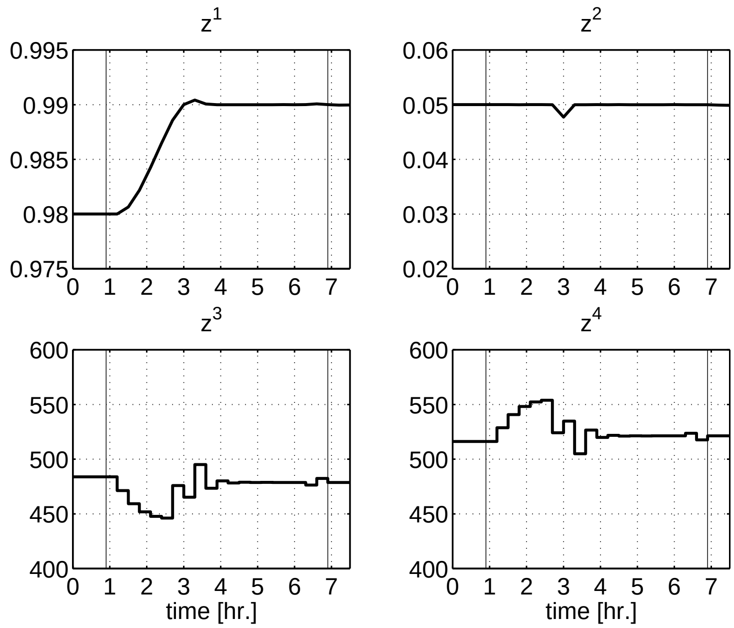


Figure 7.9: (successive MILP) Optimal trajectories of the first 4 performance variables (top purity z^1, bottom purity z^2, distillate flow z^3, bottom flow z^4) for a transition from grade 3 to grade 5 with market scenario 2.

Initial guess

In real-time optimization, successive solutions will typically be close. Consider the formulation of the LHOP in Section 6.6. An adequate initial guess for the l-th optimization cycle can be obtained by taking the remaining part of the previous solution and extending it (if required) by the steady state solution. A useful extension of this idea may be to correct the initial guess for the most recent estimation of the effect of the persistent disturbance. This way, the steady state effect of the persistent disturbance is compensated for so that the initial state trajectories will presumably get closer to the desired end-point. Let the steady state optimum input in the l-th cycle be denoted $\bar{u}^{sop,l}$. Further, let the LHOP solution in the l-th cycle be denoted $\bar{u}^{lhop,l}$. Then, an adequate initial guess is computed as follows

$$u^{p,l}(t) = \begin{cases} \bar{u}^{lhop,l-1}(t + \Delta T_{lhop}) + (\bar{u}^{sop,l} - \bar{u}^{sop,l-1}), & 0 < t < H^L - \Delta T_{lhop}, \\ \bar{u}^{sop,l}, & H^L - \Delta T_{lhop} < t < H^L, \end{cases} \tag{7.25}$$

where ΔT_{lhop} is the sampling time of the LHOP and H^L is its horizon length (for simplicity assumed constant here). If a uniform discretization basis is used to parametrize the controls and if the discretization interval fits the sampling time a whole number of times, then (7.25) directly yields an initial guess for the parameters. In case of different parametrizations (polynomial ones for example), an additional fit procedure will be required to compute the initial guess for the parameters on the basis of (7.25).

Initialization of the Hessian

The inner loop problem of the SSQP is solved using an SQP algorithm. The problem is strongly nonlinear so that many iterations may be required to converge. Although function and gradient evaluations for this SQP are comparatively fast, there is a clear incentive to limit the number of iterations required to a minimum. One way to enhance the convergence is via an adequate initialization of the Hessian. In real-time optimization a reasonable estimate of the Hessian is available from the previous cycle.

For simplicity, we consider only the case where a uniform discretization basis is used to parametrize the controls and with a constant horizon for the LHOP. Similar approaches can be derived for different parametrizations and horizon lengths. Let the parameter vector be given as follows $p = [u_0^T, u_1^T, \ldots, u_N^T]^T$. Further, let $\Delta T_{lhop} = n\tau$, with τ the discretization interval and with $n \in \mathbb{N}$. Then we can partition the Hessian that is computed in the solution of the $(l-1)$-th cycle as follows

$$H^{l-1} = \begin{bmatrix} H_{11}^{l-1} & H_{12}^{l-1} \\ H_{21}^{l-1} & H_{22}^{l-1} \end{bmatrix}, \tag{7.26}$$

where $H_{22}^{l-1} \in \mathbb{R}^{(N+1-n)n_u \times (N+1-n)n_u}$ is the part of the Hessian that concerns future inputs only. It is this part of the Hessian that is used in the construction of an initial estimate of the Hessian for the l-th optimization cycle:

$$H^{p,l} = \begin{bmatrix} H_{22}^{l-1} & H_{12}^{l} \\ H_{21}^{l} & H_{22}^{l} \end{bmatrix}. \tag{7.27}$$

There is no unambiguous initialization of H_{12}^l, H_{21}^l, and H_{22}^l. A pragmatic choice is $H_{12}^l, H_{21}^l = 0$ and H_{22}^l a unity matrix of appropriate dimension.

7.6 Contributions of this chapter

The grade change optimization problem is a crucial ingredient in our approach to market-focused operation. The focus on the market requires a flexible response of the entire company, which makes quick and cheap changeovers to customer-specific product grades an essential part of the operating strategy. Unfortunately, due to the strongly nonlinear dependency of the product rates for different grades on the quality variables, the economic optimization problem is a tedious one. In this chapter two new, tailor-made solutions were proposed for solving it.

In the first approach, a smooth approximation of the production rates is used. The SSQP method is developed for the optimization of this smooth approximation, motivated from the poor performance of SQP approaches for problems with strongly nonlinear objectives like this one. In the SSQP method, instead of using quadratic approximations based on successive gradients, we use an approximation in which only the process dynamics are linearized and the original nonlinear objective function is used. The optimization of this nonlinear approximation using the SQP method produces search steps for the original problem. Supposed that these search steps are of much better quality then in the conventional approach, fewer iterations and hence fewer costly evaluations of the model and the sensitivity equations are required to converge to a local minimum. The better performance of this method in comparison with the conventional SQP approach was demonstrated for a grade change problem on a binary distillation column.

In the second approach, the production rates are coupled to the quality variables via the introduction of a set of binary variables and linear equality and inequality constraints. Together with a linearization of the process dynamics these equations constitute a MILP inner loop optimization problem which can be used to generate search steps in the original nonlinear problem. The advantage of this approach over the SSQP method is that a guarantee on the (local) quality of the search steps (more precise: on the quality of the solution to the inner loop problem) can be obtained. The optimization procedure then reduces to the solution of a series of MILP's. This of course may be computationally demanding for large problems, which is a possible disadvantage of this approach. Some confidence was gained through the application of the successive MILP approach to the grade change problem on a binary distillation column, where computations spent on the MILP's were very fast.

Chapter 8

case III: HDPE production

This chapter presents the application of grade change optimization and production scheduling to a realistic simulation case study: production of HDPE in a gas-phase reactor. The aim of this study is to demonstrate for a specific case the feasibility and the potential benefits of the optimization approaches presented in this thesis. First, a process description is given (8.1). Next, the application of the SSQP method presented in Section 7.3 to the HDPE grade change optimization problem is treated (8.2). Finally we describe the application of the flexible, business-wide production scheduling and compare the performance to traditional slate scheduling for a specific market scenario.

8.1 The gas phase HDPE plant

A process schematic of the HDPE plant under consideration is given in Figure 8.1. The gaseous monomers, together with hydrogen and nitrogen enter the reactor at the bottom. Only part of the gas flow reacts on the catalyst surface in the fluidized bed; the rest leaves the reactor through the gas cap and is recycled through the counter current flow heat exchanger in which the heat of reaction is removed. Part of the content of the reactor can be flaired through the purge.

A grade of polymer is here defined by its density and melt index. The *density* of HDPE typically varies between 930 and 970 kg/m^3 [93] and is influenced by the amount of co-polymer (butylene in our case) that is injected into the reactor. The short branches that the co-polymer induces create sparser structures of the polymer, hence leading to decreased densities. The *melt index* is a measure of the polymer's viscosity. Different definitions of the melt index exist. In our model it is defined as the velocity with which the polymer moves through a standard die under standard conditions. The melt index is mainly influenced

performance channels (z)
1 polymer density
2 polymer melt index
3 production flow
4 cooling water flow
5 ethylene feed flow
6 butylene feed flow
7 hydrogen feed flow
8 catalyst feed flow
9 setpoint pressure controller

inputs (u)
1 butylene feed flow
2 hydrogen feed flow
3 catalyst feed flow
4 setpoint pressure controller

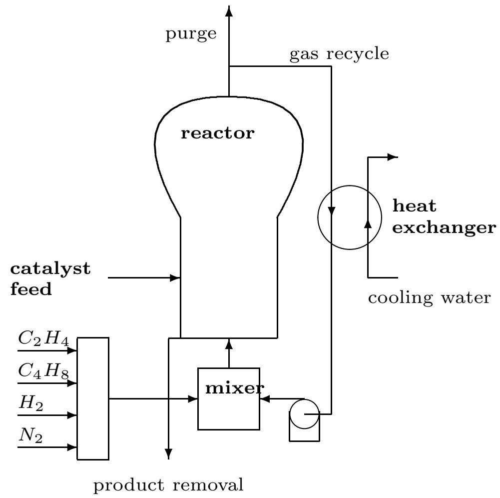


Figure 8.1: Schematic process flow sheet of the gas phase HDPE polymerization process.

g	constraints	
1	$932.8 < z^1 < 933.2$	$0.8 < z^2 < 1.2$
2	$937.8 < z^1 < 938.2$	$0.8 < z^2 < 1.2$
3	$937.8 < z^1 < 938.2$	$2.8 < z^2 < 3.2$
4	$932.8 < z^1 < 933.2$	$2.8 < z^2 < 3.2$
5	$942.8 < z^1 < 943.2$	$0.8 < z^2 < 1.2$

Table 8.1: The five production grades for the HDPE reactor.

by the amount of hydrogen added during production: hydrogen acts as a chain terminator hence more hydrogen leads to shorter chain lengths in the average and thus to higher melt indices. Melt indices vary over a wide range, typically 1e-3 through 1e3, therefore generally the logarithm of the melt index is used.

In this study we consider 5 different product grades. The product grades are defined by bounds on the density (z^1) and the natural logarithm of the melt index (z^2) of the polymer as given in Table 8.1.

Model of the HDPE plant

In our optimization studies we have at our disposal a DAE model of the HDPE plant. The model is based on [16] and the thesis of McAuley [55] and further refined by the author together with Wim van Brempt[1] in the IMPACT project.

[1] IPCOS Technology, Leuven

The model has the following properties:

- The fluidized bed is modeled as a 3-phase system, consisting of a bubble phase, an emulsion gas phase and an emulsion polymer phase. Both emulsion phases are assumed perfectly mixed. Mass transfer between the bubble phase and the emulsion gas phase is modeled using Fick's law. The emulsion gas phase and the emulsion polymer phase are assumed to be in phase equilibrium. The dynamics of the bubble phase are neglected. Instead, a static spatial concentration distribution (function of height) is modeled.

- Co-polymerization reactions (butylene co-monomer) occur on the surface of Ziegler-Natta catalyst particles in the emulsion polymer phase. The following reactions are modeled according to Ziegler-Natta kinetics [19]: 1. catalyst activation, 2. chain initiation, 3. chain propagation, 4. chain transfer, 5. catalyst deactivation. Zeroeth, first and second order moments of the polymer chain length distribution are calculated on the basis of which density and melt index are inferred using empirical relations.

- On top of the reactor a wide gas cap is placed in order to avoid catalyst and polymer particles to be entrained towards the cooler. The gas cap is modeled as being ideally mixed.

- The counter current heat exchanger is modeled using a multi-compartment model.

- A purge outlet flow makes it possible to remove nitrogen (and other gases) from the reactor.

- Four low-level PI controllers stabilize the process: a gas cap pressure controller (manipulating the ethylene input flow), a gas cap temperature controller (manipulating the heat exchanger cooling water flow), a fluidized bed level controller (manipulating the production outlet flow), and a nitrogen content controller (manipulating the nitrogen input flow).

- A flow driven representation is used.

The resulting model contains about 1000 variables amongst which 40 differential variables.

8.2 Grade change optimization

Nowadays, the control of grade changes in HDPE production is often a task for the operators. They typically use experience-based recipes for the manipulation of the controls so as to realize the transition in reasonable time. It is not likely that the operators use the plant to its full potential, simply because their insight in the plant dynamics is naturally limited. These limitations can be overcome using model-based optimization.

Model-based optimization of grade changes for HDPE processes has been studied before in literature, significant contributions were made by McAuley and McGregor [56, 55]. McAuley and McGregor mention several criteria that can be used to distinguish desirable transitions from undesirable ones: transition time, off-spec production, safety, economically desirable end-conditions. The optimization procedure that they present however does not reflect the economics of the transition, instead more or less arbitrary quadratic weightings on the deviation of the quality index variables from the target setpoints were used. We believe that the framework for economic optimization of grade transitions that we introduced in Section 5.2.3 and for which solution methods were presented in Chapter 7 is better suited to capture the different criteria for desirable grade transitions. To demonstrate this, the application of the SSQP method for the optimization of grade changes will be described next.

8.2.1 Problem formulation

The general mathematical formulation of the grade change problem is given in Section 5.2.3. The cost function is constituted by a part that represents the economics and an additional control type penalty. For the HDPE process, the economic objective is defined as

$$V_{ec} = \int_0^T \left(\sum_{r=1}^{3} p_F^r C_r(z) - \sum_{e \in \{g,h,6\}} p_P^e Y_e(z) \right) dt, \tag{8.1}$$

where the feed flows are given by $C_1(z) = z^5$, $C_2(z) = z^6$, and $C_3(z) = z^7$. Y_g and Y_h refer to the production flows of the departure grade and the target grade, respectively and are given by (7.4), where $F(z) = z^3$, G^g are defined by (7.5) and $M_g^e = 1$ if $g = e$ and zero otherwise. Y_6 refers to the production of off-spec material. It is assumed that during a transition, all material that is not within the specifications of either one of the grades connected by the transition is *off-spec* material. This leads to the introduction of a transition-dependent grade variable G^6 which is equal to one if the specifications of both grades are violated and zero otherwise. Hence, for a grade transition from grade g to h we have $G^6 = 1 - G^g - G^h$.

The horizon over which the optimization is done is fixed to 12 hours. Piecewise constant controls are sought with a sampling time equal to half an hour. To avoid solutions with unacceptably aggressive controls we consider in addition to the economic objective a control-type of objective. This objective function,

constraints		
0	$< z^4 <$	10^4
0	$< z^5 <$	10^4
0	$< z^6 <$	10^4
0	$< z^7 <$	5.2×10^4
0	$< z^{10} <$	1
24	$< z^{11} <$	30

Table 8.2: Process constraints for the HDPE reactor.

which we must admit is chosen rather arbitrarily, penalizes quadratically the rate of change of the input variables. The control objective is given as follows:

$$V_{co} = \begin{pmatrix} z_0^6 \\ z_0^7 \\ z_0^8 \\ z_0^9 \end{pmatrix}^T R_\Delta \begin{pmatrix} z_0^6 \\ z_0^7 \\ z_0^8 \\ z_0^9 \end{pmatrix} + \sum_{i=1}^{24} \begin{pmatrix} z_i^6 - z_{i-1}^6 \\ z_i^7 - z_{i-1}^7 \\ z_i^8 - z_{i-1}^8 \\ z_i^9 - z_{i-1}^9 \end{pmatrix}^T R_\Delta \begin{pmatrix} z_i^6 - z_{i-1}^6 \\ z_i^7 - z_{i-1}^7 \\ z_i^8 - z_{i-1}^8 \\ z_i^9 - z_{i-1}^9 \end{pmatrix},$$

The overall objective is obtained by combining the economic and control objective

$$V = V_{ec} + V_{co}.$$

The operation of the reactor is subject to operating constraints as given in Table 8.2. The most vital constraint in relation to safety of the process is the constraint on the cooling water flow. During normal operation of the plant strict bounds on the cooling water flow must be obeyed so as to guarantee a satisfactory safety margin in case of unexpected peaks in the heat production. The same safety margin must be guaranteed during transitions.

It was argued in 5.2.3 that different changeover strategies may need to be considered for a variety of market conditions. The sensitivity of the solutions with respect to the market conditions will be studied by varying the prices of the different grades of polymer and the feedstock.

Optimal steady state operating conditions are sought by static optimization. Provided the revenues on polymers exceed the cost of the raw material, the maximization of the added value reduces to the maximization of the production. The static optimization is performed using gPROMS' internal optimizer gOPT.

8.2.2 SSQP optimization

The SSQP approach to grade change optimization as outlined in Section 7.3 utilizes a smooth approximation of the objective function. The approximation that we use here is given by the Riemann sum of an approximation of the integral (8.1), $V^{d,0} = \tau \sum_{i=0}^{N-1} \tilde{L}^d(z_i)$, where $\tilde{L}^d$ is a smooth approximation of the function in (8.1), given by

$$\tilde{L}^d(z) = \sum_{r=1}^{3} p_F^r C_r(z) - \left(z^3 p_P^6 + z^3(p_P^g - p_P^6)\tilde{G}^g + z^3(p_P^h - p_P^6)\tilde{G}^h \right). \quad (8.2)$$

$\tilde{G}^g$ and $\tilde{G}^h$ are smooth approximations of G^g and G^h defined by

$$\tilde{G}^g := 1/\pi^2 \left(\arctan(\gamma_1(z^1 - z_l^{1,g})) + \arctan(\gamma_1(z_u^{1,g} - z^1)) \right) \cdot \\ \left(\arctan(\gamma_2(z^2 - z_l^{2,g})) + \arctan(\gamma_2(z_u^{2,g} - z^2)) \right), \quad (8.3)$$

where $z_l^{1,g}$, $z_l^{2,g}$ and $z_u^{1,g}$, $z_u^{2,g}$ are the lower and upper bounds, respectively on the density and melt index of the polymer for grade g. In our optimizations we choose γ_1 and γ_2 fixed and both equal to 200.

The end point constraint is incorporated by means of a penalty term added to the objective. The penalty term is given by $\sum_{i=1}^{n_x} q_{N,i}(x^i - \bar{x}^{h,i})^2$ with weighting factors $q_{N,i}$. Because most of the states are different physical quantities and numerical values can differ by orders of magnitude, $q_{N,i}$ are chosen so as to scale the contribution of the different states to the penalty. The scaling we apply is a division by the square of the steady state value of the corresponding state in the departure grade g, $q_{N,i} = \frac{q_N}{(\bar{x}^{g,i})^2+1}$, with q_N a positive scalar which we select equal to 100.

Analysis of the process nonlinearity shows the strong nonlinear dependency of some of the states on the inputs. This makes the optimization problem very hard to solve. To help fulfillment of the end-point constraint we force the trailing part (8 hours) of the input trajectory to be equal to the steady state values corresponding to the target grade. This is a very pragmatic way to enforce steady state behavior at the end of the horizon which has its roots in the very early industrial developments of MPC, see e.g. [24]. Because the controls are not allowed to vary over the trailing part of the horizon the states naturally converge to a steady state, assuming open loop stable behavior of the plant. An obvious disadvantage of this approach is that longer horizons are required and thus longer computation times. However, the combination with the quadratic penalty proves very effective in enforcing solutions that are close to the desired end-point without requiring the horizon over which the controls were fixed to be excessively long.

8.2.3 Results

First, as an example of the application of the SSQP method to the grade change optimization problem we consider the transition from grade 3 to 5 with $p_P^3 = 0.7$,

$p_P^5 = 1.5$, and $p_P^6 = 0.3$. Prices for the raw materials (ethylene, butylene, hydrogen) are chosen fixed for all optimization studies, respectively $p_F^1 = 0.45$, $p_F^2 = 0.6$, and $p_F^3 = 0.11$.

Step-wise input manipulation An indication of the open loop dynamics of the plant (under basic control) can be obtained from Figure 8.2 where the open loop controlled transition from grade 3 to 5 is plotted. Observe that it takes almost 10 hours for the density and the melt index to arrive within the specifications of grade 5. Further, the production and cooling water flow are increased due to the slower reactions of the ethylene in comparison with the co-polymer butylene. The cooling water flow even increases beyond the maximum cooling capacity, hence this transition is not even feasible in practice (the saturation on the cooling water flow is not coded in the model, instead it will be enforced in the optimization). The characteristics of the grade transition can be enhanced using model-based optimization as will be shown next.

SQP optimitization To demonstrate the performance of the SSQP method in comparison to the standard SQP approach we first apply the latter to the problem. The optimization is warm-started by providing an estimate of the Hessian like in the example of Section 7.3. Over 75 iterations and 100 function evaluations are required to converge to a local optimum of -29,978.9.

SSQP optimitization Next the SSQP method is applied to the same problem. Only 3 iterations are required to converge to a slightly better optimum, namely -30.1452. The resulting trajectories of the density (z^1), the melt index (z^2), the production (z^3) and the cooling water flow (z^4) are plotted in Figure 8.3. The bounds on density and melt index that define respectively grade 3 and 5 are included in the picture. The corresponding controls, the butylene feed (u^1), the hydrogen feed (u^2), the catalyst feed (u^3) and the pressure setpoint (u^4) are plotted in Figure 8.4. The actual changeover time is only 5 hours. During the changeover the production is reduced in order to minimize the losses due to off-spec production. This reduction of the production is established through a temporary reduction of the catalyst feed and the pressure setpoint. The cooling water flow is below a level of 5.2e4 at all times.

Different market situations

Next, the dependency of the optimal changeover strategy on different market situations is studied. Whether or not to consider different transition *modes* is an important decision in relation to the construction of the production database for the scheduler, see the discussion in Section 5.2.2. We explained in Section 5.2.3

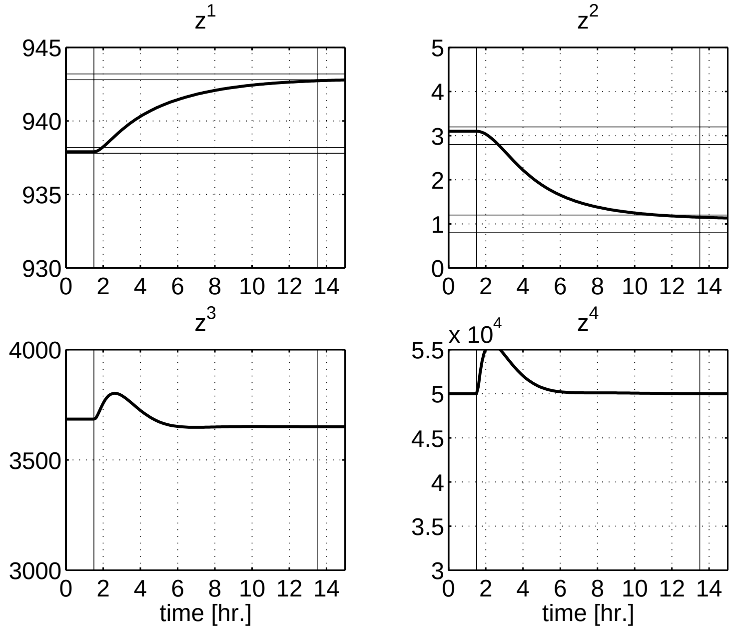


Figure 8.2: (SSQP) Trajectories of the density (z^1), the melt index (z^2), the production (z^3) and the cooling water flow (z^4) for a transition from grade 3 to grade 5 using step wise modification of the butylene feed, the hydrogen feed and the catalyst feed (u^1, u^2, and u^3).

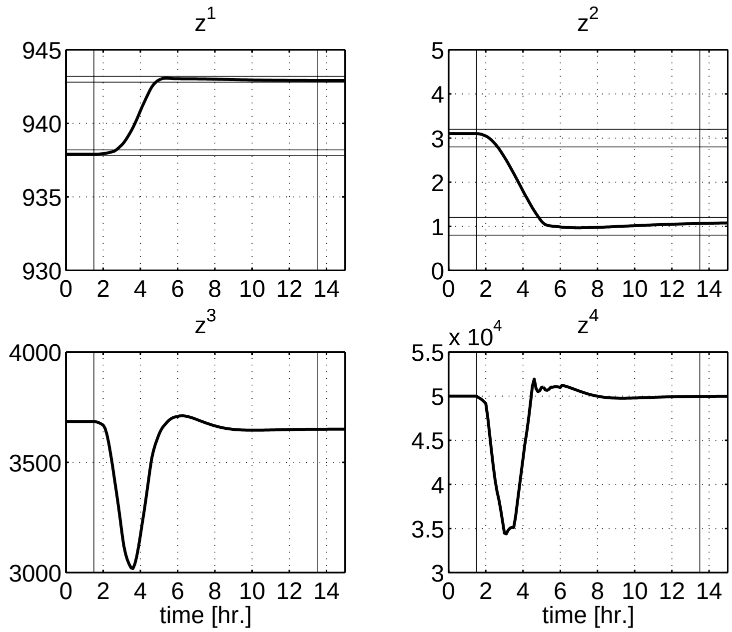


Figure 8.3: (SSQP) Optimal trajectories of the density (z^1), the melt index (z^2), the production (z^3) and the cooling water flow (z^4) for a transition from grade 3 to grade 5.

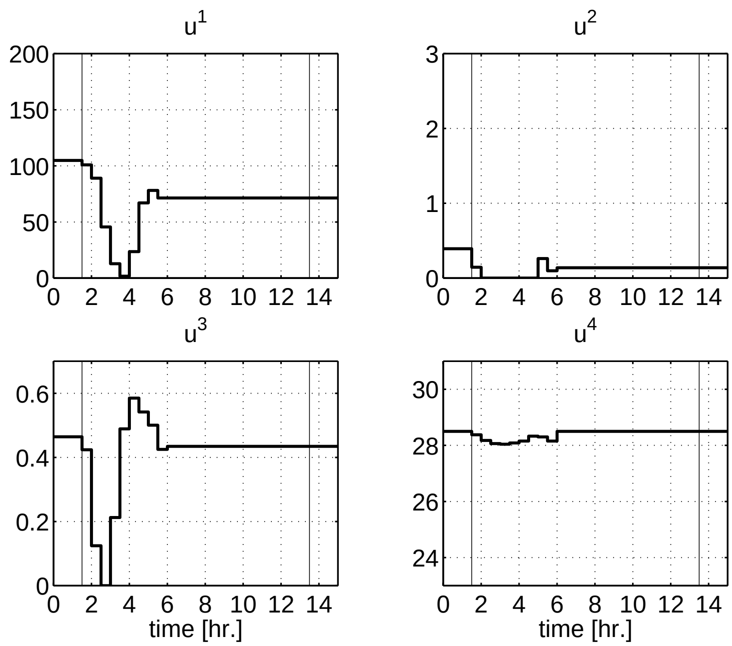


Figure 8.4: (SSQP) Optimal trajectories of the butylene feed (u^1), the hydrogen feed (u^2), the catalyst feed (u^3) and the pressure setpoint (u^4) for a transition from grade 3 to grade 5.

that the formulation of an integral economic objective function like (5.15) can be seen as a generalization of all relevant instances of the grade change problem, including the 'time-optimal' one. Different scenarios can be enforced by selecting different values for p_F^r and p_P^e. We consider again the transition from grade 3 to grade 5 for three different market scenarios. In the first scenario the prices for grade 3 and 5 are chosen equal so that there is no economic incentive to establish the grade change as early as possible. The second scenario is as described above, with a price for grade 5 that is significantly higher than that for grade 3 (1.5 compared to 0.7). In the third scenario, the only goal is to produce as much of grade 5 as possible. The trajectories of the the density (z^1), the melt index (z^2), the production (z^3) and the cooling water flow (z^4) are plotted in Figure 8.5 for the three scenarios. Apart from minor differences between the three solutions, the changeover strategies are quite similar for different market situations. Hence there appears to be no incentive for considering different transition modes. This can be explained from the fact that in HDPE transition control, the main factor determining transition economics is the amount of off-spec production. Economically optimal changeover strategies will tend to the minimization of off-spec production, pretty much independent of the factual prices of the grades.

Optimization of all transitions With the product prices chosen according to the second scenario, 20 grade transitions are optimized. These are used to construct the production database for the scheduler.

8.3 Production scheduling in compliance with process and market dynamics

Traditional production scheduling in HDPE plants is done using so-called grade slates, i.e. by running through fixed sequences of neighboring grades. Obviously, the flexibility of such an operating strategy in coping with changing market situations and attractive sales opportunities is limited. The dynamic optimization studies from the previous section demonstrate the feasibility of a more flexible operating strategy where the production schedule is determined on the basis of the most recent information from the market and the status of the plant and the stocks. How such a scheduling problem can be formulated was shown in Chapter 5.

In this section, we will investigate the potential improvement of this flexible plant scheduling in comparison with the traditional operation along product slates for the HDPE production plant. To this end we will introduce a specific market scenario (Section 8.3.1) for which the traditional and improved scheduling approach are implemented (Sections 8.3.2 and 8.3.3, respectively).

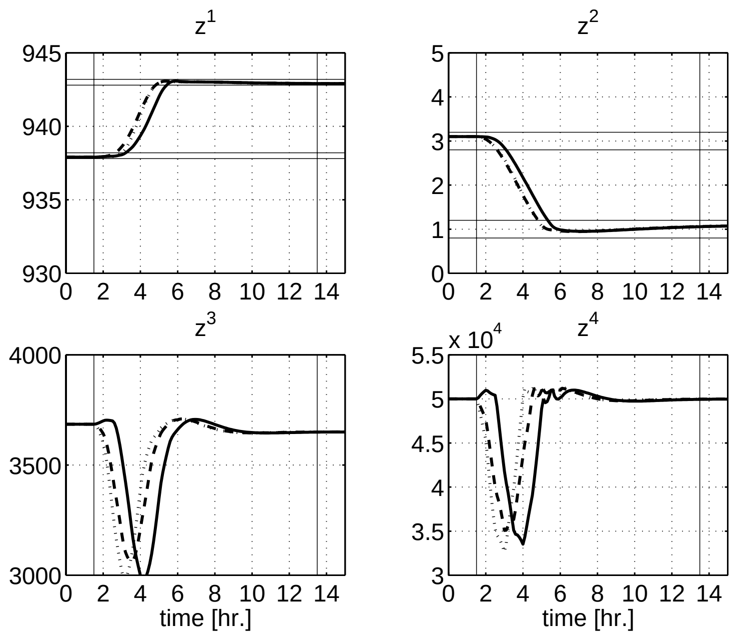


Figure 8.5: (SSQP) Optimal trajectories of the density (z^1), the melt index (z^2), the production (z^3) and the cooling water flow (z^4) for a transition from grade 3 to grade 5 for three different prices of grade 5: $p_P^5 = 0.7$ (solid), $p_P^5 = 1.5$ (dashed), $p_P^5 = 3$ (dotted).

g	h	$TY_1^{g,h}$	$TY_2^{g,h}$	$TY_3^{g,h}$	$TY_4^{g,h}$	$TY_5^{g,h}$	$TY_6^{g,h}$
1	1	4.455e+004	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
1	2	2.603e+003	2.999e+004	0.000e+000	0.000e+000	0.000e+000	1.170e+004
1	3	2.549e+003	0.000e+000	2.819e+004	0.000e+000	0.000e+000	1.354e+004
1	4	5.973e+003	0.000e+000	0.000e+000	2.287e+004	0.000e+000	1.557e+004
1	5	2.227e+003	0.000e+000	0.000e+000	0.000e+000	2.740e+004	1.428e+004
2	1	2.847e+004	4.411e+003	0.000e+000	0.000e+000	0.000e+000	1.071e+004
2	2	0.000e+000	4.413e+004	0.000e+000	0.000e+000	0.000e+000	0.000e+000
2	3	0.000e+000	9.550e+003	1.896e+004	0.000e+000	0.000e+000	1.550e+004
2	4	0.000e+000	2.207e+003	0.000e+000	2.668e+004	0.000e+000	1.475e+004
2	5	0.000e+000	3.928e+003	0.000e+000	0.000e+000	2.938e+004	1.057e+004
3	1	2.847e+004	0.000e+000	4.414e+003	0.000e+000	0.000e+000	1.066e+004
3	2	0.000e+000	2.956e+004	7.489e+003	0.000e+000	0.000e+000	6.957e+003
3	3	0.000e+000	0.000e+000	4.411e+004	0.000e+000	0.000e+000	0.000e+000
3	4	0.000e+000	0.000e+000	1.137e+004	2.427e+004	0.000e+000	7.476e+003
3	5	0.000e+000	0.000e+000	3.948e+003	0.000e+000	2.792e+004	1.171e+004
4	1	3.257e+004	0.000e+000	0.000e+000	4.467e+003	0.000e+000	7.304e+003
4	2	0.000e+000	2.812e+004	0.000e+000	2.602e+003	0.000e+000	1.333e+004
4	3	0.000e+000	0.000e+000	2.967e+004	3.894e+003	0.000e+000	1.063e+004
4	4	0.000e+000	0.000e+000	0.000e+000	4.462e+004	0.000e+000	0.000e+000
4	5	0.000e+000	0.000e+000	0.000e+000	2.228e+003	2.742e+004	1.427e+004
5	1	2.810e+004	0.000e+000	0.000e+000	0.000e+000	1.090e+003	1.408e+004
5	2	0.000e+000	2.782e+004	0.000e+000	0.000e+000	7.655e+003	7.585e+003
5	3	0.000e+000	0.000e+000	2.309e+004	0.000e+000	4.403e+003	1.610e+004
5	4	0.000e+000	0.000e+000	0.000e+000	2.447e+004	4.027e+003	1.490e+004
5	5	0.000e+000	0.000e+000	0.000e+000	0.000e+000	4.378e+004	0.000e+000

Table 8.3: Production data for the HDPE plant.

The process data is based on the results of the static and dynamic optimization described in the previous section. More details on the example can be found in [68].

8.3.1 Production, market and inventory data

A uniform discretization of time is chosen with production intervals of 12 hours. All transition times being smaller than 12 hours we can use the single-interval transition model described in Section 5.3.2. The production data which is computed on the basis of the static optimization of the grades and the dynamic optimization of grade transitions using (5.19,5.20) is given in Table 8.3. The consumption of raw materials for the grades and grade changes are given in Table 8.4.

A fictional order/opportunity database is constructed. The database is constructed in such a way that about 80% of the production capacity is used for production orders. The remaining production capacity can be used for attractive sales opportunities. Such opportunities frequently arise in the HDPE market, for example in case a competitor cannot meet his delivery contracts due to production problems or wrong-scheduling. The sales order/opportunity database is given in Table 8.5. The sets of time instances at which transactions can take

g	h	$TC_1^{g,h}$	$TC_2^{g,h}$	$TC_3^{g,h}$
1	1	4.300e+004	0.000e+000	0.000e+000
1	2	4.328e+004	2.999e+004	0.000e+000
1	3	4.326e+004	0.000e+000	2.819e+004
1	4	4.289e+004	0.000e+000	0.000e+000
1	5	4.330e+004	0.000e+000	0.000e+000
2	1	4.206e+004	4.411e+003	0.000e+000
2	2	4.304e+004	4.413e+004	0.000e+000
2	3	4.294e+004	9.550e+003	1.896e+004
2	4	4.209e+004	2.207e+003	0.000e+000
2	5	4.323e+004	3.928e+003	0.000e+000
3	1	4.202e+004	0.000e+000	4.414e+003
3	2	4.293e+004	2.956e+004	7.489e+003
3	3	4.302e+004	0.000e+000	4.411e+004
3	4	4.164e+004	0.000e+000	1.137e+004
3	5	4.293e+004	0.000e+000	3.948e+003
4	1	4.283e+004	0.000e+000	0.000e+000
4	2	4.304e+004	2.812e+004	0.000e+000
4	3	4.318e+004	0.000e+000	2.967e+004
4	4	4.307e+004	0.000e+000	0.000e+000
4	5	4.332e+004	0.000e+000	0.000e+000
5	1	4.170e+004	0.000e+000	0.000e+000
5	2	4.200e+004	2.782e+004	0.000e+000
5	3	4.251e+004	0.000e+000	2.309e+004
5	4	4.186e+004	0.000e+000	0.000e+000
5	5	4.308e+004	0.000e+000	0.000e+000

Table 8.4: Raw material consumption data for the HDPE plant.

place are chosen sparse in order to limit the number of binary decision variables. It is important to note that the scenario that we define is a snapshot of the supposedly true behavior of the internal supply chain and its interaction with the market in time. The market database should hence be seen as being the result of previous interaction with the market and the orders are negotiated preferably on the basis of earlier feedback from the scheduler to the sales managers. This being the setting that we consider we can without doing harm to reality assume (and enforce) that the order opportunity database is *feasible* i.e. that all orders can indeed be delivered. To be able to compare the performance achieved with the traditional slate scheduling to the performance with the flexible scheduling, feasibility is ensured for the inflexible slate scheduling approach too.

The purchasing strategy for HDPE production is of little interest in this study. Observe from Table 8.4 that the consumption rate of ethylene, the main raw material, is almost similar for all grades. Consumption of butylene and hydrogen is relatively low for all grades and so will be the economic impact of how these are acquired from the market. Moreover, HDPE production often takes place in the near vicinity of ethylene production facilities which provide a limitless supply of ethylene. If this is not the case, still average consumption rates can be used to predict the necessary consumption on the basis of which a purchase strategy can be chosen independent of production and sales decisions. For these reasons and to avoid the dimension of the optimization problem to be

Sales of grade 1

s	$SA^{1,s}$	$S\$^{1,s}$	$\Omega_{1,s}$	$SO^{1,s}$
1	300,000	0.7	{8}	1
2	150,000	1.55	{15,22}	0
3	200,000	0.71	{15,22}	1
4	250,000	0.72	{43,50}	1
5	180,000	1.20	{71,78}	0

Sales of grade 2

s	$SA^{2,s}$	$S\$^{2,s}$	$\Omega_{2,s}$	$SO^{2,s}$
1	250,000	0.70	{8,15}	1
2	200,000	1.31	{22,29}	0
3	250,000	1.60	{28,35}	0
4	150,000	1.20	{43,50,57}	0
5	200,000	0.65	{64,71}	1

Sales of grade 3

s	$SA^{3,s}$	$S\$^{3,s}$	$\Omega_{3,s}$	$SO^{3,s}$
1	250,000	1.60	{8,15}	0
2	300,000	0.70	{22,29}	1
3	200,000	1.65	{50,57}	0
4	150,000	1.30	{64,65}	0

Sales of grade 4

s	$SA^{4,s}$	$S\$^{4,s}$	$\Omega_{4,s}$	$SO^{4,s}$
1	250,000	0.70	{8}	1
2	200,000	1.15	{22,29,36}	0
3	300,000	0.71	{36,43,50}	1
4	150,000	1.20	{57,64,71}	0

Sales of grade 5

s	$SA^{5,s}$	$S\$^{5,s}$	$\Omega_{5,s}$	$SO^{5,s}$
1	200,000	0.60	{8,15}	1
2	250,000	1.35	{15,22,29}	0
3	200,000	1.50	{29,36,43}	0
4	220,000	0.73	{50,57,64}	1
5	150,000	1.25	{71,78}	0

Sales of off-spec material

s	$SA^{6,s}$	$S\$^{6,s}$	$\Omega_{6,s}$	$SO^{6,s}$
1	100,000	0.32	{8,..,36}	0
2	100,000	0.33	{43,..,78}	0

Table 8.5: Sales order and opportunity database for the HDPE production facility.

enlarged unnecessarily, the purchase decisions are not included in the scheduling problem. The economic objective is modified likewise. Instead of including the contribution of the purchase expenses, a fixed-priced cost of raw-material is instituted. The objective recursion (5.32) then becomes:

$$V_{t+1} = (1+\gamma)V_t + \sum_e \sum_s S_{t+1}^{e,s} SA_S^{e,s} \$^{e,s} - \sum_r \sum_g \sum_h T_t^{g,h} TC_r^{g,h} p_F^r,$$

with $p_F^1 = 0.45$ (ethylene), $p_F^2 = 0.6$ (butylene), and $p_F^3 = 0.11$ (hydrogen) Initial inventory levels, the storage constraints and the end-storage appreciation of respectively the raw materials and the end products are finally given in Tables 8.6 and 8.7. To represent a practical situation as realistically as possible non-zero initial storage levels are chosen, denoted respectively RS_1^r and ES_1^e in the aforementioned tables. These values are chosen rather high so as to avoid infeasibility of orders, especially when considering the less flexible slate scheduling scheme. To avoid a surplus of profit due to the large initial storage levels an equal amount of material in storage is required at the end of the horizon. Thereto the problem formulation is extended with the following inequality constraints:

$$ES_H^e > ES_{H,l}^e, \quad RS_H^r > RS_{H,r}^r.$$

r	RS_l^r	RS_u^r	RS_1^r	$RS_{H,l}^r$	$R\$^r$
1	0	10,000,000	1,100,000	600,000	0.45
2	0	450,000	60,000	35,000	0.60
3	0	2,000	250	100	3.30

Table 8.6: Raw material storage attributes for the HDPE plant.

e	ES_l^e	ES_u^e	ES_1^e	$ES_{H,l}^e$	$E\$^e$
1	0	5,000,000	325,000	300,000	1.02
2	0	5,000,000	315,000	300,000	0.98
3	0	5,000,000	270,000	300,000	1.06
4	0	5,000,000	270,000	300,000	1.05
5	0	5,000,000	306,000	300,000	1.03
6	0	5,000,000	22,000	0	0.33

Table 8.7: End product storage attributes for the HDPE plant.

8.3.2 Traditional slate scheduling

Sinclair [77] elaborates on how slates for polymer production are determined. The slate he considers is going back and forth through a sequence of grades. The sequence is determined in such a way that the overall grade change effort, which can be characterized for example by grade change time or off-spec production, is minimized. We assume that the off-spec production during a grade change is characteristic for its undesirability. The minimization of the total amount of off-spec production leads to the following MILP optimization:

$$\min_{G_{g,t}\in\{0,1\}} \left\{ \sum_g \sum_h \sum_t T_{g,h,t} TY_{6,g,h} \mid \exists T_{g,h,t} \text{ s.t. } \begin{array}{l} \sum_g G_{g,t} = 1, \\ \sum_{t=1}^5 G_{g,t} = 1, \\ G_{g,t} = G_{g,10-t}, \forall t \in \{2,\dots,4\} \\ \sum_g \sum_h T_{g,h,t} = 1, \\ \sum_h T_{g,h,t} \leq G_{g,t}, \\ \sum_g T_{g,h,t} \leq G_{h,t+1}, \forall t \in \{1,\dots,7\},\ \sum_g T_{g,h,8} \leq G_{h,1} \end{array} \right\}, \tag{8.4}$$

where $G_{g,t}$ are the binary decision variables representing the grades and $T_{g,h,t}$ are the transition variables (see also Section 5.3.2). The first constraint implies that only one grade can be performed at a time, the second states that each of the 5 grades should appear once in the first half of the slate, the third enforces the slate to be symmetric along the middle grade. The last three constraints enforce that the corresponding transition variables are selected, like in (5.17). The solution of (8.4) is given by the grade sequence $\{5, 2, 1, 4, 3, 4, 1, 2\}$. The repeated execution of this sequence of grades defines the production slate.

Literature is not very explicit on how the timing of product slates is executed in a practical setting. Sinclair [77] tends to an a priori fixation of the durations of the slate, however an operating strategy that never adapts production to actual sales seems unrealistic. The alternative is to determine the duration of the grades using a model-based optimization approach as proposed for the flexible scheduling. Prinssen [68] analyzes both approaches, assuming that realistic operation should probably be somewhere in the middle. We will follow the same approach.

Fixed duration

This strategy represents the least flexible operation that we consider. Production is scheduled on the basis of average demand figures. No flexibility is present to adjust the operating strategy to the market situation. Instead, the best one can do is to adjust the sales strategy to the market situation for as long as inventory levels permit this. Sinclair [77] describes how an optimal cycle time can be computed by balancing the transition costs against the cost of inventory. He shows how this problem leads to NLP's of moderate dimension which can be solved using standard software. Prinssen [68] analyzes this approach and outlines some limitations, the main one being the assumption of constant demand rates. Relaxing this assumption means that one must pragmatically add minimum buffer storage to cope with time-varying demands which makes the use of determining the optimal cycle time via optimization at least questionable. Based on a few test optimizations Prinssen concludes that a cycle time of 6 weeks seems reasonable for the problem at hand. The starting grade for the grade slate and the order base are selected such that all orders can be delivered. Because the production decisions are fixed according to the a priori determined grade slate the only remaining degree of freedom is purchase management, i.e. the fixation of delivery times and the negotiation with customers to turn sales opportunities into orders. To optimally support this decision making we construct an optimization problem using the mathematical formulation of the scheduling problem given in Chapter 5 where all the grade decision variables are fixed corresponding to the product slate. The optimal sales decisions are computed using CPLEX, which takes only a fraction of a second.

The optimum found is 2,857,900. The optimal sales strategy is depicted in Figure 8.6 where the production schedule as well as variations in the storage levels of the 6 end products are given for the 6 weeks horizon that is under consideration. Storage levels increase gradually during production and decrease abruptly due to sales actions. The corresponding transaction number is given in the figure where a star is used to indicate when the corresponding transaction concerns a sales opportunity. All orders are delivered in time which is a logical consequence of the fact that the order database was constructed to be feasible.

Besides the product orders the scheduler selects the sales opportunities 5 for grade 1, 4 for grade 2, 4 for grade 4 and 2 for the off-spec material. At this stage we cannot conclude whether and to what extent the inflexible production strategey leads to a performance that is far off from the true potential of the plant. Therefore we need to compare the obtained results with the more flexible scheduling strategies which will be treated next.

Flexible duration

The mathematical formulation of the flexible slate scheduling problem is almost equivalent to that of the flexible scheduling problem which will be described next with the exception that only the appropriate transitions are allowed. This amounts to fixing all the grade transition variables associated with transitions that are not allowed in the slate to zero.

The slate scheduling problem is implemented GAMS. The BB solver CPLEX is used to solve it. Approximately 3 hours of computation on a moderate personal computer were required to solve the problem to a solution with a guaranteed distance of 3.5% from the best open node. The resulting objective value was 3,245,032 which is over 13% better than the optimum objective obtained with the slate with fixed duration. The corresponding course of the main variables in the problem is displayed in Figure 8.7. Observe that many transitions are made so that the entire product slate is executed twice within the period of 6 weeks. More transitions lead to increased off-spec production, however the increased flexibility makes it possible to select more and more attractive sales opportunities. Opportunity 3 for grade 2 is selected, 1 and 3 for grade 3, 3 for grade 5, and finally 2 for the off-spec material. From Table 8.5 it can be observed that these are indeed more attractive sales opportunities than the ones selected in case of the fixed-duration slate scheduling.

We can conclude that the scheduling of the durations in the product slate in compliance with the market situation can yield large benefits compared to the inflexible operation with fixed durations. The reader should note however that realistic operation of the slate is probably somewhere in between the fixed and optimal duration schedules that were treated here.

Next we will investigate what further improvements can be achieved if, by means of advanced process control technology, all transitions are enabled, leading to the flexible scheduling approach discussed in Chapter 5.

8.3.3 Flexible production scheduling

The inherent inflexibility of the slate scheduling approach can be overcome using the flexible scheduling approach outlined in Chapter 5. In this approach the production is allowed to switch to any other grade at each production interval,

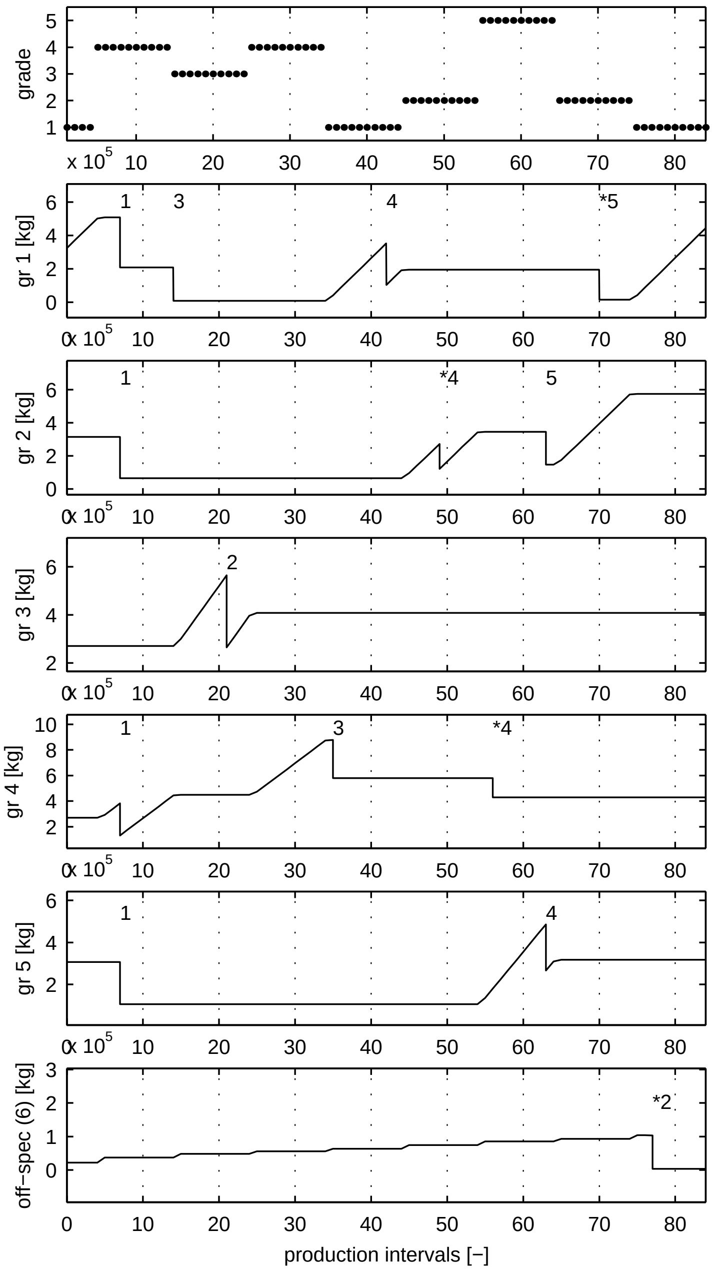


Figure 8.6: Fixed duration slate schedule for HDPE production. Grades (top) and storage levels of the end-products (bottom).

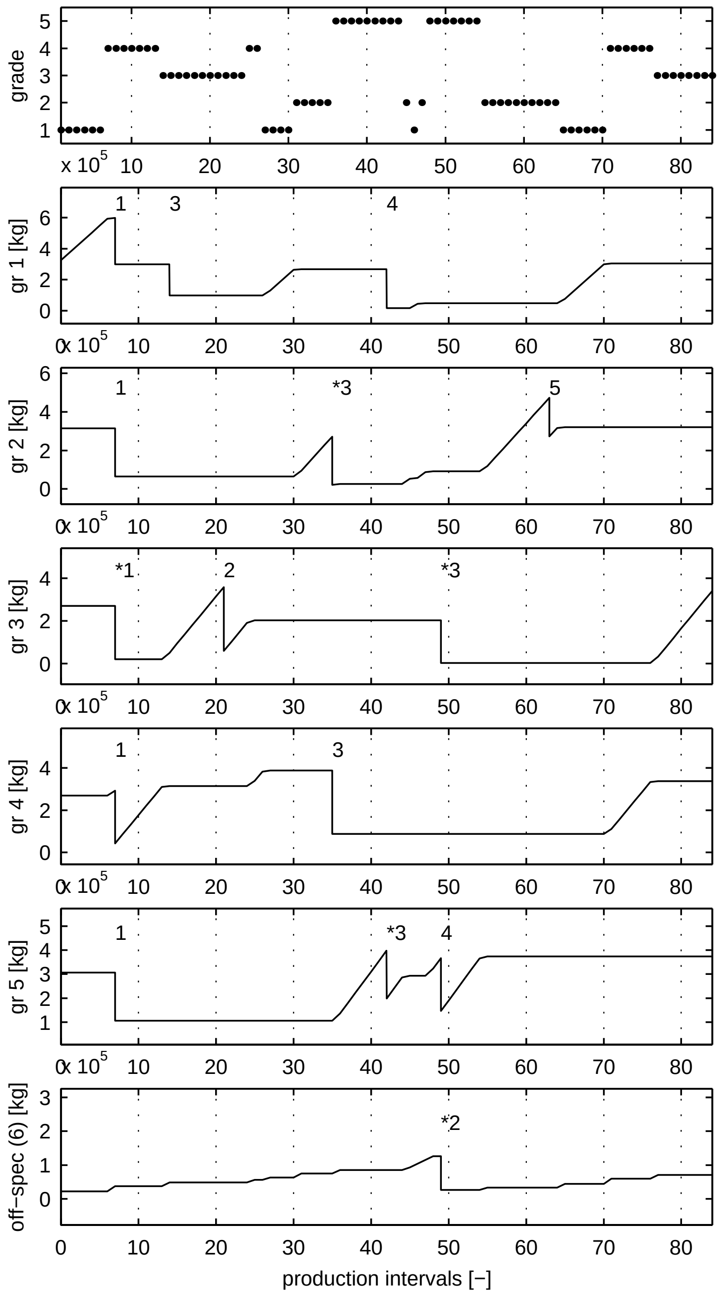


Figure 8.7: Flexible duration slate schedule for HDPE production. Grades (top) and storage levels of the end-products (bottom)

providing much improved flexibility to deal with changes in the market situation and to react to attractive sales opportunities. Whether and to what quantitative extent this improved flexibility can be useful in case of HDPE production scheduling is studied next.

A solution to the flexible scheduling problem was found in several hours and to a guaranteed optimality of slightly more than 2.3 %. The objective value was equal to 3,339,845 which is over 16.8 % better than the performance achieved with the fixed-duration slate and 2.9 % better than the flexible-slate scheduling. The flexible scheduler selects all the sales opportunities that were also selected by the flexible-duration slate scheduler. However, in addition to that the attractive sales opportunity 2 for grade 1 is selected, which makes the performance significantly better.

Although the improvement compared to the flexible-duration slate scheduling is less spectacular than the improvement of the latter over the fixed-duration slate scheduling it should be noted that the flexible scheduling approach leads to fewer transitions (11) than the flexible-duration slate scheduling (14) which is attractive for other than economic reasons as well.

8.3.4 Discussion

The results presented in this section demonstrate the potential benefits of the flexible scheduling approach in comparison to the inflexible slate-mode of operation, however a few remarks may be needed to put the presented results in the right perspective.

First, *all* schedules, also the least flexible ones, assume the presence of an advanced, dynamic-optimization-based control systems for grade changes. If we were to compare the flexible scheduling performance to a practical situation the results would probably be even more in favour of our approach because of the often highly inefficient changeover strategies that occur in current practice.

Second, the difference between the performance achieved using the flexible-duration slate scheduler and the flexible scheduler is somewhat blurred due to the fact that both problems were not solved to guaranteed optimality. In the worst case the performance would be equal for both approaches however this is not likely because even if the flexible slate scheduler would select the same sales opportunities it is likely to be able to do so only at the expense of more transitions.

Third, one must be careful not to be over-optimistic in estimating the potential benefits of the solutions that we propose. Of course, the whole case is fictional, and the presence of so many attractive sales opportunities is probably an exceptional situation in practice. Still, *if* attractive sales opportunities arise the flexible scheduler is a lot more likely to honor them than the slate scheduler,

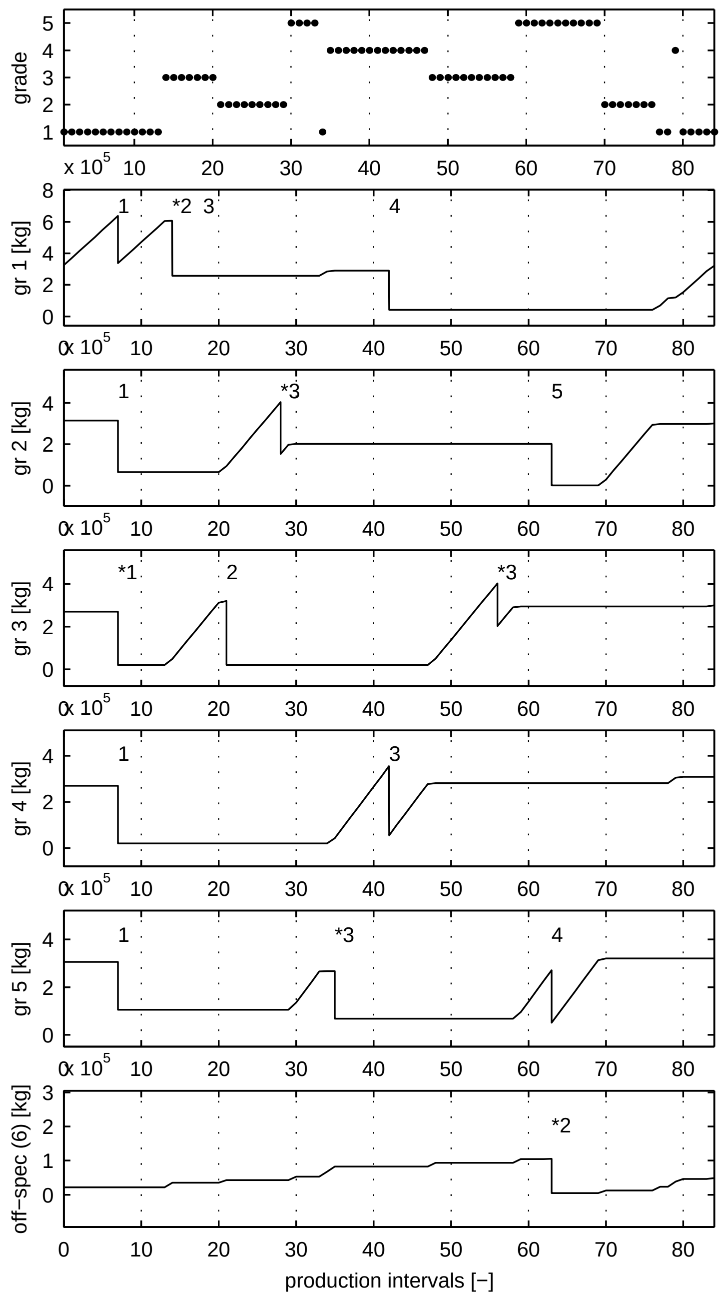


Figure 8.8: Flexible schedule for HDPE production. Grades (top) and storage levels of the end-products (bottom)

sufficient confidence of which is provided by the results presented in this section. Another practical issue that is not represented in this example is the possibility for *blending* different grades. In practice, blending provides an additional means to achieve production flexibility.

Finally, it should be noted that only a single, open-loop optimization result has been shown. The closed loop performance of the internal supply chain, where the scheduler responds to deviations of the market and the process from the prediction, is not analyzed here since this would require extensive and very time-consuming simulations. Such an exercise is required however to gain insight in the true benefit of the solutions that are proposed.

8.4 Contributions of this chapter

This chapter presents the application of the off-line model based grade change optimization techniques presented in Chapter 7 and the supply-chain-conscious production scheduling of Chapter 5 to a realistic simulation of HDPE production. The aim of this chapter is to demonstrate the *feasibility* as well as the *potential* of the developed methods for a realistic simulation case that is relevant to chemical process industry.

The *off-line grade change optimization studies* demonstrate both the feasibility and the potential of economics-based optimization of grade transitions in HDPE production using the methods presented in this thesis. Despite the considerable dimension of the model (approximately 1000 variables) and a total number of 96 optimization parameters, local minima were attained in tens of minutes on a moderate PC. Using the newly developed SSQP method convergence was attained in no more than 15 iterations. For the same problem, the SQP method uses over 75 iterations and as many costly evaluations of the model and the sensitivities. As to the operational benefits for this specific case, model based optimization reduces grade change times from a typical 10-12 hours (for step wise modification of the controls) to a typical 5-6 hours. Also, the optimizer successfully reduces production levels during the transition in order to minimize *off-spec* production.

The application of the flexible production scheduler to the HDPE case demonstrates the possibility to support decision making of production and sales managers in such a way that the economic performance of the entire internal supply chain is optimized. A six week production schedule and sales strategy are optimized for a 5-grade HDPE plant using MILP optimization. The optimization is done for a specific, fictional order/opportunity database that represents the market situation. The predicted added value for this flexible scheduling approach is compared to the added value achieved using the more traditional slate scheduling and significant improvements in the order of several per cents of the

CAV are concluded.

Chapter 9

Conclusions and recommendations

This thesis concerns the development of new, market-focused operating strategies for continuous chemical manufacturing plants. To this end two main problems were formulated in Chapter 2:

1. How can we schedule the production of continuous chemical processes in compliance with market demands and the capacity of the process, and to a company- (or supply-chain-wide-) optimum ?
2. How can we control the operation of continuous chemical plants subject to disturbances in compliance with the production schedule and to an economic optimum ?

Answers to these questions are given in Section 9.1. Finally, recommendations for further research are given in Section 9.2.

9.1 Conclusions

The conclusions are categorized according to the sub-problems that were outlined in Chapter 2.

1. Scheduling

For a chemical manufacturing company to merge to market-focused operation purchasing, production and sales decision making should be geared to one another and strive for a common, company-wide goal. This can be achieved through the institution of a scheduler that continuously selects the most desirable decisions regarding purchasing, production and sales so as to optimize the predicted behavior of the entire company. **For single-machine multi-grade processes, such a scheduler can be designed by capturing the purchasing, production and sales decisions and their effect on the company's objective into a MILP which can be solved using standard software.**

In particular, three design aspects were treated in this thesis: how to model the decision making, how to optimize it, and finally, how to fit the scheduler in the company organization.

Modeling of the internal supply chain The scheduling methodology has been developed for a simple supply chain model, consisting of a multi-grade single-machine continuous chemical plant with raw material storage, end product storage and two markets at both sides. The modeling of storage is done by mass balancing. Modeling of production decision making and purchasing/sales decision making is an essential contribution of this thesis.

Production decision making is modeled using a task description of the plant. Two types of tasks are distinguished: finite interval stationary tasks and transition tasks. Each tasks has an associated production interval and a production decision is to switch from one quasi stationary task to another. In order to reflect the true potential of the plant, the characteristics of both types of task (amount of used raw material and produced end product) are computed via model-based optimization.

Regarding the modeling of the *purchasing/sales decision making* we looked for ways to enable the scheduler to respond naturally to changes in the market. The resulting approach models company-market interaction using a transaction-based framework. In this framework two types of transactions can be described: orders and opportunities. Orders are deliveries or acquisitions according to contracts, opportunities are foreseen purchasing or sales possibilities and in those the expected status of the market can be expressed. Using this framework the interaction with different market types, amongst which monopoly, oligopoly and the free competition, can be modeled.

Mathematical formulation and optimization The scheduler oversees the union of all possible decisions and selects a sequence of decisions that is desirable with respect to a company-wide objective. We showed in Chapter 5 that this selection can be done via the solution of a MP, more specifically a MILP. In the formulation of this MILP time is discretized uniformly and purchasing, production and sales actions are defined for each time interval. Binary variables are introduced to describe whether or not these actions are executed. Process transitions and their effect on material flows are included in the formulation without the need to introduce additional binary variables. Reasonable solution times were encountered for the two test problems that were considered in this thesis, the simple blending example (Chapter 5) and the HDPE production example (Chapter 8), however no guarantee on the solution time can be obtained. For practical use of the scheduler sub-optimal heuristic solutions may need to be considered.

Decision support and organization We believe that *cooperation* is the most suitable organizational concept when it comes to the (re-)organization of purchasing, production and sales decision so as to achieve market-focused operation. The assumption in a cooperative decision structure is that all players strive for a common goal, the remaining problem being how to make sure that the player's perception of the company-wide goal and his contribution to it is accurate enough so to achieve action-taking that is indeed in line with the company-wide objective. This is where the role of the scheduler is imperative. The scheduler selects out of the union of all foreseen purchasing, production and sales actions a set of 'optimal ones'. This way, the scheduler provides feedback to the players and hence a basis to assess the value of their local decisions and initiatives.

2. Control

Through the use of the scheduler large operational benefits can be gained potentially, provided that the control system is designed in such a way that a market-focused operating strategy is sustained. **In this thesis we show how for single machine, multi-grade plants this can be realized through the institution of a NMPC-type control law that includes constraints on the production to enforce a consistent coupling with the scheduler and an economic objective to maintain operating conditions that are economically attractive.** In particular, this thesis considers the following design aspects: how to guarantee that the production is realized according to schedule, and how to ensure acceptable computation times so as to make real-time implementation possible. The latter aspect is approached from two different perspectives. One is the decomposition of the control law in different control layers on the basis of time scale analysis. The other is the tailoring of dynamic optimization methods in order to reduce computation times.

Design strategy The basic control solution that we propose consists of a state estimator in combination with a deterministic receding horizon optimization, largely inspired by existing NMPC schemes. To make the plant a predictable and reliable link in the internal supply chain, satisfaction of the production schedule (and hence satisfaction of customer demand) should be guaranteed when possible. This can be achieved by including in the definition of the receding horizon optimization problem constraints on the production and the product quality in accordance with the product schedule. Remaining degrees of freedom are used to optimize the process economics. This way, a true integration of process control and economic optimization is achieved.

Decomposition The basic optimization-and-control scheme that we propose combines nonlinear dynamics, long horizons and fast sampling times. This leads to problems that are computationally intractable. To resolve this, we propose several decompositions of the control problem for different disturbance scenarios. The most challenging scenario that we consider is the one in which a multi-grade processes is operated in the presence of disturbances. The decomposition that we propose is based on the distinction of different time scales at which disturbances occur. We distinguish fast, stochastic type disturbancess and slow, persistent type disturbances. The latter have a long term effect but because of their slow nature we need not respond to them immediately. Instead, we compute at a relatively low sampling frequency and based on estimates of the slow disturbances the steady state optimal operating conditions and the optimal trajectories towards those. The fast disturbances make immediate control action necessary. To this end, the short term control decisions are computed on the basis of a short-horizon optimization problem that aims to steer back to a point on the long-term trajectory in an economically optimal fashion. Constructive finite-horizon control laws are proposed accordingly and demonstrated successfully on the binary distillation example.

Tailored dynamic optimization strategies The control and optimization of multi-grade plants entails non-smooth optimization problems. This is due to the discontinuous dependence of the product flows on certain product quality variables. Due to the non-smoothness, gradient based methods will fail to yield satisfactory performance. This thesis describes two new approaches to solving dynamic-economic optimization problems for multi-grade processes. Both methods use control parametrization to transform the infinite-dimensional dynamic optimization problem in a parameter optimization problem.

The first method, denoted Successive Sequential Quadratic Programming (SSQP), solves a smooth approximation of the non-smooth grade change problem by solving in each iteration a SQP that is constructed via a linearization of the dynamics only. The inner loop SQP is supposed to yield a much better approximation of the original optimization problem than a QP would, so that much fewer iterations are required to converge to an optimum. Simulation studies on a distillation column and a HDPE reactor confirm this.

The second method, denoted Successive MILP, uses a finite set of binary decision variables to relate the production flows to the product quality variables. Search steps are computed using MILP via successive linearization of the plant dynamics. The advantage of this approach over the SSQP method is that in each iteration a guarantee on the quality of the solution to the inner loop (search step) problem is achieved. However, this method does not allow to include additional quadratic penalties on for example input deviations or the deviation of the final state from the desired end point. The feasibility of this approach is demonstrated on a distillation example.

9.2 Recommendations for further research

The recommendations for further research are categorized according to the two research questions that were considered in this thesis.

Production scheduling

- The framework for modeling the chemical factory and its interaction with the marketplace is very simple. An extension of this framework that captures more of the typical mechanisms characterizing continuous chemical manufacturing sites is recommended. Such an extension may involve multiple plants, combined continuous and batch operations, blending operations and more complex interactions with the market.
- The solution of MILP problems is often an intricate task. This is also true for the scheduling problem defined in this thesis: although computation times were reasonable for the HDPE case, other cases or even other instances of the HDPE case may require very long computation times. This is not acceptable in a real-time decision support tool. To circumvent this problem, heuristic or semi-exact, semi-heuristic solution approaches to the scheduling problem have to be developed. Such solutions naturally sacrifice solution quality, however possibly at the benefit of shorter and better predictable computation times.
- The proposed scheduling strategy for continuous chemical manufacturing plants is the result of an academic effort. The application of this strategy to practical cases is recommended so as to investigate the true potential and limitations of the proposed method.

Economic optimization and control

- The most crucial ingredient in the economic optimization and control solutions that we propose is a model of the plant. The derivation of such models, typically by combining first principles with data obtained from dedicated identification experiments, is a very difficult and expensive task. Another big problem is the reduction of the model size and its computation time to acceptable levels. Research towards systematic, efficient nonlinear modeling and model reduction is believed to be the key-enabler of the model-based solutions that we propose.

- The control solution that we propose consists of a state estimator and a deterministic receding horizon controller. Stochastic disturbances are dealt with in the estimation part only. For the constrained, nonlinear control problems that we are faced with, this may not be sufficient. One of the problems that may occur is that the receding horizon controller runs into infeasibilities. Such problems can be circumvented if the presence of stochastic disturbances in combination with process constraints is taken into account in the controller design.

- Currently, very few implementations of NMPC and other nonlinear-model based controllers in chemical process applications exist. As a consequence, there is little feedback to the process control research community regarding the functioning and the applicability of the solutions that are proposed by this community. Academia should take a cooperative attitude and strive for more implementations through cooperation with process industries and process control software suppliers. The results from such implementations can be used to (re-)focus the research activities that are ongoing in the field of nonlinear model-based process control. Interesting questions in this respect may be the following:

  - To what extent is computation time limiting the performance? Can computation time be traded against the accuracy of the solution?
  - To what extent is plant-model mismatch limiting the performance? How can robustness be achieved?
  - Can we, based on control implementation results, identify the critical parts in the model, so as to focus modeling or model refinement effort to those parts?

9.3 A challenge for future process control research

This thesis defines the problem of process control in the wide context of business-wide optimization. This is an important feature that distinguishes this research from most other academic contributions in the area of process control. The investigation of process control within a business-wide context is believed to be an appealing direction for future process control research for various reasons. First, the business-wide context forces the process control researcher to think of performance specifications that make sense: the fact that the process is considered in relation to its (economic) environment will provide increased insight in the requirements of future process control solutions and will guide the development of these.

Second, the extension of the system boundary to capture not only the process itself but also its interaction with other processing units and the marketplace provides researchers new, interesting challenges, both of theoretical and practical nature. Some of these were mentioned in the previous section.

Finally, for academia choosing a business-wide context of their process control research, will make their contributions easier interpretable by and more appealing to industry. Therefore, such a focus may help to bridge the theory-practice gap in process control.

Bibliography

[1] Z. Amini, J. Lin, and P.D. Roberts. Single iterative algorithm with global feedback for integrated system optimisation an parameter estimation of large scale industrial processes: Optimality, convergence and simulation. *IEEE Proceedings-D*, 139(5):447–459, September 1992.

[2] G. Applequist, O. Samikoglu, J.F. Pekny, and G.V. Reklaitis. Issues in the use, design and evolution of process scheduling and planning systems. *ISA Transactions*, 36(2):81–121, 1997.

[3] K.R. Baker. *Introduction to sequencing and scheduling.* Series in discrete mathematics and optimisation. Wiley Interscience, 1974.

[4] J.A. Bandoni, J.A. Romagnoli, and G.W. Barton. On optimising control and the effect of disturbances: calculation of the open-loop backoffs. *Computers and Chemical Engineering Suppl.*, 18:S505–S509, 1994.

[5] M.H. Bassett, P. Dave, F.J. Doyle III, G.K. Kudva, J.F. Pekny, G.V. Reklaitis, S. Subrahmanyam, D.L. Miller, and M.G. Zentner. Perspectives on model based integration of process operations. *Computers and Chemical Engineering*, 20(6-7):821–844, 1996.

[6] M.L. Bell and R.W.H. Sargent. Optimal control of inequality constrained dae systems. *Computers and Chemical Engineering*, 24(11):2385–2404, 2000.

[7] A. Bemporad and M. Morari. Control of systems integrating logic, dynamics, and constraints. *Automatica*, 3:407–427, 1999.

[8] D. Berry, M.M. Naim, and D.R. Towill. Business process re-engineering an electronic products supply chain. *IEE Proceedings of Science, Measurement and Technology*, 142(5):395–403, September 1995.

[9] G.G. Betts and F.J. Plenard. *Future changes in the chemical industry.* EFCE Publications Series No. 20. Rugby, 1981.

[10] H.G. Bock, M.M. Diehl, D.B. Leineweber, and J.P. Schloder. A direct multiple shooting method for real-time optimization of nonlinear dae processes. In F. Allgőwer and A. Zheng, editors, *Nonlinear Model Predictive Control; Progress in Systems and Control Theory Vol. 26*, pages 245–267. Birkhäuser Verlag, Basel, 2000.

[11] M.L. Brisk and W.A. Walker. The economic benefits of advanced process control. In D. Behrens, editor, *Strategies 2000. Proceedings of the 4th World Congress of Chemical Engineering, Karlsruhe, Germany, 16-21 June 1991.*, pages 1040–1046, Frankfurt am Main, Deutschland, 1992. Dechema Verlag.

[12] A.E. Bryson. *Dynamic optimization.* Addison-Wesley, 1999.

[13] A.E. Jr. Bryson and Y.C. Ho. *Applied optimal control.* Washington: Hemisphere, 1975.

[14] A.K. Chakravarty. *Market driven enterprise : product development, supply chains, and manufacturing.* Wiley, New York, 2001.

[15] H. Chen and F. Algőwer. A quasi-infinite horizon nonlinear model predictive control scheme with guaranteed stability. *Computers and Chemical Engineering*, 34(10):1205–1217, 1998.

[16] K.Y. Choi and W.H. Ray. The dynamic behavior of fluidized bed reactors for solid catalyzed gas phase olefin polymerization. *Chemical Engineering*, 40:2261–2279, 1992.

[17] M.L. Darby and D.C. White. On-line optimization of complex process units. *Chemical Engineering Progress*, 84(10):51–59, 1988.

[18] V.D. Dimitriadis and E.N. Pistikopoulos. Flexibility analysis of dynamic systems. *Ind. Eng. Chem. Res.*, 34:4451–4462, 1995.

[19] N.A. Dotson, R. Galvan, R.L. Laurence, and M. Tirell. *Polymerization process modelling.* VCH Publishers, USA, 1996.

[20] S.A.W. Drew. The application of hierarchical control methods to a managerial problem. *Int. J. of Systems Science*, 6(4):371–395, 1975.

[21] W. Findeisen, F.N. Bailey, M. Brdys, K. Malinowski, P. Tatjewski, and A. Wozniak. *Control and coordination in hierarchical systems.* Chicester - John Wiley and Sons, New York, 1980.

[22] C.A. Floudas. *Nonlinear and mixed-integer optimization: fundamentals and applications.* Topics in chemical engineering. Oxford University Press, 1995.

[23] J.W. Forrester. *Industrial dynamics.* MIT Press, 1961.

[24] J.B. Froisy. Model predictive control: past, present and future. *ISA Transactions 22*, pages 235–243, 1994.

[25] J.B. Froisy and J. Richalet. Industrial applications of IDCOM. *In T.J. McAvoy, Y. Arkun and E. Zafiriou (editors), Model based proces control of the 1988 IFAC Workshop, Georgia, USA*, pages 233–244, 1986.

[26] D.E. Garrett. *Chemical engineering economics.* Van Nostrand Reinhold, New York, 1989.

[27] Gangadhar Gattu and Evanghelos Zafiriou. Observer based nonlinear quadratic dynamic matirx control for state space and input/output models. *The Canadian Journal of Chem. Eng.*, 73:883–895, December 1995.

[28] I.E. Grossmann and Z. Kravanja. Mixed-integer nonlinear programming: A survey of algorithms and applications. In L.T. Biegler, T.F. Coleman, and A.R. Conn, editors, *Large-scale optimisation with applications. Part II: Optimal design and control*, pages 73–100. Springer Verlag, 1997.

[29] S.K. Gupta and J. Kyparisis. Single machine scheduling research. *OMEGA*, 15(3):207–227, 1987.

[30] A. Heaton. *The chemical industry.* Blackie academic & professionals, 1994.

[31] A. Helbig, O. Abel, and W. Marquardt. Structural concepts for optimization based control of transient processes. In F. Allgőwer and A. Zheng, editors, *Nonlinear Model Predictive Control; Progress in Systems and Control Theory Vol. 26*, pages 295–311. Birkhäuser Verlag, Basel, 2000.

[32] M.A. Henson. Nonlinear model predictive control: current status and future directions. *Computers and Chemical Engineering 23*, pages 187–202, 1998.

[33] A. Hertz, E. Taillard, and D. de Werra. Tabu search. In E.H.L. Aarts and J.K. Lenstra, editors, *Local search algorithms*, Series in discrete mathematics and optimization, chapter 5, pages 121–136. Wiley Interscience, 1997.

[34] D.H. van Hessem, C. Scherer, and O.H. Bosgra. LMI-based closed-loop economic optimization of stochastic process operation under state and input constraints. In *Proceedings of the 40th IEEE CDC 2001, Orlando, USA*, 2001.

[35] F.S. Hillier and G.J. Lieberman. *Introduction to operations research.* McGraw-Hill, sixth edition, 1995.

[36] J. Ingham, I.J. Dunn, E. Heinzle, and J.E. Prenosil. *Chemical Engineering Dynamics*. VCH, New York, 1994.

[37] N. Karmarkar. A new polynomial-time algorithm for linear programming. *Combinatorica*, 4:373–395, 1984.

[38] S. Kirkpatrick, C.D. Gelatt jr., and M.P. Vecchi. Optimisation by simulated annealing. *Science*, 220:671–679, May 1983.

[39] E. Kondili, C.C. Pantelides, and R.W.H. Sargent. A general algorithm for short-term scheduling of batch operations - i. MILP formulation. *Computers and Chemical Engineering*, 17(2):211–227, 1993.

[40] H. Kwakernaak and R. Sivan. *Linear optimal control systems*. Wiley New-York, 1972.

[41] J.H. Lee and N.L. Ricker. Extended kalman filter based nonlinear model *Ind. Eng. Chem. Res.*, 33:1530–1541, 1994.

[42] J.H. Lee and Zhenghong Yu. Worst-case formulations of model predictive control for systems with bounded parameters. *Automatica*, 33:763–781, 1997.

[43] F.L. Lewis. *Optimal estimation; with an introduction to stochastic control theory*. Wiley, New York, 1986.

[44] F.L. Lewis and V.L. Syrmos. *Optimal control*. Wiley, New York, 1995.

[45] W.C. Li and L.T. Biegler. Multistep, newton-type control strategies for constrained nonlinear processes. *Chem. Engng. Res. Dev.*, 67:562–577, 1989.

[46] W.C. Li, L.T. Biegler, C.G. Economou, and M. Morari. A constrained pseudo-newton control strategy for nonlinear systems. *Computers and Chemical Engineering*, 14:451–468, 1990.

[47] C. Loeblein and J.D. Perkins. Economic analysis of different structures of on-line process optimization systems. *Computers and Chemical Engineering Suppl.*, 20:S551–S556, 1996.

[48] C. Loeblein and J.D. Perkins. Analysis and structural design of integrated on-line optimization and regulatory control systems. *Aiche Journal*, 45:1030–1040, 1999.

[49] J. Z. Lu. Multi-zone control under enterprise optimization: needs, challenges and requirements. In F. Allgwer and A. Zheng, editors, *Nonlinear Model Predictive Control; Progress in Systems and Control Theory Vol. 26*, pages 394–402. Birkhäuser Verlag, Basel, 2000.

[50] R. Luus. Optimal control of batch reactors by iterative dynamic programming. *Journal of Process Control*, 4(4):218–226, 1994.

[51] W.J. Luyben, B.D. Tyréus, and M.L. Luyben. *Plantwide process control*. McGraw-Hill, 1999.

[52] S. Macchietto. Bridging the gap - integration of design, operations scheduling and control. In D.W.T. Rippin, J.C. Hale, and J.F. Davis, editors, *Proceedings second International Conference on Foundations Of Computer Aided Process Operations, Crested Butte, Colorado, USA*, pages 207–230, 1993.

[53] W. Marquardt, O.H. Bosgra, and T. Backx. Towards intentional dynamics in supply chain conscious process operations. In *Proceedings third International Conference on Foundations Of Computer Aided Process Operations, Snowbird, Utah, USA*, 1998.

[54] D. Mayne. Nonlinear model predictive control: challenges and opportunities. In F. Algower and A. Zheng, editors, *Nonlinear Model Predictive Control; Progress in Systems and Control Theory Vol. 26*, pages 394–402. Birkhäuser Verlag, Basel, 2000.

[55] K.B. McAuley. *Modelling, estimation and control of product properties in a gas phase polyethylene reactor*. PhD thesis, McMaster University, 1991.

[56] K.B. McAuley and J.F. MacGregor. Optimal grade transitions in a gas phase polyethylene reactor. *Aiche Journal*, 38:1564–1576, 1992.

[57] D. Mesarovic, M.D. Macko and Y. Takahara. *Theory of hierarchical, multilevel systems*. Academic Press, New York, 1970.

[58] H. Michalska and D. Mayne. Robust receding horizon control of constrained nonlinear systems. *IEEE Trans. on Automatic Control*, 38:1512–1516, 1993.

[59] H. Mühlenbein. Genetic algorithms. In E.H.L. Aarts and J.K. Lenstra, editors, *Local search algorithms*, Series in discrete mathematics and optimization, chapter 6, pages 137–171. Wiley Interscience, 1997.

[60] S.G. Nash and A. Sofer. *Linear and Nonlinear Programming*. McGraw-Hill, 1996.

[61] V. Nevistic. Mpc with linear time-varying prediction models. Technical report, Automatic control laboratory, ETH Zurich, Switzerland, 1997.

[62] G. De Nicolao, L. Magi, and R. Scattolini. Stability and robustness of nonlinear receding horizon control. In F. Allgőwer and A. Zheng, editors, *Nonlinear Model Predictive Control; Progress in Systems and Control Theory Vol. 26*, pages 394–402. Birkhäuser Verlag, Basel, 2000.

[63] C.C. Pantelides. Unified frameworks for optimal process planning and scheduling. In D.W.T. Rippin, J.C. Hale, and J.F. Davis, editors, *Proceedings second International Conference on Foundations Of Computer Aided Process Operations, Crested Butte, Colorado, USA*, pages 253–274, 1993.

[64] L.R. Petzold. A description of dassl: A differential/algebraic system solver. *Scientific computing*, pages 65–68, 1983.

[65] M. Pinedo. *Scheduling: theory, algorithms and systems*. Prentice-Hall, 1995.

[66] L.S. Pontryagin. *The mathematical theory of optimal processes*. Interscience, New York, 1962.

[67] B. Prasad. Decentralized cooperation: a distributed approach to team design in a concurrent engineering organization. *Team Performance Management*, 4(4):138–165, 1998.

[68] W. Prinssen. Supply-chain-conscious scheduling of single-machine multi-product continuous chemical processes, M.Sc. thesis. Technical report, Mechanical Engineering Systems and Control Group, Delft University of Technology, The Netherlands, 2000.

[69] Y. Ramamurthi, P.B. Sistu, and B.W. Bequette. Control-relevant dynamic data reconciliation and parameter estimation. *Computers and Chemical Engineering*, 17(1):41–59, 1993.

[70] G.V. Reklaitis. Overview of scheduling and planning of batch process operations. In *Proceedings NATO ASI on Batch processing systems engineering, Antalya, Turkey*, pages 660–705, 1992.

[71] J. Richalet, A. Rault, J.L. Testud, and J. Papon. Model predictive heuristic control: applications to industrial processes. *Automatica*, 14:413–428, 1978.

[72] P.D. Roberts. An algorithm for steady-stae system optimization and parameter estimation. *International Journal of Systems Science*, 10(7):719–734, 1979.

[73] D.G. Robertson and J.H. Lee. A least squares formulation for state estimation. *Journal of Process Control*, 5(4):291–299, 1995.

[74] P.O.M. Scokaert and J.B. Rawlings. Constrained linear quadratic regulation. *IEEE Trans. on Automatic Control*, 43(8):1163 –1169, 1998.

[75] R. Selpulchre, M. Janković, and P. Kokotović. *Constructive nonlinear control*. Springer, 1997.

[76] M.D. Simmons and G.W.T. White. The decentralized profit maximization of interconnected production systems. part i. the theory of price coordination. *Int. J. of Control*, 25(5):705–719, 1977.

[77] K.B. Sinclair. Grade change flexibility - defined, determined, compared. In *Proceedings fifth International Conference on Polyolefins, Houston, Texas, USA*, pages 2–19, 1987.

[78] J. Stevens. Integrating the supply chain. *International Journal of Physical distribution and Material Management*, 19:3–8, 1989.

[79] S. Støren and T. Hertzberg. The sequential linear quadratic programming algorithm for solving dynamic optimization problems - a review. *Computers and Chemical Engineering*, 19:495–500, 1994.

[80] P. Tanartkit and L.T. Biegler. A nested, simultaneous approach for dynamic optimization problems - i. *Computers and Chemical Engineering*, 20:735–741, 1996.

[81] P. Tanartkit and L.T. Biegler. A nested, simultaneous approach for dynamic optimization problems - ii: the outer problem. *Computers and Chemical Engineering*, 21:1365–1388, 1997.

[82] S. Tayur, R. Ganeshan, and M. Magazine. *Quantitative models for supply chain management*. Kluwer academic, Boston, 1999.

[83] W.Dahmen T.Binder, L.Blank and W.Marquardt. Towards multiscale dynamic data reconciliation. Technical report, Aachen University of Technology, 1998.

[84] V.J. Terpstra. *Batch scheduling within the context of intelligent supervisory process control*. PhD thesis, Delft University of Technology, 1996.

[85] R.L. Tousain and O.H. Bosgra. Efficient dynamic optimization for nonlinear model predictive control - application to a high-density poly-ethylene grade change problem. In *Proceedings of the 39th IEEE CDC 2000, Sydney, Australia*, 2000.

[86] R.L. Tousain, C.W.J. Hol, and O.H. Bosgra. Measured variable selection and nonlinear state estimation for mpc, with application to a high-density poly-ethylene reactor. In *Proceedings of the Process Control and Instrumentation Conference 2000, Glasgow, Scotland*, 2000.

[87] D.R. Towill. Industrial dynamics modelling of supply chains. *Int. J. of Phys. Distr. & Log. Man. 26*, pages 23–42, 1995.

[88] J.J. van der Schot, R.L. Tousain, A.C.P.M. Backx, and O.H. Bosgra. Ssqp for the solution of large-scale dynamic-economic optimization problems. *Computers and Chemical Engineering Supplement*, pages S507 – S510, 1999.

[89] V.S. Vassiliadis. *Computational Solution of Dynamic Optimisation Problems with General Differential-Algebraic Constraints*. PhD thesis, University of London, 1993.

[90] T.T.L. Vu, P.A. Bahri, and J.A. Romagnoli. Operability considerations in chemical processes: a switchability analysis. *Computers and Chemical Engineering*, 21(Suppl.):S143–S148, 1997.

[91] V. White, J.D. Perkins, and D.M. Espie. Switchability analysis. *Computers and Chemical Engineering*, 20(4):469–474, 1996.

[92] D.A. Wismer. *Optimization methods for large-scale systems with applications*. McGraw-Hill, New York, 1971.

[93] T. Xie, K.B. McAuley, J.C.C. Hsu, and D.W. Bacon. Gas phase ethylene polymerizations: Production processes, polymer properties, and reactor modelling. *Ind. Eng. Chem. Res.*, 33:449–479, 1994.

[94] M.G. Zentner, A. Elkamel, J.F. Pekny, and G.V. Reklaitis. A language for describing process scheduling problems. *Computers and Chemical Engineering*, 22(1-2):125–145, 1998.

[95] M.G. Zentner, J.F. Pekny, G.V. Reklaitis, and J.N.D. Gupta. Practical considerations in using model-based optimization for the scheduling and planning of batch/semicontinuous processes. *Journal of Process Control*, 4(4):259–280, 1994.

[96] Z. Zhang, R.W. Pike, and T. A. Hertwig. An approach to on-line optimization of chemical plants. *Computers and Chemical Engineering*, 19:305–310, 1995.

[97] K. Zhou, J.C. Doyle, and K. Glover. *Robust and optimal control*. Prentice Hall, New Jersey, 1996.

List of symbols

Symbol	Description
A	continuous time state space state transition matrix
B	continuous time state space input-to-state matrix
	Hessian approximation
c	mole fraction in liquid phase
c_K	feed composition (distillation example)
C	raw material consumption (rate)
C_x	state selection matrix in DAE plant description
C_u	input selection matrix in DAE plant description
d	disturbance
D	distillate flow
ES	end product storage
EV	end product storage end-appreciation
(f, g)	vector functions used to represent DAE plant model
$\mathcal{F}$	set of feasible operating conditions
F	vector function representing material flows
g	grade
	vector function representing grade constraints
G	grade variable
	coefficient in the p to z sensitivity matrix
$\mathcal{G}_g$	set of operating conditions for grade g
h	vector function used to represent process constraints
H	horizon length
H^L	horizon length LHOP
H^S	horizon length SHOP
I	liquid flow
J	objective value
	vapour flow
k	time index
K	feed flow (distillation example)

l	(linear) weight factor
L/L^d	added value function
$\mathcal{L}$	Lagrangian function
	objective map
M	matrix mapping material flow to end-product flow
M_l	lower bound holdup blender
M_u	upper bound holdup blender
$\mathcal{M}$	merit function
	model map
n	number
O	molar holdup on tray
O_d	molar holdup in the reflux drum
O_R	molar holdup in the reboiler
p	price, optimization parameters
P	purchase variable
	realized production level
$P\$$	sales unit price
PA	sales amount
PI	set of time spans
PO	sales order/opportunity variable
q	quality variable,
	quadratic weight factor
q_K	feed condition (distillation example)
Q	constant
	weighting matrix
r	relaxation variable
R	covariance matrix
	weighting matrix
R_r	Reflux ratio
RS	raw material storage
RV	raw material storage end-appreciation
S	sales variable
SA	sales amount
$S\$$	sales unit price
SO	sales order/opportunity variable
t	time
T	(end-) time
$T^{g,h,m}$	transition variable (from grade g to grade h in mode m)
T_g^h	transition from grade g to grade h
T_u	input to performance variable sensitivity
T_{Nx}	input to final-state sensitivity
ΔT_{shop}	SHOP sampling time

ΔT_{sop}	SOP sampling time
ΔT_{lhop}	LHOP sampling time
TC	consumption of raw material during transition
TM	transition mode
TY	yield of end product during transition
$\mathcal{T}$	set of transitions
u	input variables
$\mathcal{U}$	set of input trajectories
v	mole fraction in vapour flow
V	objective value
V_{ec}	economic objective value
V_{co}	control objective value
V_E	final state penalty value
w	Gaussian white noise signal
W	bottom outflow (in distillation column)
x	state variables
y	algebraic variable in DAE plant description
y^m	measured output
Y	end product yield (rate)
z	performance variable
α	weight factor
α_v	relative volatility
β	weight factor
γ	interest rate (per time span)
ϵ	constant
Γ	discrete time state space input-to-state matrix
λ	Lagrange multiplier
Φ	discrete time state space state transition matrix
τ	(transition) time interval
Ω	set of time spans

Sub/superscript	**Description**
C	consumption
d	disturbance
e	end product index
f	fast
g, h	grade index
G	production action
i	time index
$initial$	initial value
k	time index
l	lower bound

L	LHOP
m	transition mode
p	purchasing order/opportunity index
P	purchasing action
r	raw material index
R	reference
s	sales order/opportunity index
	slow
S	sales action
	SHOP
u	upper bound
Y	yield
$\bar{\cdot}$	optimal value
$\hat{\cdot}$	estimated/approximated value

List of abbreviations

Abbreviation	**Description**
APC	Advanced Process Control
B2B	Business-to-Business
BB	Branch and Bound
BFGS	Broyden, Fletcher, Goldfarb, and Shannon
CAV	Cumulative Added Value
DAE	Differential Algebraic Equations
DCS	Distributed Control System
DMC	Dynamic Matrix Control
EFCE	European Federation of Chemical Engineering
EKF	Extended Kalman Filter
EQP	Equality constrained Quadratic Programme
GRG	Generalized Reduced Gradient
HDPE	High-Density Poly-Ethylene
IDCOM	Identification and Command
IMPACT	Improved Polymers Advanced Control Technology
INCOOP	INtegration of process COntrol and plant-wide OPtimization
IQP	Inequality constrained Quadratic Programme
LHOP	Long Horizon Optimization Problem
LP	Linear Programme/Programming
LPV	Linear Parameter-Varying
LTV	Linear Time-Varying
MILP	Mixed Integer Linear Programme/Programming
MIP	Mixed Integer Programme/Programming
MINLP	Mixed Integer NonLinear Programme/Programming
MP	Mathematical Programme/Programming
MPC	Model Predictive Control
NLP	NonLinear Programme/Programming
NMPC	Nonlinear Model Predictive Control
NP	Nondeterministic Polynomial

OPC	OLE for Process Control
OR	Operations Research
PC	Personal Computer
QP	Quadratic Programme/Programming
RTPO	Real Time Process Optimization/Optimizer
SHOP	Short Horizon Optimization/Optimizer
SOP	Static Optimization/Optimizer
SSQP	Successive Sequential Quadratic Programme/Programming
TCP-IP	Transport Control Protocol-Internet Protocol
UA(-factor)	product of the heat transfer coefficient (U) and the heat-passing surface (A)
UDM	Uniform Discretization of time Modeling

Appendix A

Review of scheduling approaches and solution methods

A.1 Formulations of scheduling problems

Literature displays many different classes of more or less generic scheduling problems and corresponding formulations. Production scheduling in chemical manufacturing is an interesting application area for operations research (OR) sciences. Overviews of scheduling methods derived from OR can be found in e.g. [3, 65]. In OR, scheduling problems are typically classified according to the $\{\alpha|\beta|\gamma\}$ notation, where α describes the machine environment, β the processing constraints and γ the objective. The machine environment defines amongst others the processing times, release dates (earliest time at which a job may start) and due dates (latest time at which it may finish) of the processing jobs on the different machines. Processing constraints may include precedence constraints, sequence-dependent setup times and alike. Typical objectives used are 'minimum makespan', 'minimum lateness', or 'weighted completion time'. Many different combinations of these characteristics have been studied in literature. Also, efficient solution methods have been developed for a range of such problems, some of which are derivations of solutions to well known OR problems as the traveling salesman problem like the knapsack problem. Extensive and specific research has been done on the problem of scheduling jobs on a single machine. An excellent though somewhat outdated overview can be found in [29].

The scheduling problem at hand has a few typical characteristics which make it hard to fit in the existing OR framework. The main problem is that the OR-framework assumes that it has already been determined *which* jobs are to be scheduled, which leads to a *sequencing* problem rather than the scheduling problem we intend to examine. Also, the objectives typically used in OR are too simple to express economically optimal operation. In the definition of OR-objectives it is generally assumed that the production scheduling is subjected to production orders only. According to our view on horizontal integration, the scheduler should support the purchase and sales decision making and a basic consequence of this is that it is *not* determined a priori which of the orders and opportunities are to be met. Finally, the scheduling problem for continuous chemical manufacturing leads to the introduction of sequence-dependent transition tasks which are characterized by a transition time and the corresponding raw material consumption and production. Although sequence-dependent changeover times are mentioned in many papers on production scheduling, to our knowledge there exists no general scheduling formulation which takes the sequence-dependent consumption and production, and the existence of multiple transition modes as discussed in this thesis into account as well.

A.2 Solution methods for scheduling problem

The solution of scheduling problems can not be seen independent from their mathematical formulation. Because of the combinatorial nature of scheduling problems in general, one must be very careful (and sometimes a bit fortunate) not to end up with problems of unmanageable dimension and/or complexity. Therefore, in formulating scheduling problems there is a clear trade-off between the accuracy of the formulation and the tractability of the problem. We can mainly distinguish two classes of solution methods, *mathematical programming methods* and *heuristic methods*.

A.2.1 Mathematical programming (MP) methods

The most thorough way to describe a combinatorial problem is as MP. Common formulations are Mixed-integer Programmes (MIP) and disjunctive programmes. We will consider MIP's only.

MIP's are defined as follows.

$$\min_{x \in \mathbb{R}^m, y \in \mathbb{N}^n} \{f(x,y) \mid g(x,y) \leq 0, h(x,y) = 0\}. \tag{A.1}$$

If $n \neq 0$, $m \neq 0$ and f, g and h are all linear the problem is a Mixed Integer Linear Programme (MILP). If either f, g or h is nonlinear, the problem is a

Mixed Integer Nonlinear Programme (MINLP). Popular solution methods for MILP's are Branch and bound (BB), Benders decomposition, and cutting planes methods. MINLP's can be solved using BB, generalized benders decomposition, extended cutting planes, and outer approximation methods, see e.g. [28] or [22] for recent reviews. BB methods are the most popular and most broadly used methods in literature on scheduling. A short description of BB optimization for MILP's is given in Appendix B, for more details we refer to [35]. The main advantage of using MP tools for solving scheduling problems is that the solution quality is guaranteed. *If* an integer solution is available, then a worst-case distance from the optimum is available as well because the best possible relaxation acts as a lower bound on the optimum (in case of a minimization problem). Of course, the integer solution itself provides an upper bound. The solution process can be terminated if the worst case distance is within the desired accuracy. This way, the lengthy computations required to converge to the real optimum can be avoided. Another advantage of exact methods is their relative transparency. A clear disadvantage of exact methods is computation time. A large number of integer decision variables typically leads to lengthy computations; nonlinearity of the objective or the constraints often decreases the computational feasibility dramatically.

A.2.2 Heuristic methods

Heuristic methods exist for solving scheduling problems of any type and in any form and hence heuristic solvers provide an alternative or an add-on to exact methods. We can roughly distinguish two different types of heuristic methods: local search methods and rule-based methods. *Local search methods* try to improve on the solution quality by updating in an iterative fashion the parameter set. The quality of the update is determined by simulation. The different types of local search methods are differentiated according to the update mechanism that is being used. We mention Tabu search (see e.g. [33]), Simulated Annealing [38], and genetic algorithms (see e.g. [59]); many other exotic search methods have been proposed. *Rule based methods* rely on the derivation of a set of generic rules which transform the scheduler input into an acceptable solution. In order for an appropriate rule base to be derived, the main mechanisms underlying the original scheduling problem must be analyzed and understood as well as the dependency of the 'solution' on the scheduler input. Applequist et al. [2] discuss rule-based scheduling of chemical processes. According to their findings, rule-based methods combine a reasonable performance with minimum computational effort. Still, it seems that the derivation of a suitable rule-base is in most cases as complicated as the original scheduling problem itself.

Heuristic methods will generally put much lower computational demands then exact methods. A disadvantage of heuristic methods is that their operation is often difficult to interpret and understand. Lots of intuition and experience will generally be required to tune these methods such to arrive at acceptable solutions. As a major drawback no guarantee on the solution quality is obtained.

Appendix B

Introduction to the branch and bound (BB) method for the solution of MILP's

The optimal control problem in Chapter 4 as well as the scheduling problem in Chapter 5 are formulated as MILP's. The inner loop optimization problem in Section 7.4 constitutes a MILP as well. Solving MILP's is fundamentally different from solving optimization problems with continuous variables only. Due to the discrete nature of the MILP gradient based methods are useless. Instead, the presence of discrete decision variables gives rise to a decision tree which is typically of very large dimension. Solution approaches for MILP's try to restrict the section of the decision tree that needs to be considered in search for the optimum. The most popular and by far best known solution method for MILP's is the BB method. In the following the basic operation of the BB method will be explained. For a more thorough investigation we refer to Hillier [35].

B.1 Branch and Bound method - basic operation

We consider the following MILP formulation with continuous variables x and binary integer decision variables y:

$$\min_{x \in \mathbb{R}^m, y \in \{0,1\}} \{f_x^T x + f_y^T y \mid g_x x + g_y y \leq 0, h_x x + h_y y = 0\}. \tag{B.1}$$

Initialization

The BB solution process initializes via the solution of a relaxation of (B.1) which is obtained by substituting the integrality constraint by the following: $y \in [0, 1]$. This relaxation is an LP and its solution can be obtained efficiently using e.g. the Simplex method or Interior Point optimization [60]. Depending on the solution of the initial relaxation the following can be concluded. (1) If the initial relaxation is infeasible, then the MILP will be infeasible as well and the solution process can be terminated. (2) If a fractional (i.e. integer-*infeasible*) solution results then there exists no integer solution with a lower objective value, so the obtained minimum acts as a lower bound for the integer optimal solution (if one exists). (3) If the solution of the relaxed problem satisfies the integrality constraint then it is also optimal for the MILP and the solution process can be terminated.

Branching, bounding and fathoming

After initialization a first node of the BB decision tree is created by selecting a single integer variable on which the branching is started. Branching refers to the fixation of an integer variable to respectively 0 and 1. The construction of the decision tree proceeds via branching on successive integer variables. For each branch a relaxation is solved, where the integrality constraints of the remaining integer variables are removed. Depending on the solution of the relaxations, the following conclusions may be drawn. (1) If the relaxation is infeasible, then there can not be a feasible integer solution in the corresponding branch so we can omit the branch from further consideration. Coming to such a conclusion is referred to as *fathoming*. (2) If the solution to the relaxation satisfies the integrality constraints, then an *upper bound* to the solution of the MILP is found. The lowest upper bound is denoted *incumbent*. If the upper bound is lower than the incumbent then the incumbent is updated accordingly. (3) If the solution to the relaxation is fractional (i.e. does *not* satisfy the integrality constraint), then further investigation in the branch is required. The corresponding node is referred to as an *open node*. However, if an upper bound is present and the relaxed solution for the open node is higher (i.e. worse) than the upper bound, then we can conclude that the optimum is not located in the corresponding branch after which fathoming can take place. As soon as a better incumbent is found all open nodes are checked for fathoming. When no further fathoming is possible new nodes are introduced by selecting the next integer variable that is branched upon.

Optimality test

When there are no remaining open nodes the procedure can be terminated. The current incumbent is the optimal solution to the original MILP problem. If there is no incumbent then the MILP is infeasible.

B.2 Branch and Bound method - tuning

The basic BB process as outlined above is theoretically guaranteed to find the exact optimum. However, there is no guarantee on the solution speed, which may be inpractically slow even for problems of moderate size. Nevertheless, if an incumbent is present, then the worst-case distance from the optimum is known (this is the difference between the incumbent and the 'best' open node) so practically the solution process can be terminated as soon as a solution is found for which this worst-case distance is acceptably small.

The BB procedure can be customised to enhance its efficiency for specific problems. First, to promote fathoming it is important to get a good incumbent quickly. One way to get a good incumbent is by inputting a user-specified solution. Of course this requires sufficient insight in the approximate optimum value. Another way to get an incumbent fast is by executing a so-called *depth-first* search in which the lastly created node is always branched on first. This rather opportunistic search attempts to arrive at an integer solution quickly by fixing successive integer variables.

As soon as an incumbent has been found, all branches with a lower bound worse than the incumbent will be fathomed. Clearly, fathoming will happen more frequently when the objective values for the relaxations are close to the incumbent. The typical distance between incumbents and relaxations of a MILP is denoted the 'integrality gap'. Problems with a large integrality gap are generally more difficult to solve because fathoming will only occur due to infeasibility. Sometimes the integrality gap can be modified by trying different formulations of the same problem. The idea then is to introduce additional or alternative inequality constraints that force the solution of the relaxed problem to be closer to integral solutions.

An important tuning factor in the solution of MILP's is the branching order. The branching order determines how quickly incumbents are found, how often fathoming occurs and so on. Intuitively it seems wise to branch earliest on those variables that are most decisive for feasibility and optimality. Further it may be wise to select the branching order in such a way as to reduce the integrality gap quickly. Whether or not this is possible depends on the specific problem.

Most solvers can distinguish so-called *specially ordered sets* (sos) which they can deal with efficiently. An important sos in relation to the MILP's encountered in this thesis is the sos of type 1 where the set consists of binary integer variables that sum up to 1. Observe that fixing one of those variables to 1 fixes all other values (to zero obviously). For this sos it is clearly unnecessary to branch on all individual variables; instead, in each node we need to consider only a number of branches equal to the number of variables. This clearly reduces the number of branches and can speed up the solution significantly.

Appendix C

Tailoring the solution of the scheduling MILP's

This chapter discusses a few computational aspects of the scheduling problem defined in Chapter 5. First, it will be described how the problem can be modified such that infeasibility of the MILP is avoided a priori. Next, the sources that contribute to the relaxation gap are identified and a few rules of thumb for tailoring BB solution of the MILP are given.

C.1 Feasibility of the MILP

It is possible that a combination of storage, production, purchasing and sales data leads to a MILP that is infeasible. Unfortunately, infeasibility of the MILP cannot always be concluded in advance (we refer to Appendix B for a short introduction on BB methods and to what extent they can detect MILP infeasibility) in which case costly computation time may be spent on a problem that does not yield a solution anyway. One way to avoid this is via a relaxation of the constraints in the original problem. Suitable candidates for relaxation are the purchase and sales orders. Unsuitable candidates are the minimum and maximum storage capacities since these are *hard* constraints in reality. To make sure that the solution to the relaxed problem resembles the solution to the original problem as much as possible we can attach to the relaxed sales orders very high prices and to the relaxed purchase orders very low prices. This will favour those transactions that were orders in the original problem formulation to be selected. To rule out infeasibility completely we need to make a second modification to the original problem. Raw material levels may be insufficient to sustain production or end product storage capacity may be insufficient to store all production.

These sources of infeasibility can be circumvented through the introduction of a 'no-production-grade' and the corresponding shut-down and start-up transitions *from* respectively *to* all other grades.

C.2 Properties of the MILP - Tailoring the BB solution

The tuning of BB algorithms requires reasonable insight in the problem's mathematical structure. One way to analyze the mathematical properties of a MILP is by considering the properties of the relaxed problem. Most BB solvers for MILP problems use an LP relaxation in which the binary variables are substituted by continuous variables with lower bound 0 and upper bound 1. The distance between integer solutions and relaxed solutions of MILP problem is called the 'relaxation gap' or 'integrality gap' and is a measure for how difficult it is to attain good solutions. Note that a large 'relaxation gap' implies that no or hardly any bounding is likely to happen which makes the BB process tend to complete enumeration. More details on the solution of MILP's using BB methods can be found in Appendix B. The current analysis focuses on the two classes of binary variables in the scheduling problem: the grade description binary variables G_t^g and the sales decision variables $S_t^{e,s}$. For the purchasing decision variables an analysis similar to that for the sales variables can be done.

Relaxation of the grade decision variables

In the relaxed problem $G_k^g \in \{0,1\}$ are substituted by $G_k^g \in [0,1]$. This means that it is no longer enforced that in every time span only one task is being executed. The relaxed problem allows for linear combination of quasi-static tasks g_1, g_2, ... to be selected as long as $G_k^{g_1}$, $G_k^{g_2}$, ... sum up to 1. Accordingly, linear combination of *transition* tasks can be selected. There are generally more than just one combination of transition variables that satisfy the constraints (5.17); the most favorable combination will be selected. The consequences of this are best analyzed by means of an example.

We consider a certain time interval containing 10 time spans at the end of which there are three attractive sales opportunities for equal amounts of respectively product A, B and C. We further assume the end-product stores at the beginning of this interval to be empty. Whether or not these sales opportunities can be met depends on the capability of the plant to produce the required lots of A, B and C during the interval under consideration. We assume that the production rates are equal for all three end-products. In the *relaxed* solution maximum production of the three end products is attained if G_k^A, G_k^B and G_k^C as well as $T_k^{A,A}$, $T_k^{B,B}$ and $T_k^{C,C}$ are all assigned a value 1/3 for all 10 time spans. This corresponds to a *parallel* production of the three grades without any production losses due to transitions. Hence, it may well happen that the *relaxed* production description *falsely* suggests that the three sales opportunities can be met. In that case, if the sales opportunity variables are branched upon first, infeasibility will follow in a later stage so that lots of costly computing time is spent on a dead branch in the search tree. If the production losses due to transitions are minor this will not pose severe problems, however if production losses due to transitions are large then we must be aware of a significant relaxation gap related to the grade decision variables.

Relaxation of the sales decision variables

In the relaxed problem $S_k^{e,s} \in \{0,1\}$ are substituted by $S_k^{e,s} \in [0,1]$. One consequence of this is that sales orders and opportunities can be spread out over different time spans, e.g. $S_k^{e_1,s_1} = 0.5$, $S_{k+1}^{e_1,s_1} = 0.5$. This relaxation provides a means for obtaining 'interest benefits' because revenues are booked on an earlier time, however these benefits are considered negligible given the short time over which additional interest is accounted. If in the relaxed solution a single sales order or opportunity is spread out over different time spans then we can branch on the corresponding sales variables without incurring infeasibility, unless storage constraints are violated. If the latter is not the case, then a guaranteed feasible solution is obtained if the binary sales variable in the *latest* time span is chosen equal to 1. For sales *orders* the decision variables are required to sum up to 1, see (5.25), so the previous reasoning applies directly. For sales *opportunities* however it is only required that the sum of the decision variables is smaller than 1. As a consequence the relaxed solution allows sales opportunities to be executed *partly* which may cause a significant relaxation gap. This makes dealing with sales opportunities a lot more complicated than dealing with sales orders. As a rule of thumb for branching we can state that sales opportunity variables should only be branched up to 1 if the sum over the validity time set of the corresponding sales decision variables is close to 1.

Branching priority

A very important tuning factor in the BB solution of MILP's is the *branching priority* which determines the order in which the variables that are branched upon are selected. As a first step towards an appropriate branching strategy it seems instructive to consider the properties of the relaxed problem in case some of the grade decision variables are branched upon. Consider previous example with porducts A, B, and C. Based on priori knowledge about the sales transactions only we suspect that the production capacity will be equally divided amongst the three different grades and the minimum number of required tran-

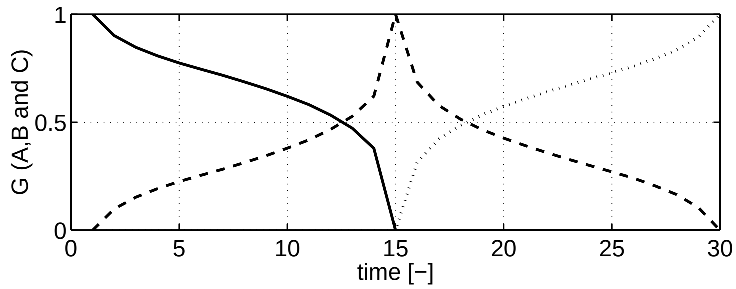


Figure C.1: Relaxed solution for the three grade/three opportunity example after fixing G_1^A, G_{15}^B and G_{30}^C to 1. Solid line: grade A, dashed line: grade B, dotted line: grade C.

sitions is hence two. Assume that we specify, based on this understanding of the required production characteristics, the production grade at the start, the middle and the end of the horizon. We choose an arbitrary order A - B - C. In Figure C.1 the resulting relaxed solution is given, for a horizon length of 30, sales opportunities for 9 units of all three products and production rates of 1 for quasi-static production and 0.5 for transitions between two different grades. This branching strategy has some obvious benefits. First, because different grades are selected during the horizon, transitions are *enforced*. This means that the attractive, though not very realistic production of different grades in parallel is no longer possible. It can further be shown that the production loss due to the transition (A $\rightarrow$ B) is bounded from below by the minimum loss of transitions (A $\rightarrow$ B) and (B $\rightarrow$ A). In case these are equal, like in the example treated here, the production loss in the relaxed solution is exactly equal to the lowest possible production loss. In general the difference between the production losses due to a transition and the production losses due to its reverse transition will not be very large, which means that a good indication is obtained on the production loss due to the transition. The attractiveness of this way of branching is obvious: *if* the initial selection of the three grades is correct than the integrality gap due to the remaining grade decision variables vanishes. If the initial guess is not correct, at least it is made less likely that infeasibility occurs in a later stage, so that feasible integer solutions can be expected earlier and more frequently. Another attractive property of this branching strategy is that the relaxed problem provides an effective indication on the production profiles and hence on how the remaining grade decision variables should be branched on. The relaxed solution plotted in Figure C.1 yields some obvious clues for the selection of the next variables that should be branched on. For example, an obvious choice is to branch *up* on variable G_2^A, G_{14}^B, G_{16}^B or G_{29}^C. Regarding the proposed branching strategy one big challenge remains: to select the time instances at which the first grade decision variables are to be fixed. Some heuristics are needed to guide this selection. For example, it may help to compute in advance the number of transitions that is expected, based on an estimation of the total number of sales transactions. A reasonable estimate of the number of transitions may be enough to provide an effective initial guess on the number of time spans at which production variables should be fixed. Because the relaxation on sales orders will not incur infeasibility in a later stage, no benefit is expected from branching on those variables in an early stage. Infeasibility *can* occur after an early branching on sales opportunity variables. To avoid this, opportunity decision variables should be branched on in the latest stage.

Appendix D

Analysis of the MILP inner loop problem in the Successive MILP approach to grade change optimization

The core of the Successive MILP approach to grade change optimization described in Section 7.4 is a MILP inner loop optimization. To analyze the properties of the MILP inner loop problem we investigate the characteristics of the relaxation of the MILP which is obtained by removing the integrality, hence by selecting $G_i^g \in [0, 1]$. There exist two obvious sources contributing to the integrality gap. First, due to the definition of the grade regions, infeasible grades can be partially selected. Therefore the relaxed problem will generally compute too large production amounts of the more favorable products. Second, if $F(z)$ is much smaller than $Y_{e,u}^g$ for a particular, favorable end product then the total production can be assigned to this favorable products, even for small values of the corresponding grade variable G^g. To limit the integrality gap to the minimum we should choose the values $Y_{e,u}^g$ and Q^g as small as possible. The proper choice of $Y_{e,u}^g$ is the maximum realistic production rate of end product e in grade g. Q^g should be selected the maximum of $g_g(z)$ over the set of all feasible z. To gain some more insight in the properties of the MILP we next consider a simple example.

Let $F(z) = z^2$. Further, we let 3 grade regions be linearly dependent on z^1

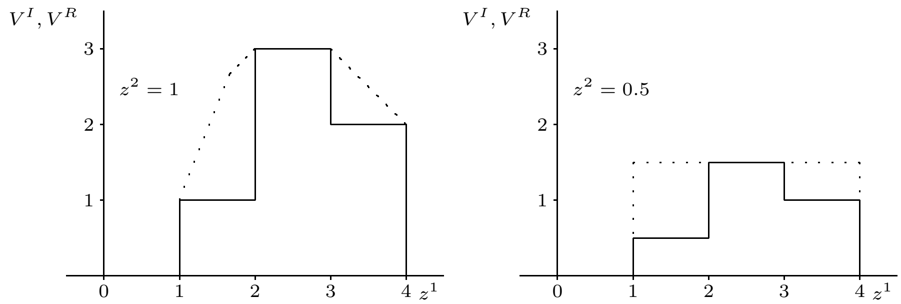


Figure D.1: The optimal integral (solid lines) and relaxed (dashed lines) costs as a function of z^1 for two choices of z^2 for the simple, three-grade example.

leading to the following grade constraints:

$$\begin{array}{lll} 1 - z^1 \leq 0, & 2 - z^1 - (1 - G^2) \leq 0, & 3 - z^1 - 2(1 - G^3) \leq 0, \\ z^1 - 2 - 2(1 - G^1) \leq 0, & z^1 - 3 - (1 - G^2) \leq 0, & z^1 - 4 \leq 0. \end{array} \tag{D.1}$$

The production rates are constrained from below by zero and from above as follows

$$\begin{array}{lll} Y_1^1 \leq G^1, & Y_1^2 \leq 0, & Y_1^3 \leq 0, \\ Y_2^1 \leq 0, & Y_2^2 \leq G^2, & Y_2^3 \leq 0, \\ Y_3^1 \leq 0, & Y_3^2 \leq 0, & Y_3^3 \leq G^3. \end{array} \tag{D.2}$$

The prices of the three end products are respectively $p_P^1 = 1$, $p_P^2 = 3$, $p_P^3 = 2$. We are interested in the difference between the integral objective and the relaxed objective function. To this end, we consider the functions

$$V^I(z^1, z^2) = \max \left(\sum_{e=1,\ldots,3} Y_g^e p_P^e \mid \text{ s.t. } \exists Y_g^e, G^g \in \{0,1\} \text{ s.t. (D.1),(D.2) hold} \right),$$

and

$$V^R(z^1, z^2) = \max \left(\sum_{e=1,\ldots,3} Y_g^e p_P^e \mid \text{ s.t. } \exists Y_g^e, G^g \in [0,1] \text{ s.t. (D.1),(D.2) hold} \right),$$

which represent the optimal integral respectively relaxed objective as a function of the process variables z^1 and z^2. Since all non-zero $Y_{e,u}^g$ are selected 1 the smallest difference between V^I and V^R is found at a production level of 1, see the left image in Figure D.1.

Clearly the relaxed problem indicates the attractiveness of the expensive grade 2. The situation however deteriorates for smaller production levels. Already at a production level of 0.5 the relaxed problem assigns the maximum integer objective value to all feasible choices of z^1. This is plotted in the right image of Figure D.1. The coupling between the performance variables at different time instances is not considered in this example, however this coupling is already continuous, so that no additional contribution to the relaxation gap is expected. Nevertheless, above-mentioned sources for the gap can become very significant, making the problem potentially difficult to solve.

The situation is even worse when the price of a certain product depends rather erratically on its quality. This is for example the case when in between two regions of specification there is an off-spec region with corresponding low prices. In the simple example if we would have selected the prices of the first and the third product to be 3 and the price of the second product to be 1, then the relaxed, optimal cost as a function of z^1 would be constant and equal to that for grades 1 and 3. The unattractiveness of grade 2 would be completely invisible in the *relaxed picture*. Whether or not this approach is feasible in practice will have to be verified for each specific application.

Appendix E

Implementation details

E.1 SHOP-1, application to case II: distillation column, Section 6.4

This section presents the details of the implementation of the SHOP-1 controller to the binary distillation grade change problem. The implementation of the SHOP-1 is a practical modification of the general SHOP-1 formulation (6.7).

Most noticeable modifications are the substitution of the end-point constraint by a penalty term that is added to the objective and the use of a discrete time linear model (6.11) instead of a continuous time nonlinear one. The horizon length (H^S) used is 2 hours with a discretization interval (ΔT_{shop}) of 0.1 hour.

The objective of the SHOP is given by $V^S = V_{ec}^{S1} + V_{co}^{S1} + V_E^{S1}$, containing respectively an economic term, a control type penalty and a penalty corresponding to the final state constraint. The three terms are given as follows:

$$
\begin{aligned}
V_{ec}^{S1} &= \Delta T_{shop} \sum_{i=0}^{20} \left(0.2 z_i^6 - (1, 2, 2, 1.5, 0.5) \sum_g \bar{G}_i^{g,R} M_g \begin{pmatrix} z_i^3 \\ z_i^4 \end{pmatrix} \right), \\
V_{co}^{S1} &= \sum_{i=0}^{20} \begin{pmatrix} z_i^5 - \bar{z}^{R,5}(t' + i\Delta T_{shop}) \\ z_i^6 - \bar{z}^{R,6}(t' + i\Delta T_{shop}) \end{pmatrix}^T \begin{pmatrix} 100.0 & 0 \\ 0 & 0.001 \end{pmatrix} \cdot \\
&\qquad \begin{pmatrix} z_i^5 - \bar{z}^{R,5}(t' + i\Delta T_{shop}) \\ z_i^6 - \bar{z}^{R,6}(t' + i\Delta T_{shop}) \end{pmatrix}, \\
V_E^{S1} &= 10^8 (x_{20} - \bar{x}^R(t''))^T (x_{20} - \bar{x}^R(t'')),
\end{aligned} \tag{E.1}
$$

where $\bar{z}^R$, $\bar{x}^R$ and $\bar{G}^{g,R}$ are available from off-line dynamic optimization and where M_g maps the material flows to the end product flows for production grade 6:

$$M_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad M_2 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad M_3 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix},$$

$$M_4 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad M_5 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad M_6 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

The constraints are respectively the process constraints, the grade constraints, the scheduling constraints, and additional constraints on the rate of change of the controls. The process constraints are given in Table 6.4 and are implemented at discrete samples:

$$z_l^j < z_i^j < z_u^j, \quad j = 1, \ldots, 6, \quad i = 1, \ldots, 20$$

The grade constraints are implemented as follows

$$\left. \begin{array}{l} z_l^{1,g} < z_i^1 < z_u^{1,g}, \\ z_l^{2,g} < z_i^2 < z_u^{2,g}, \end{array} \right\} \ \forall\, g \ s.t.\ \bar{G}_i^{g,R} = 1, \quad i = 1, \ldots, 20,$$

with $z_l^{1,g}$, $z_u^{1,g}$, $z_l^{2,g}$, and $z_u^{2,g}$ the lower and upper bounds on respectively the top purity and the bottom impurity for grade g as given in Table 6.3. The scheduling constraints are implemented as follows:

$$\sum_{i=1}^{20} z_i^3 > \sum_{i=1}^{20} \bar{z}^{R,3}(t' + i\Delta T_{shop}) - 50, \quad \sum_{i=1}^{20} z_i^4 > \sum_{i=1}^{20} \bar{z}^{R,4}(t' + i\Delta T_{shop}) - 50,$$

where the production constraints are relaxed by an amount of 50 in order to have some back off from the reference production levels. In addition to these, constraints on the rate of change of the controls are implemented:

$$\begin{array}{rcl} -1 < & z_1^5 - z^5(t') & < 1; \qquad -1 < \quad z_i^5 - z_{i-1}^5 \quad < 1, \qquad i = 2, \ldots, 20, \\ -150 < & z_1^6 - z^6(t') & < 150; \quad -150 < \quad z_i^6 - z_{i-1}^6 \quad < 150, \quad i = 2, \ldots, 20. \end{array}$$

E.2 SOP and SHOP-2, application to case II: distillation column, Section 6.5

This section presents the details of the implementation of the combination of the SOP and the SHOP-2 controller to the binary distillation grade change problem.

SOP, application to case II: distillation column

The implementation of the SOP is a practical modification of the general SOP formulation (6.20). The objective is the economic objective:

$$L(z) = 0.2z^6 - (1, 2, 2, 1.5, 0.5)Y(z),$$

where during operation in grade 3 the yield is given by $Y(z) = (0, z^3, 0, z^4, 0)^T$. The process and grade constraints are implemented according to Tables 6.3 and 6.4. The production constraints are implemented according to (6.17), (6.18), and (6.19).

Infeasibility of the SOP can occur in case of large deviations of the feed composition from the nominal value of 0.5. Physical insight in the process can be used to indicate that infeasibility of the constraint on the top production can result in case of positive deviations and infeasibility of the constraint on the bottom impurity in case of negative deviations. Therefore, *if* the SOP appears infeasible, the corresponding production constraint is omitted and the objective is modified so as to minimize the constraint violation:

$$L(z) = \begin{cases} -z^3, & \text{if } \hat{x}^{ds} < 0.5, \\ -z^4, & \text{if } \hat{x}^{ds} > 0.5. \end{cases} \tag{E.2}$$

SHOP-2, application to case II: distillation column

The formulation of SHOP-2 is based on the general definition given by (6.21). The model used is given by the LTV dynamics (6.11) derived along the trajectories generated according to (6.22) and (6.23). The horizon length is chosen 2 hours with the length of the discretization interval equal to 0.1 hour. Similar to the design of SHOP-1, the objective contains three terms, V_{ec}^{S2}, V_{co}^{S2}, and V_E^{S2}, where the control objective constitutes a quadratic penalty on the rate of change of the controls:

$$\begin{aligned} V_{ec}^{S2} &= \Delta T_{shop} \sum_{i=0}^{20} \left(0.2z_i^6 - (1, 2, 2, 1.5, 0.5)(0, z_i^3, 0, z_i^4, 0)^T\right), \\ V_{co}^{S2} &= \begin{pmatrix} z_0^5 - z^5(t') \\ z_0^6 - z^6(t') \end{pmatrix}^T \begin{pmatrix} 1000.0 & 0 \\ 0 & 0.02 \end{pmatrix} \begin{pmatrix} z_0^5 - z^5(t') \\ z_0^6 - z^6(t') \end{pmatrix} \\ &\quad + \sum_{i=1}^{20} \begin{pmatrix} z_i^5 - z_{i-1}^5 \\ z_i^6 - z_{i-1}^6 \end{pmatrix}^T \begin{pmatrix} 1000.0 & 0 \\ 0 & 0.02 \end{pmatrix} \begin{pmatrix} z_i^5 - z_{i-1}^5 \\ z_i^6 - z_{i-1}^6 \end{pmatrix}, \\ V_E^{S2} &= 10^8 (x_{20} - \bar{x}^{sop})^T (x_{20} - \bar{x}^{sop}). \end{aligned} \tag{E.3}$$

Process constraints are implemented as in the design of the SHOP-1. Scheduling constraints are implemented in a straigtforward manner as in (6.21) with an additional relaxation of 5 per cent.

E.3 SOP, LHOP and SHOP-1, application to case II: distillation column, Section 6.6

The implementation of the control configuration treated in Section 6.6 on the binary distillation example uses the implementation of the SHOP-1 discussed in E.1 and the SOP as in E.2. The implementation of the LHOP will be discussed here. The basic problem formulation for the LHOP is given by (6.33).

Determination of the prediction horizon

The horizon length and the set of production intervals for which the production constraints need to be enforced (6.26) are determined according to the following decision scheme.

Let interval i be the current production interval,

if $t^i + \tau - t' > H_l^L$
[*the remaining length of the current production interval is larger than the minimum LHOP horizon length*]
    if $G_{i-1}^g = G_i^g, \;\; \forall g$
    [*the current production interval is a quasi-static interval*]
        $H^L = H_l^L$
        $PI_{t'} = \varnothing$
    else
    [*the current production interval is a transition interval*]
        $H^L = t^i + \tau - t'$
        $PI_{t'} = \{i\}$
    end
else if $G_{i+1}^g = G_i^g$
[*the next production interval is a quasi-static interval*]
    $H^L = H_l^L$
    $PI_{t'} = \{i\}$
else
[*the next production interval is a transition interval*]
    $H^L = t^i + 2\tau - t'$
    $PI_{t'} = \{i, i+1\}$
end

The minimum horizon length is chosen $H_l^L = 3.6$ hours.

Implementation of the objective and the scheduling constraints

The objective function used is constituted by respectively an economic term, a control type penalty and a penalty corresponding to the final state constraint.

The three terms are given as follows:

$$
\begin{aligned}
V_{ec}^{L1} &= \Delta T_{lhop} \sum_{i=0}^{N-1} \left(0.2 z_i^6 - (1, 2, 3, 1.5, 0.5) Y(z_i)\right), \\
V_{co}^{L1} &= \begin{pmatrix} z_0^5 - z^5(t') \\ z_0^6 - z^6(t') \end{pmatrix}^T \begin{pmatrix} 1000.0 & 0 \\ 0 & 0.02 \end{pmatrix} \begin{pmatrix} z_0^5 - z^5(t') \\ z_0^6 - z^6(t') \end{pmatrix} \\
&\quad + \sum_{i=1}^{N-1} \begin{pmatrix} z_i^5 - z_{i-1}^5 \\ z_i^6 - z_{i-1}^6 \end{pmatrix}^T \begin{pmatrix} 1000.0 & 0 \\ 0 & 0.02 \end{pmatrix} \begin{pmatrix} z_i^5 - z_{i-1}^5 \\ z_i^6 - z_{i-1}^6 \end{pmatrix}, \\
V_E^{L1} &= 10^7 (x_N - \bar{x}^{sop})^T (x_N - \bar{x}^{sop}),
\end{aligned}
\tag{E.4}
$$

where $N = H^L/\Delta T_{lhop} + 1$ is the number of samples considered in the horizon of the LHOP, with a discretization interval ΔT_{lhop} of length 0.6 hour. The production is given by $Y(z) = [Y_1(z), Y_2(z), Y_3(z), Y_4(z), Y_5(z)]^T$.

The scheduling constraints in the LHOP are implemented according to (6.27), (6.28), (6.29), (6.30), (6.31), and (6.32).

The evaluation of the production rates $Y_e(z)$ which appear in the objective function as well as in the scheduling constraints is done using the smooth approximation of the grade functions as given on page 137 in the treatment of the SSQP approach to the optimization of grade changes for the binary distillation column. This smooth approximation underestimates the actual production when the top purity and the bottom impurity reach the specification boundaries. To avoid wrongful infeasibility of the scheduling constraints a relaxation of the production constraints by 20 per cent is introduced.

SSQP optimization

The SSQP optimization method is used to solve the LHOP's. How this method works is treated in Chapter 7. For accurate solution of the LHOP's a two stage approach is adopted. First, a rough approximation of the solution is obtained in a few iterations using $\gamma = 1000$ in the first stage. In the second stage, γ is increased to 10000 and the LHOP is solved again using the solution from the first stage as an initial guess.

E.4 Linearization of dynamics

Linearizations of the plant dynamics along state/input trajectories are used in the optimal control solutions of Chapter 6 and the optimization routines of Chapter 7.

Throughout the thesis we utilized piece-wise constant parametrizations of the controls. If we stack the values of the inputs at the piece-wise constant intervals the parameter vector is given by $p = [u_0^T, u_1^T, \ldots, u_N^T]$. For this choice of parametrization the linearized dynamics can be expressed as

$$\begin{pmatrix} \Delta z_0 \\ \Delta z_1 \\ \vdots \\ \Delta z_N \end{pmatrix} = \begin{pmatrix} G_{01} & \cdot & \cdots & \cdot \\ G_{11} & G_{12} & \cdots & \cdot \\ \vdots & \vdots & \ddots & \vdots \\ G_{N1} & G_{N2} & \cdots & G_{NN} \end{pmatrix} \begin{pmatrix} \Delta u_0 \\ \Delta u_1 \\ \vdots \\ \Delta u_N \end{pmatrix},$$

$$\Delta x_N = \begin{pmatrix} H_{N1} & H_{N2} & \cdots & H_{NN} \end{pmatrix} \begin{pmatrix} \Delta u_0 \\ \Delta u_1 \\ \vdots \\ \Delta u_N \end{pmatrix}.$$

where $G_{ij} = \frac{\partial z_i}{\partial u_j} := \left[\frac{\partial z_i}{\partial u_j^1}, \ldots, \frac{\partial z_i}{\partial u_j^{n_u}}\right]$ and $H_{Nj} = \frac{\partial x_N}{\partial u_j} := \left[\frac{\partial x_N}{\partial u_j^1}, \ldots, \frac{\partial x_N}{\partial u_j^{n_u}}\right]$. The determination of G_{ij} and H_{Nj} normally proceeds via the sampling of the solution of the sensitivity equations (7.2) for a piece-wise constant parametrization of the controls.

The following notation shows how the sampling of the solution of the sensitivity equations can be interpreted in terms of the state transition matrix Φ_j and the input-to-state transition matrices Γ_j (introduced on page 100):

$$\frac{\partial z_i}{\partial u_j} = \begin{cases} C_u, & \text{if } i = j, \\ C_x \prod_{m=j+1}^{i-1} \Phi_m \Gamma_j, & \text{if } i > j, \\ 0, & \text{if } i < j, \end{cases} \tag{E.5}$$

$$\frac{\partial x_N}{\partial u_j} = \begin{cases} \prod_{m=j+1}^{N-1} \Phi_m \Gamma_j, & \text{if } j < N-1, \\ \Gamma_{N-1}, & \text{if } j = N-1, \\ 0, & \text{if } j = N-1, \end{cases} \tag{E.6}$$

In our linearizations we use an approximation of the state transition matrix and the input-to-state transition matrix that is based on a local linearity assumption. The expressions are given as follows $\Phi_m = e^{A(mT)T}$ and $\Gamma_k = \int\limits_{mT}^{(m+1)T} e^{A(mT)\tau} B(mT)\, d\tau$ where $A(\cdot)$ and $B(\cdot)$ are as defined in (6.9) and (6.10) respectively.

Appendix F

Nonlinear optimization

This chapter provides a brief introduction to two categories of methods for solving constrained NLP's. Sequential Quadratic Programming shall be treated in Section F.1. Penalty and barrier methods are discussed in Section F.2. The notation used in this appendix does not comply with the list of symbols.

F.1 Sequential Quadratic Programming (SQP)

The SQP approach is at present one of the most popular methods for solving equality-constrained as well as inequality-constrained NLP's. The method was originally developed for the solution of equality-constrained NLP's only. The following discussion is based mainly on [60]. For ease of notation we consider the following general formulation of an equality-constrained NLP:

$$\min_x \{f(x) \mid g(x) = 0\}.$$

The Lagrangian for this problem is

$$\mathcal{L}(x, \lambda) = f(x) - \lambda^T g(x),$$

and the first-order optimality condition is

$$\nabla \mathcal{L}(x, \lambda) = 0.$$

Applying Newton's method to this system of nonlinear equations yields the following update formula for x and λ: $x_{k+1} = x_k + p_k$ and $\lambda_{k+1} = \lambda_k + v_k$ where the search steps p_k and v_k are given by the solution to the linear system

$$\begin{pmatrix} \nabla^2_{xx} \mathcal{L}(x_k, \lambda_k) & \nabla g(x_k) \\ -\nabla g(x_k)^T & 0 \end{pmatrix} \begin{pmatrix} p_k \\ v_k \end{pmatrix} = \begin{pmatrix} -\nabla_x \mathcal{L}(x_k, \lambda_k) \\ g(x_k) \end{pmatrix}.$$

These equations represent the first-order optimality conditions for the following quadratic programme (QP)

$$\min_{p_k}\left\{\frac{1}{2}p_k^T\nabla^2_{xx}\mathcal{L}(x_k,\lambda_k)p_k+p_k^T\nabla_x\mathcal{L}(x_k,\lambda_k)\mid(\nabla g(x_k))^Tp_k+g(x_k)=0\right\}. \tag{F.1}$$

The SQP approach solves a sequence of such QP's to converge to a local minimizer of the NLP. Generally, several modifications to this basic scheme are made. One such a modification is the use of a positive definite approximation of the Hessian $\nabla^2_{xx}\mathcal{L}(x_k,\lambda_k)$ instead of the Hessian itself. A practical reason for using such an approximation is that the true Hessian is not always available at low computational costs. An additional advantage of using approximate Hessians is that we can guarantee positive-definiteness of the reduced Hessian which is required for the solution of the QP to be a descent direction. Alternatively, when using the true Hessian, positive-definiteness would need to be checked and resolved (by regularization) in every iteration. Typical Hessian updating strategies guarantee some nice properties of the approximated Hessian such as symmetry and positiveness. Probably the most famous update scheme is the BFGS (Broyden, Fletcher, Goldfarb, and Shannon) formula

$$B_{k+1}=B_k-\frac{(B_ks_k)(B_ks_k)^T}{s_k^TB_ks_k}+\frac{y_ky_k^T}{y_k^Ts_k},$$

where $s_k=x_{k+1}-x_k$, and $y_k=\nabla_x\mathcal{L}(x_{k+1},\lambda_{k+1})-\nabla_x\mathcal{L}(x_k,\lambda_k)$.

Because the solutions obtained from the sequence of QP's can possibly diverge, a line search is instituted to insist that in each iteration (x_{k+1},λ_{k+1}) is a 'better estimate' of the true optimum than (x_k,λ_k). Progress is measured in terms of an auxiliary *merit function* which typically includes two terms: the objective function and a measure of constraint infeasibility. One example of a merit function is the following

$$\mathcal{M}(x)=f(x)+\rho g(x)^Tg(x),$$

with ρ a positive number. In the line search, a step size α is determined such that $\mathcal{M}(x_{k+1},\lambda_{k+1})<\mathcal{M}(x_k,\lambda_k)$, where $x_{k+1}=x_k+\alpha p_k$ and $\lambda_{k+1}=\lambda_k+\alpha v_k$. Alternatively $\mathcal{M}(x_{k+1},\lambda_{k+1})$ can be minimized over α in a one-dimensional search or optimization problem.

Inequality constraints

Next we consider the following problem with equality and *in*equality constraints:

$$\min_x\{f(x)\mid g(x)=0,\ h(x)\le 0\}.$$

The investigation of the equality-constrained case suggests that the solution of this problem can be obtained through the solution of a sequence of QP's, and this approach was indeed proposed in literature. In fact, two approaches exist, which differ mainly in how the inequality constraints are treated. In the *Inequality constrained* version (IQP) the inequality constraints are included in the formulation of the QP

$$\min_p \left\{ \frac{1}{2} p^T \nabla^2_{xx} \mathcal{L}(x_k, \lambda_k) p + p^T \nabla_x \mathcal{L}(x_k, \lambda_k) \mid (\nabla g(x_k))^T p + g(x_k) = 0 \right.$$
$$\left. (\nabla h(x_k))^T p + h(x_k) = 0 \right\}.$$

The active set of constraints is determined in each iteration by the QP subprogramme. The *Equality constrained* version (EQP) assumes that an *active set strategy* be implemented by an additional procedure and solves in each iteration an *equality*-constrained QP. The big advantage of the EQP is that the solution of the equality-constrained QP's proceeds very fast. However, the development of a suitable active-set strategy may be very involved in practice.

F.2 Penalty and barrier methods

Penalty and barrier methods solve a constrained optimization problem by solving a sequence of unconstrained optimization problems. These methods have been studied rather extensively before being abandoned in the 1970s due to the typical ill conditioning problems in the linear algebra these methods require. A renewed interest in and a further development of barrier methods was initiated in 1984 with the introduction of Karmakar's interior point method for linear programming [37]. Nowadays, penalty and barrier functions are extensively studied and used in many applications. The main idea in barrier and penalty methods is to incorporate the constraints by means of a penalty function in the objective and to solve the resulting unconstrained optimization problem.

F.2.1 Barrier methods

Barrier methods are strictly feasible methods which means that all iterates lie inside the feasible region. Feasibility is maintained by creating a barrier that keeps the iterates away from the boundary of the feasible region. To this end, the objective function is extended by a barrier term resulting in a so-called *barrier* function that is continuous on the interior of the feasible set and becomes unbounded as the boundary of the set is approached from the interior. In general, barrier methods handle only *in*equality constraints. We consider the general inequality constrained problem

$$\min_x \{f(x) \mid h_i(x) \leq 0, \;\; i = 1, \ldots, m\}.$$

Typical barrier functions employ the logarithmic or the inverse function:

$$\text{logarithmic barrier function :} \qquad \beta(x, u) = f(x) - \mu \sum_{i=1}^{m} \log(-h_i(x)),$$

$$\text{inverse barrier function :} \qquad \beta(x, u) = f(x) + \mu \sum_{i=1}^{m} \frac{1}{-h_i(x)},$$

with a positive valued μ. Observe that for small μ the barrier function will resemble the original objective on the interior of the feasible region while still having infinite value at the boundaries. Theoretically, a good approximation of the constrained optimum can hence be achieved if we minimize the barrier function (an *un*constrained minimization problem) for a sufficiently small value of μ. The reason why this is not done in practice is that for small values of μ the problems are difficult to solve. Practically, barrier methods solve a sequence of unconstrained minimization problems of for a sequence $\{\mu_k\}$ that decrease monotonically to zero. The solution of one unconstrained problem is used as a starting point for the next problem, making the unconstrained problems much easier to solve than would be the case if we attempted to solve the problem directly for a small value of μ.

Many variations to this basic scheme for barrier methods exist which we will not describe here. Convergence of the barrier method can be proved under mild assumptions, see [60]. Barrier methods can be of use in the type of optimization problems formulated in this thesis, for example to account for the presence of path inequality constraints. Also, as is shown in Section 7.3, the idea of approximating a discontinuous function (i.e. the 'ideal barrier') by a continuously differentiable one can also be applied to derive a computationally feasible approach to the economic grade change optimization problem.

F.2.2 Penalty methods

Penalty methods do not require feasibility in each iteration. Thus, unlike barrier methods, they are suitable for problems with equality constraints. We consider general equality-constrained problems of the form

$$\min_x \{f(x) \mid g_i(x) = 0, \;\; i = 1, \ldots, m\}.$$

In penalty methods the constrained optimization problem is replaced by a series of unconstrained optimization problems in which the objective is extended by a term that penalizes the constraint violation. As this penalty is increased iterates are forced towards the feasible region. The resulting extended objective is referred to as the *penalty function*. Typical penalty functions employ a quadratic penalty on the constraints:

$$\pi(x, \rho) = f(x) + \rho \frac{1}{2} \sum_{i=1}^{m} g_i(x)^2,$$

with ρ a positive number. Similar to the barrier methods, the penalty methods solve a sequence of unconstrained minimization problems, in this case for increasing ρ to converge to the minimum of the constrained problem. Convergence can be proved under mild conditions. The penalty method is of particular interest in relation to the dynamic optimization problems we encountered in this thesis, as it may provide for a computationally feasible approach to dealing with the end-point equality constraints.

Summary

The chemical marketplace is a global one with strong competition between manufacturers. To continuously meet the customer demands regarding product quality and delivery conditions without the need to maintain very large storage levels chemical manufactures need to strive for *production on demand*. In this thesis we research how market-oriented production can be realized for the particular class of multi-grade continuous processes. For this class of processes production on demand is particularly challenging due to the the complex trade-off between performing costly and time-consuming changeovers and maintaining high storage levels.

The first requirement for market-oriented production is that production management cooperates with purchasing and sales management. We propose the use of a scheduler as a decision support system in a cooperative organization constituted by these players. In such a scheduler, decision making is represented using decision variables and their effect on the company-wide objective, which is chosen to be the added value of the company, is modeled. The scheduler then selects a decision strategy that is optimal with respect to the objective and presents this strategy to the decision makers who use it to base their actual decision taking on.

The company-market interaction is modeled using a transaction-based modeling framework. Therein not the actual market behavior is modeled but the expected effect of the interaction of the company *with* the market. Two types of transactions can be modeled in this framework: orders, which result from contracts with suppliers and customers, and opportunities, which express the expected sales and purchases. Two different approaches to the modeling of production decisions are taken, the choice of which depends largely on the implementation of the process control hierarchy that is assumed. In the first approach, production management and control is performed by a single level controller and the control decisions are the minute to minute manipulation of the valves. This approach is academically interesting, though practically intractable due to the combination of long horizons and fast sampling times. In the second approach the process control hierarchy consists of a scheduling layer

at which it is determined *what* products will be produced *when*, and a process control layer which determines *how* this production is realized. This approach is taken in the rest of the thesis.

The design of the *scheduling layer* is done by transforming the question “what is produced when” into a Mixed Integer Linear Programming (MILP) decision problem. The formulation of this MILP uses a parametrization of the behavior of the plant in terms of “finite horizon quasi-stationary” production tasks and “transition tasks”. The production characteristics for these tasks are computed using model based static and dynamic optimization.

The *process control layer* basically consists of a nonlinear state estimator in combination with a deterministic Nonlinear Model Predictive Controller (NMPC). The objective function used is a finite horizon expression of the process economics and is based on an evaluation of the added value. The constraints comprise amongst others a bound on the production levels in accordance with the production schedule. A decomposition based on a distinction of two time scales of disturbances (fast, stochastic type disturbances and slow, persistent disturbances) is proposed which combines fast short-term control with a lower frequent update of the long term target trajectories to retain consistency with the production schedule and to retain economically attractive operating conditions in the presence of persistent disturbances.

The economic optimization of multi-grade process transitions in the derivation of the production database used by the scheduler and in the real-time control configuration leads to a specific non-smooth optimization problem for which two solution approaches are proposed. One uses a smooth approximation of the definition of the grade region and exploits the structure of the problem in the definition of a Nonlinear Programming (NLP) based inner loop optimization to compute accurate search directions. The second approach uses integer variables to describe the grade regions and solves a sequence of MILP’s to converge to a solution.

The arguments given in this thesis are mainly constructive. Proofs of performance are lacking mainly due to the complexity such analysis would entail. Nevertheless the potential of the methods is demonstrated on several interesting cases. Case I, the market-oriented operation of a blending system is treated in relation to the design of the scheduler. Both the single level approach and the scheduling approach resulting from the decomposition are applied to this case with illustrative results. On case II, the optimal operation of a binary distillation column, the excellent performance of the proposed grade change optimization techniques is demonstrated. Also, promising behavior of the real-time control and optimization strategies is exposed in this case. The third and largest case study comprises the model-based optimization and production scheduling for a HDPE gas phase reactor. Interesting improvements of the grade change efficiency and the overall process added value in comparison with traditional operating strategies are shown, demonstrating clearly the potential of the solutions that were presented in this thesis.

Samenvatting

De markt voor chemische produkten is te karakteriseren als een zeer globale markt met harde concurrentie. Om aan de eisen van de klanten met betrekking tot produktkwaliteit en levering te kunnen voldoen zonder daar extreem hoge voorraadniveaus voor nodig te hebben, dienen chemische producenten te streven naar een vraaggestuurde produktie. Dit proefschrift beschrijft de resultaten van een onderzoek naar de realisatie van vraaggedreven produktie voor de speciale klasse van continue chemische processen die in verschillende werkpunten bedreven worden teneinde daarmee verschillende produkten of produktkwaliteiten te realiseren. Voor dit type proces is vraaggedreven produktie lastig te realizeren vanwege de afweging die telkens gemaakt moet worden tussen het uitvoeren van dure en tijdrovende procesovergangen en het aanhouden van hoge voorraadniveaus.

De eerste vereiste voor vraaggedreven produktie is dat de verantwoordelijken voor produktie goed samenwerken met de verantwoordelijken voor inkoop en verkoop. Om deze samenwerking op een goede manier te laten verlopen stellen wij voor de besluitvorming van deze verantwoordelijken te ondersteunen met behulp van een *scheduler*. In deze *scheduler* is de besluitvorming van de verantwoordelijken en de gevolgen daarvan op de bedrijfsprestatie, in dit proefschrift gekozen als de toegevoegde waarde, gemodelleerd. De scheduler bepaalt een beslissingsstrategie die de toegevoegde waarde maximaliseert. De verantwoordelijken baseren hun besluitvorming op de uitkomsten van de *scheduler*.

De interactie tussen het bedrijf en de markt is in de *scheduler* gemodelleerd in de vorm van een verzameling met inkoop/verkoop transacties. Er zijn twee typen transacties: *orders*, als gevolg van bijvoorbeeld langlopende verkoopcontracten en *opportunities* waarmee verwachte transacties worden gekarakteriseerd. Twee verschillende aanpakken voor het modelleren van het proces zelf zijn bestudeerd. In de eerste aanpak zijn alle produktiebeslissingen tot op het niveau van de regeltechniek samengepakt, wat betekent dat de *scheduler* over een gedetailleerd en tevens zeer uitgebreid model moet beschikken waarin zowel de dag-tot-dag produktiebeslissingen als de minuut-tot-minuut regelbeslissingen dienen te worden meegenomen. Deze aanpak is academisch interessant, echter praktisch niet haalbaar door de combinatie van een lange voorspelhorizon en korte bemonstertijden. De tweede aanpak bestaat uit een hiërarchische beslissingsstructuur met een *produktie-scheduling* laag waarin bepaald wordt *welke* produkten *wanneer* worden gemaakt en een *procesregelingslaag* die bepaalt *hoe* de produktie wordt gerealiseerd.

Het ontwerpen van de *produktie-scheduler* is gedaan door de vraag "*welke* produkten *wanneer* worden gemaakt" te vertalen in een *Mixed Integer Linear Programme* (MILP) beslissingsprobleem. In de formulering van deze MILP is het procesgedrag gekarakteriseerd in termen van "eindige horizon quasi-stationaire taken" en "transitie taken". De eigenschappen van deze taken worden bepaald met behulp van modelgebaseerde statische respectievelijk dynamische optimalisatie.

De *procesregelingslaag* bestaat uit een niet-lineaire toestandsschatter in combinatie met een deterministische *Nonlinear Model Predictive Controller* (NMPC). De doelfunctie bestaat uit een eindige-horizon-berekening van de toegevoegde waarde van het proces. In de begrenzingen van het regelprobleem zijn de minimum produktie eisen die de scheduler stelt meegenomen. Ten behoeve van praktische haalbaarheid (met name met betrekking tot rekentijden) is de regelaar, op basis van de verschillende tijdschalen waarin verstoringen kunnen worden onderscheiden, opgedeeld in een aantal lagen. In deze opdeling worden snelle verstoringen met een snel bemonsterende korte-horizon regelaar aangepakt terwijl een lange-horizon regelaar die op een lagere frequentie draait ervoor zorgt dat de produktie-schedules worden gehaald onder economisch aantrekkelijke procescondities.

De optimalisatie van procesovergangen leidt, door de sprongGewijze afhankelijkheid van de doelfunctie voor veranderingen in de kwaliteit, tot een niet-glad optimalisatieprobleem waar gebruikelijke standaard oplossingen zoals de *Sequential Quadratic Programming control parametrization* aanpak niet geschikt voor zijn. Twee optimalisatieaanpakken zijn voorgesteld. In de eerste aanpak wordt het probleem eerst benaderd door een glad probleem. Voor dit gladde probleem is een optimalisatieprocedure ontwikkeld die gebruik maakt van Nietlineair Programmeren (NLP) in de binnenlus om tot goede zoekstappen te komen. De tweede aanpak maakt gebruik van diskrete beslissingsvariabelen om de veranderingen in kwaliteit te beschrijven. In deze aanpak wordt, met in elke iteratie een linearisatie van de procesdynamica, een serie van MILP's opgelost om een lokaal minimum te vinden.

Voor de methodieken die worden beschreven in dit proefschrift blijft, met name vanwege hun complexiteit, bewijsvoering van de prestatie achterwege. Om toch vertrouwen te krijgen in de werking, wordt de toepassing van deze methodieken op enkele voorbeeldprocessen in simulatie getoond. De eerste casus, vraaggedreven bedrijfsvoering van een mengproces, wordt behandeld in relatie tot produktie-scheduling en toont de haalbaarheid van de gekozen scheduling aanpak. De tweede casus, de optimale bedrijfsvoering van een destillatiekolom, toont de werking van de dynamische optimalisatietechnieken en de implementatie van de procesregelingslaag zoals hierboven omschreven. De derde en laatste casus betreft modelgebaseerde optimalisatie en produktie-scheduling voor een gasfase HDPE proces. Toepassing van de technieken die besproken zijn in dit proefschrift leidt tot het inzicht dat een significante verbetering van de transitieprestatie en, ten opzichte van de traditionele *slate-scheduling*, een hogere toegevoegde waarde van de totale bedrijfsvoering mogelijk zijn.