THE OPTIMIZATION ALGORITHM iFSQP
WITH APPLICATION TO NONLINEAR MODEL
PREDICTIVE CONTROL OF grate sinterING

THESIS BY

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Preface

This thesis has been submitted to the Norwegian University of Science and Technology (NTNU) in partial fulfillment of the requirements for the degree of Doktor Ingeniør.

The doctoral project has been accomplished at the Department of engineering cybernetics, NTNU, in cooperation with Elkem Sauda, Norway, and the Department of Chemical Engineering at the Carnegie Mellon University. The Elkem ASA plant at Sauda is now a part of Eramet Norway AS, a subsidiary of the Eramet Group. My supervisors have been professor Bjarne A. Foss and associate professor Tor A. Johansen. One semester of the doctoral project was spent at the Department of Chemical Engineering at Carnegie Mellon University under the supervision of professor Lorenz T. Biegler. The work has been supported by the Norwegian Research Council (NFR) grant # 119314/221.

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Due to professor Lorenz T. Biegler’s well-known experience in optimization, he taught me virtually all there is to know about practical optimization. He included me in his work-group as one of his students and shared with me from his long scientific experience. He also provided access to his optimization codes which has been of paramount importance in my work. His hospitality and friendly nature have made him a highly regarded mentor. A particular thanks to Ph.D. student Andreas Wächter from professor Biegler’s group for his hospitality during my stay at Carnegie Mellon University, and for always answering my questions by email during the last two years.

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I am grateful for receiving the opportunity of working on industrial problems within the frame of a doctoral degree. I acknowledge the cooperative
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The last three years of this work, my son, Magnus, has been my greatest source of inspiration. Thank you.

Frode Martinsen

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\(^1\)Stein Wasbø, Ragnar Tronstad, Bente Baugstø and Leif-Idar Rossemýr are presently with Eramet Norway AS.
Summary

This thesis contributes to the research on optimization algorithms for non-linear programming, and to the application of such algorithms to nonlinear model predictive control.

Regarding the contribution to research on algorithms for nonlinear programming, a novel algorithm is put forward with a complete theory for global and local convergence. This is the main contribution of the thesis. The algorithm, named rFSQP, is a reduced Hessian Feasible Sequential Quadratic Programming method. It remains feasible with respect to nonlinear inequalities at all SQP iterations, but nonlinear equality constraints are treated as in general reduced Hessian SQP methods. The rFSQP algorithm is implemented in MATLAB and tested on a number of small scale problems with encouraging results. However, the algorithm is designed for large scale problems with few degrees of freedom. Some preliminary testing of the algorithm on large scale problems are investigated.

The thesis also contributes to the understanding of the relation between sequential and simultaneous reduced gradient methods, and to the understanding of the relation between discretization methods for dynamical systems and the choice of optimization algorithms.

The thesis also contributes to model based control approaches of grate sintering. Grate sintering is a complex metallurgical process, where melting of solids and fast gas dynamics give rise to stiff process models, i.e. the "time constants" of the system differ by many decades in magnitude. Hence, application of real-time optimization methods like nonlinear model predictive control to the grate sintering process is challenging. The thesis gives a framework for implementing nonlinear model based control of grate sintering by giving a control objective, a nonlinear model and choosing an appropriate discretization scheme. The thesis gives a reduced order model which is less computationally demanding. Data from industrial experiments are used to adapt the model and to assess the control objective.
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Chapter 1

Introduction

1.1 Motivation

Optimality is a natural phenomenon which has engaged scientists in various guises for centuries. The following quote illustrates its generality and importance:

"Since the fabric of the universe is most perfect, and is the work of a most wise Creator, nothing whatsoever takes place in the universe in which some form of maximum and minimum does not appear."

Leonhard Euler, 1744

A creek always taking the steepest path downhill is an example of minimization of energy. Consider another example; imagine a blind person, call him Mr. Iterate, on top of the mountain Besseggen and ask him to find his way down on his own. By careful steps he explores the downhill path, going one step at a time, adapting his step lengths to the terrain and possibly using his memory to correct zig-zagging. Eventually, he arrives at the saddle point between the two lakes, and after testing for further descent directions, declares that he is now at the lowest point. Of course, if he strayed, say 5 meters, towards any of the two lakes he would have sensed a descent direction and continued his path. However, from his point of view there

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2 A famous mountain hike in Norway crosses this ridge which has a saddle point between a grey and a green colored lake on each side of the trek between two peaks. It is commonly believed that Ibsen’s character Peer Gynt jumped off this ridge on his buck.
is nothing to gain by moving away from his present position. The terrain seems to be flat, i.e. he has stopped at a local solution.

Although there exists a considerable body of optimization examples that can be handled by pen-and-paper calculations, computerized solutions of optimality problems have emerged during the last few decades as a powerful tool for solving larger and harder optimization problems.

A computer program for solving optimization problems commonly iterates the problem, and tries to improve on the present solution. If the problem is nonlinear but smooth and analytic (exists and is differentiable), a common approach is to linearize and solve simpler subproblems. The solutions to these subproblems become search directions, and it is then customary to moderate the step lengths to compensate for the error in the linearization. Linearization only provides local information and extrapolating information too far can be hazardous.

Returning to Mr. Iterate, this could be the way he chooses where to place his next step; he perturbs ("linearizes") the terrain in front to find the steepest descent and moderates his step length if the terrain is rugged or very steep. Note that Mr. Iterate does not have a look-ahead property, but he has a memory. Using his memory he can speed up his descent if the steepest descent path tend to zig-zag. I.e. if he experiences zig-zagging he can bend his step directions towards what seems to be the historical average direction towards the minimum. Needless to say, he would not be pleased if the terrain suddenly revealed a discontinuous vertical wall.

If there are fences in the terrain and it is required that the optimal point should be within the fences, Mr. Iterate may consider searching within the fences, or to cross them and search for the lowest topological point on the outside, but keeping in mind that he should return to the inside for the final point. Perhaps it is reasonable that he would make only conservative strolls outside the fences, and hesitate straying too far away from them?

If there are stronger requirements, e.g. that the optimal point should lie on a fence or a trek, Mr. Iterate could be forced to follow the trek or to stray from it. If there are many treks it could then be time consuming to trace them all.

Summarizing the various ways and reasonings of Mr. Iterate in an algorithm and implementing this in a computer program is precisely what is undertaken in this thesis. The algorithm shall be a generic and effective set of rules that applies to all problems falling within a specified set of assumptions. The proposed algorithm, termed rFSQP, is designed to solve nonlinear optimization problems with thousands of variables subject to nonlinear constraints. Specifically, rFSQP is designed to always remain within
1.2 Contributions

The main contribution of this thesis is the optimization algorithm rFSQP. A complete convergence analysis is given, considering both global and local properties, and the algorithm is implemented and tested on a number of problems.

The main case is grate sintering. For this case a reduced order model is developed from models available in the literature. Industrial experiments including special measurements were conducted, and the data was used for model adaption and assessing the control objective.

Various implementation issues concerning the interplay between discretization and optimization nonlinear MPC are explored. This provides insight into how a continuous time model must be discretized to allow optimization.

Appendix D gives a generic approach to representing hyperbolic PDE’s as multi-models. Due to numerical difficulties the approach has not been pursued further.

1.3 Outline

This chapter has presented the motivation for the present work, what is believed to be its main contribution, and placed it in a broader context. More detailed background, including references, are given in the introductions to chapter 2 and 3.

\footnote{Such problems belong to the class of nonlinear programming problems, which is a subclass of mathematical programming problems.}
Chapter 2 presents the grate sintering case, with a nonlinear PDE model, control objective, industrial experiments and data analysis.

Chapter 3 presents the optimization algorithm rFSQP with global and local convergence analysis, implementation details and numerical results on a selection of small sample problems.

Chapter 4 applies the optimization algorithm rFSQP to two different nonlinear model predictive control (NMPC) examples of different complexity. The second example is the grate sintering example.

Chapter 5 ends the thesis and gives its conclusions.

Appendices A to C provide some additional details for the various chapters.

Appendix D is a reprint of the paper Martinsen, Johansen, and Foss (1999).

The notation is consistent within each chapter, but to conform to the common notation within the sintering and optimization literature, respectively, the notation is not consistent between different chapters. The notation for chapter 2 is given in section 2.1.
Chapter 2

Sintering

This chapter considers the metallurgical process of grate sintering. The purpose is to develop and assess a dynamic model suitable for model-based control. The model is adapted to industrial data from experiments conducted at the sintering plant at Sauda in south-west Norway. The process at Sauda is batch-wise sintering of manganese ore, but much of the discussion, and in particular the model, is equally relevant for travelling grate sintering. It should be noted that manganese is in many aspects similar to iron which is most frequently considered in the literature.

This chapter starts with some background on sintering in section 2.2, i.e. the process is described with some comments on the sintering plant as a whole. The underlying principles governing the quality and production rate of sintering are reviewed. In section 2.3 the model is documented and discussed, while the industrial experiments and measurements are described in section 2.4. Model adaptation to the industrial data and model validation are addressed in section 2.5, while data reconciliation and analysis is considered in section 2.6. Some concluding remarks and a summary of the contributions of this chapter follows in section 2.7. The notation used in this chapter is summarized in section 2.1. Parts of this chapter have been published in Martinsen, Johansen, and Foss (1999), which is reprinted in appendix D.

2.1 Notation for chapter 2

Arabic letters

\( a_i \) - polynomial coefficient [\( \cdot \) ]
$A_b$ - specific surface area $[m^2/m^3]$

$A_f$ - frequency factor $[m/s\sqrt{K}]$

$c_p$ - specific heat capacities of solid $[J/kgK]$ and gas $[J/m\cdot d\cdot K]$

$d_p$ - average particle diameter $[m]$

$D_{ON}$ - axial gas dispersion coefficient $(O_2-N_2) [m^2/s]$

$E$ - activation energy $[kJ/mol]$

$G$ - mass flow rate of gas used in equation (2.2) $[m^2\cdot t/h]$

$G_s$ - gas volume per sinter mass used in equation (2.2) and (2.3) $[m^3/t]$

$F_i$ - liquid fraction

$h_c$ - convective heat transfer coefficient $[J/m^2\cdot s\cdot K]$

$h_m$ - mass transfer coefficient $[m/s]$

$\Delta H$ - heat of reaction $[kJ/mol]$

$k_{th}$ - thermal conductivity of gas $[J/m\cdot K]$

$k_r$ - chemical reaction rate $[m/s]$

$K_r$ - overall combustion rate constant $[m/s]$

$L$ - height of bed $[m]$

$L_f$ - latent heat of fusion $[kJ/mol]$

$L_v$ - latent heat of evaporation $[J/kg]$

$m_i$ - exponent $[-]$

$M_i$ - molecular weight $[kg/mol]$

$n_C$ - number of coke particles per unit bed volume $[1/m^3]$

$n_i$ - molar flow $[mol/m^2\cdot s]$

$p_i, \Delta p$ - (partial) pressure, differential pressure $[Pa]$

$P_{l,t}^{voice}$ - Laminar or turbulent Voice gas permeability of bed (units vary according to exponent $m_1$ in equation (2.1))
2.1 Notation for chapter 2

\( r_i \) - reaction rate \([mol/m^3s]\)

\( R \) - universal gas constant 8.314 \([J/molK]\)

\( \bar{R}_R, R_R \) - reaction rate for water \([mol/m^3s]\)

\( s_i \) - stoichiometric constant \([-]\)

\( T_{s,g} \) - temperature, solid or gas \([K]\)

\( T_{fu} \) - incipient melting temperature of solids \([K]\)

\( T_w \) - wet-bulb temperature \([K]\)

\( v \) - gas velocity \([m/s]\)

\( \nu_0 \) - gas velocity as referred to the empty bed used in equation (2.2) and (2.3) \([m/h]\)

\( \nu_w \) - heat wave velocity used in equation (2.3) \([m/h]\)

\( W \) - actual moisture content \(= x_{H_2O}(g)\) \([kg/m^3]\)

\( W_\alpha \) - critical moisture content \([kg/m^3]\)

\( x_i \) - component concentration of solids \([kg/m^3]\) or gas \([mol/m^3]\)

**Greek letters**

\( \varepsilon \) - void fraction \([-]\)

\( \varphi \) - scaling factor for the Sherwood relation \([-]\)

\( \kappa_g \) - adiabatic constant \([-]\)

\( \mu \) - viscosity \([kg/ms]\)

\( \rho \) - density \([kg/m^3]\)

\( \omega \) - specific humidity \([-]\)
Dimensionless numbers

Re - Reynolds number: $Re = \frac{d_0G}{\mu}$

Sh - Sherwood number: $Sh = \frac{h_{oa}d_0}{D_{ON}}$

Sc - Schmid number: $Sc = \frac{\mu}{\rho D_{ON}}$

Nu - Nusselt number: $Nu = \frac{h_{oa}d_0}{k}$

Pr - Prandtl number: $Pr = \frac{c_p\mu}{k}$

2.2 Background

The main purpose of sintering is to convert weakly-bounded granules into a partially fused porous sinter cake suitable for feeding a furnace. In the furnace the sintered ore is reduced with carbon. Sintering is an agglomeration process in which fine graded materials are partially fused into larger lumps by heating the charge through coke combustion. Fusion occurs when the solid charge particles undergo re-crystallization across the old grain boundaries, and possibly by simultaneous softening and partial melting. Sintering is a complex process involving flow of gas through a packed bed, heat and mass transfer between gas and solids, heterogeneous chemical reactions, and melting of solids. The heat for sintering of oxidic ores like $Fe_xO_y$ and $Mn_xO_y$ is provided by heat exchange between gas and solids and by combustion of coke. Typically the temperature must be raised to the range of $1000^\circ C - 1400^\circ C$. Since only approximately 5% (weight) of coke is needed to raise the temperature to this level, the process is generally considered to be economic in terms of energy. Water is added to micro-agglomerize finer granules by the capillary forces of water. Micro-agglomeration increases the gas permeability of the bed allowing a larger gasflow, which in turn improves sintering conditions. The critical water content is typically below 8% (weight). Typical granule sizes of the incoming material are in the range 3mm to 6mm. A large fraction of finer grades can cause low gas permeability of the bed, while coarser grades can give poor micro-agglomeration. Both cases give poor sintering conditions.

Sintering plants are commonly located close to a furnace, since, due to its low mechanical strength, sinter is ill-suited for transportation and extensive handling. The mechanical strength of the sinter can be increased by adding more coke and thereby increasing the sintering temperature. Increased sintering temperature allows a larger fraction of the solids to melt...
2.2 Background

thereby giving a stronger sinter. However, this also gives a glassy surface of the sinter, which impairs its reducibility since the effective surface area is reduced. Hence, there is a compromise between mechanical strength and reducibility which is mainly controlled by the coke weight percent.

The metallurgical process of sintering prepares the ore to form suitable feed for a (blast) furnace. Granulated ore and coke are mixed, moistened with water and micro-pelletized to form the charge. The charge is loaded onto a grate and levelled to form a bed which is ignited by a gas-fuelled ignition hood. A heat wave and coke combustion zone travels down through the bed under the influence of a suction pressure. Hot gas from the combustion zone passes through moist charge deeper in the bed where water evaporates. The process can be divided into five subsequent zones; heat exchange, fusion, combustion, drying and overmoist charge. This is illustrated in figure 2.1. A number of operations, such as feed mixing, feed charging, crushing of the produced sinter cake, screening and recycling of fines are needed. A simplified outline of the overall sintering plant is shown in figure 2.2. The sintering plant as a whole is only considered in section 2.4 where the experiments conducted at the plant are described. The dynamic model in section 2.3 is concerned with the sintering process itself, i.e. the process taking place inside the sintering pan.

The industrial plant at Sauda produces manganese alloys, such as ferromanganese \((FeMn)\) and silicomanganese \((SiMn)\) from manganese ore in electric furnaces. \(FeMn\) is typically used as an addition in the steel industry to produce certain steel qualities. Such steel qualities are used in rail-way tracks, wear-plates, etc. Because of the high reduction temperature the electric furnace is competitive with the blast furnace, especially for high purity qualities where the carbon content of \(FeMn\) must be low. \(FeMn\)-alloys with low and medium carbon \((LC/MC)\) content are produced in a subsequent refining process \((MOR)\). Limestone, \(CaO\), is commonly added in ironmaking to adjust the basicity defined by the weight-ratio of \((CaO + MgO)/(SiO2 + Al2O3)\). Limestone is not used at the sintering plant in Sauda, and is not included in the model. For a discussion of basicity in the context of manganese reduction, see Rosenqvist (1983), p. 357. General properties of the sintering process are described in Schluter and Bilsianes (1962).

2.2.1 Process goals

For the sintering process the overall goal is to produce sinter at a prescribed quality and rate at the lowest possible cost. The process dependent outputs
Figure 2.1: Zones 1-5 in the sintering bed. The figure shows a snapshot of a vertical slice of the sintering bed approximately mid-way through the process. The five zones are described to the left, with the corresponding temperature profile to the right. As time goes by the temperature profile proceeds down through the bed, i.e. at a time earlier than the snapshot in the figure the temperature profile is shifted upwards, and at later times the profile is shifted downwards relative to the one shown in the figure. The offgas is led through pipes to a cyclone, and the pressure below the pan is less than 1 atm. At the time instance shown in the figure cool air from the surroundings is being sucked into zone 1 where it heat-exchanges with the hot sinter cake. I.e. the air is preheated, and the sinter is cooled. At level 5 the temperature is 1200°C, which is the approximate freezing point of the sinter. In zone 2 the temperature is above the freezing point, and the solids are partly melted depending on the heat available for fusion. At level 4 all the coke in the bed has been combusted. Hence, above this point there are no sources of energy and the available energy between level 4 and 5 is being used for fusion and heat-exchange. At level 3 the heat from coke combustion has raised the temperature in the bed to the melting point of the charge. From level 3 to 4 coke is combusted and fusion commences. At level 2 the ignition temperature of coke is reached, and the heat from coke combustion quickly raises the temperature. In zone 4, hot gas from zone 3 pre-heats the charge, and evaporates water. Water vapor is being transported down through the bed to zone 5 where it may recondensate. At level 1 the temperature of the charge is at the boiling point of water, and above this level water evaporates.

are the quality in terms of mechanical strength and reducibility (Dawson 1993), and the production rate.
2.2 Background

Figure 2.2: *Simplified sintering plant.* Feed, consisting of a mix of various ores, coke and usually lime stone, enters to the left. The composition of the feed is known, but not the moisture content. The feed is mixed with water and (hot) recycle of undersized particles. The adhesive capillary forces of water gives micro-agglomeration of the finer particles. Only fine particles are micro-agglomerized, and large fractions of coarser particles are usually undesirable. The temperature of the recycle can be above the boiling point of water, hence evaporation of water can make it difficult to mix in the optimal water content. The mix of ore, coke, water and recycle is then charged onto the sintering bed which is supported underneath by a grate. A suction pressure is established and air is drawn down through the bed. The sintering process commences when ignition is applied to the top of the bed. The coke in the top layer of the bed is ignited and the sintering process proceeds as described in figure 2.1. After completion of the sintering process the produced sinter cake is crushed into manageable lumps by a mechanical device. The sinter is then screened, and the fines are recycled, while coarser sinter is stored or fed to the furnace.

Production rate

The productivity is quantified by the stationary Voice gas permeability $P^\text{Voice}$ (Voice, Brooks, and Gledhill 1953) in the laminar and turbulent flow regimes:

$$
P^\text{Voice}_l = v \left( \frac{L}{\Delta p} \right)^{1.0} = \frac{1}{1.5 \mu} \cdot \left( \frac{\varepsilon^3}{1 - \varepsilon} \right)^{0.5} \cdot d_p^{0.5}
$$

$$
P^\text{Voice}_t = v \left( \frac{L}{\Delta p} \right)^{0.5} = \sqrt{\frac{1}{1.5 \rho}} \cdot \left( \frac{\varepsilon^3}{1 - \varepsilon} \right)^{0.5} \cdot d_p^{0.5}
$$

(2.1)

The productivity relation thus becomes (Olsen 1997):

$$
G = \frac{v}{G_s} = \frac{P^\text{Voice}}{G_s} \cdot \left( \frac{\Delta p}{L} \right)^{m_1}
$$

(2.2)

where $m_1 = 0.5$ for turbulent flow and $m_1 = 1$ for laminar flow. The mass air flow $G$ then serves as an on-line measure of production rate. Note that when significant melting occurs, the solids becomes a continuous media and the particle size $d_p$ is not a meaningful parameter. Dawson (1993) suggests to select $d_p$ as the minimum measured sieve fraction of incoming ores in the case
of significant melting. The process variable influencing on production rate is mainly the permeability $P$ of the bed which in turn is influenced mainly by water content. Water is added to micro-agglomerize finer particles by the capillary forces of water. This increases the average particle diameter and the void fraction of the bed if the water content is kept below a critical value $W_r$. A large air flow is promoted by a large permeability which in turn forces the heat wave to travel faster through the sintering bed, thus giving a shorter batch duration and consequently an increased production rate.

Utilizing the Voice permeability $P^{Voice}$ to estimate production rate is impractical since it does not account for the amount of recycle in the plant. In the present work, $P^{Voice}$ is discarded and the production rate is estimated from the calculated recycle. The recycle stream serves as an indirect online measure of mechanical sinter quality: Poor mechanical quality will give increased recycle rate, which in turn reduces the production rate.

Quality

The sinter quality is determined by the amplitude and shape of the heat wave. Increased coke content increases the maximum sintering temperature, $T_{s,max}$ (Venkataramana, Gupta, Kapur, and Ramachandran 1998), but to achieve high reducibility $T_{s,max}$ should not be too high (Toda, Senzaki, Isozaki, and Kato 1984). In addition, proper ignition is necessary to establish initial conditions for sintering (Dash and Rose 1977). As discussed above there is an optimal water content yielding the highest bed permeability. Hence, there is an optimum depending both on the coke (Toda et al. 1984) and water content (Hinkley, Waters, O’Dea, and Litster 1994). Due to the large (hot) recycle and time delays present, the process is considered difficult to control, with quality and production rates being hard to predict (Cumming and Thurlby 1990).

Control objective

To summarize, the control objective should balance an optimal temperature profile, while considering quality, against minimizing sintering batch time. The sintering batch time is reduced by an increased air mass flow $G$ since the heat wave velocity $v_w$ is increased by an increasing air flow. The vertical velocity of the travelling combustion zone is assumed to follow the linear
relationship (Olsen 1997), p.30:

\[ v_w = \frac{v_0}{G_s \rho_b} \]  

(2.3)

where \( v_0 \) [m/h] is the gas velocity, \( \rho_b = (1 - \varepsilon) \rho_s \) [t/m³] is the bulk density of the bed and \( G_s \) [m³/t] is the gas volume per sinter mass.

The optimal temperature profile can be quantified by integrating the part of the solid temperature that has values above the fusion temperature \( T_{fu} \). The fusion temperature \( T_{fu} \) is defined by the liquidus curves of the ore composition. Partial melting of the solids occurs when the temperature is raised above \( T_{fu} \). Fusion is discussed in more detail in section 2.3.1.

The temperature profile at various levels inside the bed should be evenly distributed during the batch to give equal sintering conditions in throughout the whole sintering bed. A measure for the temperature profile at each spatial level is

\[ \tau_z \equiv \begin{cases} \int_0^{t_{end}} (T_{s,z} - T_{fu}) dt & \text{if } T_{s,z} \geq T_{fu} \\ 0 & \text{otherwise} \end{cases} \]  

(2.4)

where the subscript \( z \) emphasizes the spatial distribution of the temperature profile and \( t_{end} \) is the batch duration time. Since the fusion temperature \( T_{fu} \) is uncertain and will vary with varying ore composition, a “smooth” switch is suggested to approximate the switch caused by equation (2.4). The smoothing function is chosen as the sigmoid function

\[ \sigma(T_s) = \frac{1}{1 + e^{-k(T_s - T_{fu})}} \]  

(2.5)

This is plotted with \( T_{fu} = 1200^\circ C \) and \( k = 0.1 \) in figure 2.3.

Hence, the control objective is to maximize an objective \( \phi \) subject to the nonlinear inequality constraint imposed by quality as discussed in section 2.2.1. This is expressed formally as

\[
\max_{T_s} \phi(T_s) = \int_0^L \int_0^{t_{end}} \sigma(T_s)(T_s - T_{fu}) dt dz \\
\text{s.t.} \quad \psi_z(T_s) = \int_{t=0}^{t_{end}} \sigma(T_s)(T_s - T_{fu}) dt \leq q
\]  

(2.6)

where the parameter \( q \) remains to be selected. Observe that \( \psi_z \) is a vector function since \( T_s \) is spatially distributed. Hence, \( \phi \) must be evaluated at
Figure 2.3: *Sigmoid function*. The figure shows the sigmoid function $\sigma$ with parameters $T_{ja} = 1200^\circ C$ and $k = 0.1$. The sigmoid function is used as a smooth switch in the control objective.

Each spatial position in the sintering bed, see appendix A.1 for details. The weighting function $w(z)$ is introduced to give varying contributions to the objective at different spatial levels. The parameter $q$ is not chosen as a function (of $T_s$) since the uncertainty is assumed to be captured by the smoothing inherent in the sigmoid function. The validity of the objective function $\phi$ is assessed in section 2.6.3. The parameter $k$ in $\sigma$ can be tuned down to reduce the negative contribution following from $T_s < T_{ja}$.

### 2.2.2 Control objectives

There are few reported results on control of the sintering process. Kim and Kwon (1998) considers a linear MPC scheme designed to control the burn-through point of travelling grate sintering, using an identified input/output model. To the best of the authors knowledge, this is the only reference on model predictive control of the sintering process reported in the literature.

**Across multiple batches**

Controlling the coke and water content as discussed above can only be done across several batches, since the composition inside each sintering pan cannot be altered once it has been charged. The experiments documented in section
2.4 make some preliminary investigations of the relationship between the coke and water inputs, and the quality and production rate outputs. Inside the sintering pan, the coke and water contents have a negative bias due to the mixing of unmeasured (hot) recycle into the measured fresh feed. Note that the accuracy of the weights measuring the fresh feed may vary considerably. Manipulated inputs are the added coke, ignition energy, water and air flow rate, while the feed is regarded as a disturbance.

**During one batch**

The model and the control strategy considered in the following only considers the process taking place inside the sintering pan, i.e. the coke and water concentrations are not considered as control inputs. The only control action that influences the sintering process as the batch proceeds is the gas velocity. The gas velocity is controlled by adjusting the choke valve in the offgas-pipe, thus altering the differential pressure drop across the bed. We also assume that there is sufficient ignition in the sense that the duration and quality of ignition allows the sintering process to start at the top of the bed. Below a qualitative assessment of the gas velocity as a control action is outlined, while a quantitative discussion is given in section 2.3.4.

The heat exchange properties of the initial raw charge is much better than the heat exchange properties of the sintered material. I.e., the heat transfer properties are altered by melting since the surface area is reduced, and the heat capacity of sintered material is altered due to the change in chemical composition. To compensate for this, a large amount of excess air is used in the sintering process, and it is not expected that the O₂ concentration will be rate limiting in coke combustion. There is an upper bound on the gas velocity, since too large gas velocities can cause the bed to collapse giving poor sintering conditions. The upper limit is dependent upon the permeability \( P^{\text{V}} \) as discussed in section 2.2.1, since a larger permeability allows a larger gasflow without collapsing the bed.

The large difference in heat exchange properties of charge and sinter causes the fusion zone to widen as the batch proceeds, giving different sintering conditions at the various layers of the bed. Commonly this is discussed in terms of "matching" of the combustion heat wave and the heat exchange wave in the literature. Adjusting the gas velocity, based on a model and the measured offgas quantities, then controls the width of the fusion zone at the various layers of the bed. This conjecture is investigated by ballistic simulations in section 2.5, and nonlinear MPC based on this control strategy is implemented in chapter 4. Preliminary experiments were conducted to
investigate this conjecture at the industrial plant, see section 2.4.3. The results of these experiments are not conclusive but the hypothesis cannot be rejected on the basis of these experiments.

Note that by assuming a constant velocity of the heat wave as it passes through the bed, simpler control schemes not depending on real-time optimization and a complex process model may be considered. This has not been considered in the present work, since it is outside the scope of the thesis which focuses on optimization and nonlinear MPC.

To summarize; the control objective is to maintain the same heat wave shape at all layers in the sintering bed. Informally the objective then is to balance the heat wave profile spatially for product quality, while simultaneously maximizing the gas velocity for production rate. These issues are revisited a number of times throughout this chapter.

2.3 Modeling

Several models of the sintering process are presented in the literature (Muchi and Higuchi 1972), (Dash and Rose 1977), (Hoislbauer and Jaquemar 1983), (Kasai, Yagi, and Omori 1984), (Cumming and Thurlby 1990), (Patisson, Bellot, Ablitzer, Marlère, Dulcy, and Steiler 1991), (Nath, Da Silva, and Chakraborti 1997), (Venkataramanana, Gupta, Kapur, and Ramachandran 1998). These models are presented as nonlinear PDE's, and mainly focus on reproducing important process quantities. Noting that nonlinear PDE models are difficult to implement in a control strategy, we seek to exploit the underlying structure of the sintering process to develop a simplified model which later on can be utilized to develop a MPC strategy for the sintering process.

The model in this section should be a control relevant model suitable for MPC. Reproduction of the internal states is important since a driving hypothesis is that synchronization of the model and process through state estimation is beneficial in an industrial implementation. If the states cannot be measured and estimation is hard, it is likely that the MPC algorithm performs poorly.

This section will emphasize the development of the control relevant model, and the control algorithm itself is to be investigated in chapter 4. The global PDE model discussed in section 2.3.1 is compiled from cited references. Modelling assumptions are summarized in section 2.3.2.
2.3 Modeling

2.3.1 Global PDE model

A global PDE model is understood as a nonlinear PDE model describing the whole sintering bed as in figure 2.1 without explicit consideration of zones. In this section a model valid for the sintering bed is compiled from cited literature. A detailed review of the various physical and empirical relations used in the literature is included.

The following states are included in the model

\[ x = [T_s, T_g, x_C, x_{H_2O(t)}, x_{O_2}, x_{N_2}, x_{CO_2}, x_{H_2O(v)}] \]

i.e. temperature of solids and gas, coke concentration in solid, liquid water content\(^1\) and gas composition including water vapor. The gas velocity and pressure drop are not included as states in the model, see section 2.3.4 for a discussion. The hyperbolic PDE’s constituting the model are, for the mass balance of gas (Patisson et al. 1991)

\[
\begin{align*}
\varepsilon & \frac{\partial x_{O_2}}{\partial t} + v \frac{\partial x_{O_2}}{\partial x} = -r_{O_2} \\
\varepsilon & \frac{\partial x_{CO_2}}{\partial t} + v \frac{\partial x_{CO_2}}{\partial x} = r_{O_2} \\
\varepsilon & \frac{\partial x_{H_2O(t)}}{\partial t} + v \frac{\partial x_{H_2O(t)}}{\partial x} = r_{H_2O} \\
\varepsilon & \frac{\partial p_a}{\partial t} + v \frac{\partial p_a}{\partial x} = M_{Cr}r_{O_2} + M_{H_2O}r_{H_2O}
\end{align*}
\]

for the mass balance of solids (Patisson et al. 1991),

\[
\begin{align*}
\frac{\partial p_{H_2O(t)}}{\partial t} & = -M_{Cr}r_{O_2} \\
\frac{\partial p_{H_2O}}{\partial p_a} & = -M_{H_2O}r_{H_2O} \\
\frac{\partial p_a}{\partial p_a} & = -M_{Cr}r_{O_2} - M_{H_2O}r_{H_2O}
\end{align*}
\]

and for the energy balance (Patisson et al. 1991)

\[
\begin{align*}
\varepsilon & \frac{\partial T_s}{\partial t} + v \frac{\partial T_s}{\partial x} = k_1(T_s - T_g) \\
\frac{\partial T_g}{\partial t} & = k_2(T_g - T_s) + k_3g(T_s)
\end{align*}
\]

\(k_1 = \frac{\lambda_a c_s}{\rho_g c_p g}, k_2 = \frac{\lambda_a c_s}{\rho_s c_p a}\) and \(k_3 = \frac{1}{\rho_s c_p a}\) are aggregated temperature dependent parameters. The gas is assumed to be ideal and we assume plug-flow. The solid states are assumed not to move, i.e. \(\partial T_s / \partial x = 0\) etc.

Kinetic parameters are only considered for coke combustion, fusion and drying in the model. The chemical reactions considered are

\[
\begin{align*}
C + O_2 & \rightarrow CO_2 \\
H_2O(t) & \leftrightarrow H_2O(v)
\end{align*}
\]

\(\text{\textsuperscript{1}}\text{Liquid and solids are lumped in one phase.}\)
The kinetic relations \( r_i \)

\[
\begin{align*}
g(T_s) &= \left(-\Delta H_r\right) r_{O_2} - I_w(T_s) M_{H_2O} r_{H_2O} - I_f r_f \\
r_{O_2}(T_s) &= s_{O_2} R_C(T_s) \\
r_{H_2O}(T_s) &= s_{H_2O} R_w(T_s) \\
r_f(T_s) &= s_f R_f(T_s)
\end{align*}
\]

are discussed in the following subsections. The kinetic parameters of coke combustion \( r_{O_2} \), fusion and solidification of solids \( r_f \) and condensation \( r_{H_2O} \) are not known in detail. The kinetic model of coke combustion is discussed in Parker and Hottel (1936) and Muchi and Higuchi (1972) assuming the reaction \( C + O_2 \rightarrow CO_2 \). The kinetics of fusion of solids is described by empirical schemes based on slag diagrams (Patisson et al. 1991) or linear schemes based on process experience (Cumming and Thurby 1990). The kinetics of condensation of water is derived from laboratory tests (Patisson et al. 1990) or by heuristics and experience (Dush and Rose 1977), (Zou, Huang, Yang, and Chen 1995). The heat of coke combustion is released to the solid phase, see discussion in Cumming and Thurby (1990). Limestone is not utilized in the industrial plant, and is not included in the model. We continue by specifying the model parameters in the next subsections.

**Introductory relations**

Some introductory relations are derived. Subscript \( b \) refers to bulk sizes, \( s \) refers to spherical particle while \( p \) refers to (non-spherical) particle. Recalling that \( A_s = \pi a_s^2 \) and \( V_s = \frac{4}{3} a_s^3 \), resembles \( \frac{A_s}{V_s} = \frac{6}{a_s^2} \) and \( \frac{A_p}{m_s} = \frac{6}{a_p \rho_s} = \frac{A_s}{\rho_s} \), where \( m_s = V_s \rho_s \). The void fraction \( \varepsilon \) is defined by:

\[
1 - \varepsilon = \frac{\text{volume of solids}}{\text{volume of bed}} = \frac{m/b}{\rho/b} = 1 - \frac{\rho_b}{\rho_a}
\]

where \( \rho_b \) is the bulk density of the bed and \( \rho_a \) is the granule apparent density (see Hinkley, Waters, and Litster (1994) for details). The volume occupied by solid (spheres) in the total volume is \( V_b = (1 - \varepsilon) V \). This implies for spherical particles that \( \frac{A_b}{V_b} = \frac{A_b}{V_b/[1-\varepsilon]} = (1 - \varepsilon) \frac{A_b}{V_b} = \frac{6(1-\varepsilon)}{a_b^2} \). For a non-spherical particle of the same density as a sphere occupying the same volume \( (\rho_s = \rho_p = \rho \text{ and } V_s = V_p) \), define the mean particle diameter as \( d_p = \frac{6m}{A_p \rho_p} = \frac{6A_s}{A_p} \). Then define the form factor \( \phi_f \) as the ratio between the surface area of a sphere and the surface area of a particle occupying the same volume:

\[
\phi_f = \frac{A_s}{A_p} = \frac{d_p A_s}{6V_s} = \frac{d_p}{d_s} \leq 1
\]
2.3 Modeling

i.e. \( A_p = A_s / \phi_f = \frac{\pi d_f^2}{\phi_f} \geq A_s \). Finally, the reaction rate per unit surface area is given by \( r_{A_b} = \frac{dn}{dt} A_b \), and per unit mass and unit volume by \( r_m = \frac{6 r_{A_b}}{d_p \rho} \) and \( r_v = \frac{6(1-\varepsilon)r_{A_b}}{d_p \rho} \), respectively. Typical values of void fraction and form factor of the present materials (prior to sintering) are \( \varepsilon \in [0.4 - 0.6] \) and \( \phi_f \approx 0.75 \), see Rosenqvist (1983), p. 143. \( A_b \) is in the order 2000 [\( m^2/m^3 \)].

The harmonic mean diameter of the charge particles is calculated from mesh analysis of the raw charge as (Hinkley, Waters, and Litster 1994):

\[
\frac{1}{d_p} = \frac{f_1}{d_1} + \frac{f_2}{d_2} + \cdots + \frac{f_n}{d_n}
\]

(2.8)

where \( f_n \) is the fraction of particles between two sieve sizes with a mean diameter \( d_n \).

**Empirical relations**

Parameter uncertainties are present in the global models, since essential parameters typically are determined from empirical formulas valid only under idealized conditions. In industrial sintering processes the formation of cracks and channels leads to areas where air passes through without interacting with the mass in the sinter bed. In particular, the mass, \( h_m \), and heat, \( h_c \), transfer coefficients are calculated from the Nusselt and Sherwood numbers. Empirical relations for \( S_h \) and \( N_u \) are stated in equations (2.10) and (2.9) (Wakao and Kaguei 1982):

\[
N_u = \frac{h_c d_p}{k_{th}} = \frac{1}{\varepsilon} \left( 2 + 1.1 Pr^{1/3} Re^{0.6} \right)
\]

(2.9)

\[
S_h = \frac{h_m d_p}{D_{ON}} = \frac{1}{\varepsilon} \left( 2 + 1.1 Sc^{1/3} Re^{0.6} \right)
\]

(2.10)

valid for an idealized bed with homogeneous packing. The Reynolds, Schmid and Prandtl numbers are given by

\[
Re = \frac{\rho_0 v d_p}{\mu}
\]

\[
Sc = \frac{\mu}{\rho_0 D_{ON}}
\]

\[
Pr = 0.7
\]
where the value $Pr = 0.7$ holds for diatomic gases\(^2\). In an industrial bed the gas flowing through channels and large cracks does not interact with the solid, and the values estimated from the empirical relations for an idealized bed will deviate from the actual values. Various heuristics are utilized to overcome this in the literature, i.e. altering the constants of the empirical relations (Dash and Rose 1977), (Hoislbauer and Jaquenar 1983), (Nath et al. 1997), and introducing a scaling factor (Cumming and Thurlby 1990), (Patisson et al. 1991). According to the discussion above the gas fraction passing through possible large cracks and channels in the sinter cake does not contribute to the mass transfer and should not be included when calculating $h_m$ from $Sh$. Therefore a factor $\varphi$ is introduced to compensate the Sherwood relation (Schluter and Bitsianses 1962):

$$h_m = \varphi \frac{D_{ON}}{\varepsilon} \left( 2 + 1.1 Sc^{1/3} Re^{0.6} \right) \quad (2.11)$$

The Nusselt relation is scaled by the same factor $\varphi$.

The heat capacity of the solid and the void fractions will change in a complicated way as sintering proceeds. The specific heat capacity of sintered material for Fe-sinter is given by (Rose and Dash 1979)

$$c_{p,s} = 753 + 24 \cdot 10^{-3} T_1 \quad [J/kgK] \quad (2.12)$$

As seen from figure 2.4 this linear approximation is suitable for iron ore. For manganese ore the situation is different, and the relation for $c_{p,s}$ used in the model is the dashed curve in the right part of figure 2.4. This relation was obtained as a linear combination of the data for the three Mn-oxides. The linear combination was chosen from plant data where the ore contained 47.0% $MnO_2$, 25.5% $Mn_2O_3$ and 27.5% $MnO$.

This model of $c_{p,s}$ does not include other elements contained in the ore, and it does not reflect changes caused by fusion, chemical reactions and thermal decomposition of the Mn-oxides.

The temperature dependence of $c_{p,g}$ is modelled as:

$$\frac{c_{p,g}}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \quad [J/kgK] \quad (2.13)$$

where $a_i$ values are specified in Moran and Shapiro (1993), p. 680. For ideal gases $c_{p,g} - c_{v,g} = R$ gives a similar expression for $c_{v,g}$. The temperature

\(^2\)A diatomic gas contains two atoms in its molecules. $O_2$ is a diatomic gas, while $H_2O_{(v)}$ has three atoms in its molecules. A small error is introduced by this, but since $H_2O_{(v)}$ is not present in the combustion zone, the error is assumed to be of minor importance.
dependence of the viscosity $\mu$ is modelled by Sutherland's formula (White 1999), p. 771:

$$\mu = \mu_0 \left[ \frac{T_g}{T_0} \right]^{3/2} \left[ \frac{113 + 273.1}{113 + T_g} \right]^{m_2} \left[ kg/ms \right]$$

(2.14)

where $\mu_0 = 1.72 \cdot 10^{-5} \left[ kg/ms \right]$ and $m_2 \approx 0.9$. The temperature dependency of the axial gas dispersion coefficient $D_{ON}$ is modelled as:

$$D_{ON} = D_{ON}^0 \left[ \frac{T_g}{273} \right]^{m_3} \left[ m^2/s \right]$$

where $m_3 \approx 1.5$. The thermal conductivity of gas $k_{th}$ is estimated from the Prandtl number:

$$k_{th} = \frac{\mu c_{p,g}}{P_r m_4}$$

where $m_4 \approx 10.7$ is determined by adapting the computed $k_{th}$ to tabulated data from Perry and Green (1984).
Coke combustion and overall heat of reaction

A number of different reactions occur during sintering of manganese ore. The equilibrium diagram in figure 2.5 shows the possible reactions at given operating conditions. These reactions contribute to the overall heat of reaction, $\Delta H_r$. Since only coke combustion is considered to be of major importance with respect to the dynamic properties, the kinetics of reduction of Mn-ore is neglected.

![Equilibrium gas ratio for reduction of Mn-oxides](image)

Figure 2.5: Equilibrium gas ratio $\log_{10}(p_{CO_2}/p_{CO})$ for reduction of Mn-oxides. The Boudouard-line ($2CO \leftrightarrow C + CO_2$) crosses the MnO – Mn line at approximately 1400°C. The measurements conducted at the Sandu plant show that the temperature in the sintering bed is nominally below this point. Hence, reduction to Mn is not likely to occur. The slopes of the other oxide-components slants upward, and reduction in the presence of CO will occur endothermic.

In a (reducing) atmosphere of CO the following endothermic reactions are observed in figure 2.5:

\[
\begin{align*}
MnO_2 + \frac{1}{2}CO & \leftrightarrow \frac{1}{2}Mn_2O_3 + \frac{1}{2}CO_2, & \Delta H_{r,1} & \approx -100 \text{ kJ/mol C} \\
\frac{1}{2}Mn_2O_3 + \frac{1}{6}CO & \leftrightarrow \frac{1}{3}Mn_3O_4 + \frac{1}{6}CO_2, & \Delta H_{r,2} & \approx -30 \text{ kJ/mol C} \\
\frac{1}{3}Mn_3O_4 + \frac{1}{6}CO & \leftrightarrow MnO + \frac{1}{3}CO_2, & \Delta H_{r,3} & \approx -22 \text{ kJ/mol C}
\end{align*}
\]

where the heat of reaction is taken as the average over the temperature range of interest. These reactions move to the right during combustion and fusion, cf. figure 2.1. However, due to the large air excess during sintering, only a small amount of CO is actually present. According to Olsen (1997) the offfgas ratio $\alpha = \frac{CO}{CO_2}$, subsequent to combustion can become as high
as 0.25 – 0.30. I.e. we have \( \log_{10} \left( \frac{p_{CO}}{p_{CO_2}} \right) \approx \log_{10}(3) \approx 0.47 \) showing by inspection of figure 2.5 that the three reactions above are possible. The Boudouard-reaction:

\[
2CO \leftrightarrow C + CO_2, \quad \Delta H_{298}^\circ = -172.5 \text{ kJ/mol C}
\]

which is strongly endothermal, prevents further reduction by CO. In addition thermal dissociation at \( p_{O_2} = 1 \text{ atm} \) occurs:

\[
500^\circ C : \quad MnO_2 \leftrightarrow \frac{1}{2} Mn_2O_3 + \frac{2}{12} O_2, \quad \Delta H_{298}^\circ = 41.8 \text{ kJ/mol C}
\]

\[
800^\circ C : \quad \frac{1}{2} Mn_2O_3 \leftrightarrow \frac{1}{3} Mn_3O_4 + \frac{1}{6} O_2, \quad \Delta H_{298}^\circ = 16.3 \text{ kJ/mol C}
\]

Expressing \( X_{CO} = \frac{\alpha}{1+\alpha} X_{CO_2} \) and assuming that coal is present as pure carbon, combustion is expressed as:

\[
C + (1+\alpha)O_2 + 3.76(1+\alpha)N_2 + L + (1-\alpha)CO_2 + \alpha CO + 3.76(1+\alpha)N_2 + L
\]

where excess air \( L \) consisting of 79% \( N_2 \) and 21% \( O_2 \) is utilized. Choosing \( \alpha = 0.25 \) gives a heat of reaction \( \Delta H_{r,c} = -335 \text{ kJ/mol C} \approx -28 \text{ MJ/kg C} \). The heat of combustion for coal is experimentally determined to approximately \( \Delta H_{r,c} \approx -35 \text{ MJ/kg C} \) (Olsen 1977), i.e. 7MJ/kg more than indicated by the enthalpy of reaction stated above. This is attributed to volatile components present in industrial coal. The overall heat of reaction used in the model is \( \Delta H_r = \Delta H_{r,c} - \Delta H_{r,1} - \Delta H_{r,2} - \Delta H_{r,3} \approx -270 \text{ kJ/mol C} \) which is close the reported values for Fe-sintering in the literature. Note that thermal dissociation is not included since it is completed before coke combustion proceeds.

The reaction rate of coke combustion is important due to the large temperature gradients present in grate sintering. Coke combustion is a heterogeneous reaction, and the overall combustion rate is controlled by two physical phenomena; the chemical combustion rate and the gas transport rate to the individual coke particle. The combustion rate for a coke particle is governed by (Parker and Hottel 1936), (March and Higuchi 1972)

\[
k_r = A_f \cdot e^{-E/RT_s} \cdot \sqrt{\tau_s} \cdot x_{O_2} \quad (2.15)
\]

with the frequency factor \( A_f = 6.53 \cdot 10^5 \text{ m/s}\sqrt{K} \) and \( E = 185 \text{ kJ/mol C} \). \( \tau_s \) is the gas temperature at the solid surface. This relationship is extensively used in the literature, but it assumes the first order reaction \( C + O_2 \rightarrow CO_2 (\alpha =\)
0) and that combustion commences on the coke particle surfaces (Muchi and Higuchi 1972). Both of these assumptions are inconsistent with industrial experience. Still, equation (2.15) is used in the present model assuming \( \tau_s = T_i \). The activation energy, however, is reduced to approximately 70 \( kJ/mol \) to fit the model to the measured data. By using the ideal gas law (2.15) can be written in terms of \( pO_2 \) instead of \( xO_2 \).

Since the transport of reactants and products to and from the coke particle surface can be rate limiting at elevated temperatures, the overall reaction rate, including both chemical and transportation phenomena, is modelled by the relation (Muchi and Higuchi 1972):

\[
K_r = \frac{k_r h_m}{k_r + h_m}
\]

where \( h_m \ [m/s] \) is calculated from equation (2.11). Pore diffusion \( D_{pd} \) may be included similarly according to

\[
\frac{1}{K_r} = \frac{1}{k_r} + \frac{1}{h_m} + \frac{1}{D_{pd}}
\]

This is not included in the present model. This gives the overall combustion rate of coke:

\[
R_r = 4\pi (d_{p,C}/2)^2 n_C K_r xO_2
\]

(2.16)

where \( n_C \ [1/m^3] \) is the number of coke particles per unit bed volume and \( d_{p,C} \) is the average coke particle diameter.

**Fusion**

Particle growth due to fusion is modelled according to Dash and Rose (1977) as

\[
d_{p,f} = d_p (1 + k_f L_f)
\]

where \( k_f \) is a constant to be determined experimentally and \( L_f \) is the enthalpy of fusion (melting). If significant melting does not occur, the scheme of Dawson (1993) where smaller particles attaches to larger particles is assumed to be prevailing. This is termed heterogeneous texture, i.e. the mean particle size of sintered particles is in the region of the larger sieve sizes of the charge. However, if significant melting occurs the situation will be completely altered, with formation of larger continuous blocks which again
forms a homogeneous texture. This is assumed to correspond to a texture of very fine particles, with particle sizes in the region of the finest mesh sizes present in the charge. The transition between these two regimes is controlled by the sintering temperature (Dawson 1993). Particle growth is not included in the present model.

Fusion itself is complex and is modelled by the following equations (Patisson et al. 1991):

\[
\begin{align*}
  r_f &= \rho_s \frac{dF_1}{dT_s} \cdot \frac{dT_s}{dt} \\
  F_1 &= (1 - x_h) \left[ a_0 + a_1(T_s - T_{df}) + a_2(T_s - T_{df})^2 + a_3(T_s - T_{df})^3 \right] \\
  F_2 &= F_m \frac{T_s - T_{fs}}{T_{sa} - T_{fs}}
\end{align*}
\]

where the function \( F_1 \) denotes the liquid fraction during melting, \( x_h \) is the hematite fraction of the ternary system FeO – MnO – SiO2, \( T_{df} \) is the incipient melting temperature, and \( a_i \) are dependent on the basicity index and can be found from a liquidus surface diagram, see Verein Deutscher Eisenhüttenleute (VDEh) (1995), figure 3.286. During solidification, composition is assumed to be constant and the simplified relation \( F_2 \) is adopted where \( F_m \) is the liquid fraction at \( T_{s, max} \) and \( T_{fs} \) is the temperature at the end of solidification.

Using the liquidus surface diagram is impractical and the present model only considers linear schemes based on process experience (Cumming and Thurlby 1990). The present model implements a quadratic approximation where the parameters were tuned to fit the data.

\[
\begin{align*}
  r_f &= \left( \hat{a}_1 \cdot (T_s - T_{df}) + \hat{a}_2 \cdot (T_s - T_{df})^2 \right) \cdot \rho_s \left[ \text{mol} / \text{s} \right] \\
  L_f &= 255 \left[ \text{kcal} / \text{mol} \right]
\end{align*}
\] (2.17)

with \( T_{df} = 1250^\circ C \) and different values of \( \hat{a}_i \) for melting and freezing following the scheme of Nath, Da Silva, and Chakraborti (1997). This simplified model gives a kink in the temperature profile when the model switches from melting to freezing. Since these parameters were selected without reference to liquidus diagrams, the model is conceptual, and refinements should be considered since the sinter quality is governed by the shape of the temperature profile. Note that fusion has a significant influence on the falling edge of the temperature profile.

**Water**

Water evaporates and condenses according to

\[
H_2O_{(l)} \leftrightarrow H_2O_{(v)}
\] (2.18)
The drying model is governed by (Patisson, Bellot, and Ablitzer 1990)

\[
\begin{align*}
\dot{R}_R &= R_M \cdot P(W_r) \\
P(W_r) &= 1 - (1 - W_r)(1 - 1.796W_r + 1.0593W_r^2) \\
R_M(T_w) &= \frac{\alpha_p \rho_v}{M_{H_2O} \Delta H_v(T_w)} \\
R_R(T_s) &= \frac{\alpha_p \rho_v}{R_T^g} \left( p_{v,sat}(T_s) - p_{H_2O} \right) \\
p_{v,sat}(T_s) &= \exp \left( 25.541 - \frac{5211}{T_s} \right) \\
k_{th} &= \frac{3.355 \rho_g}{h_c T_s \sqrt{(1-0.24x_g)(1+\frac{x_g}{x_{v,s}})(1-x_g)}}
\end{align*}
\]

(2.19)

where \( W_r = W/W_{cr} \) and the given coefficients of \( P(W_r) \) determined from laboratory tests (Patisson, Bellot, and Ablitzer 1990) are valid for a Fe-charget. Coefficients for Mn must be determined experimentally. The wet-bulb temperature \( T_w \) can be calculated by solving a nonlinear equation (Patisson et al. 1990). The present approach uses the approximation (Rose and Dash 1979)

\[
T_w = 293.4 + 324.6 \cdot W - 594.1 \cdot W^2 + 292.1 \cdot W^3
\]

which is based on tabulated data from Perry and Green (1984). \( x_{tg} \) is the logarithmic mean of the molar fraction of vapor in the bulk gas and at the saturated surface:

\[
x_{tg} = \frac{x_{v,g} - x_{v,s}}{\log \frac{x_{v,g}}{x_{v,s}}}
\]

Since \( x_{v,s} \) is unknown the present model implements \( x_{tg} = 0.5 \cdot x_{v,g} \). The heat transfer coefficient \( h_c \) for the water-vapor system may differ from the overall heat transfer coefficient from equation (2.9). This is not considered in the present model. If \( R_R > 0 \) and \( W \geq W_{cr} \) (falling rate) \( r_{H_2O} = \dot{R}_R \). If \( R_R > 0 \) and \( W < W_{cr} \) (constant rate) \( r_{H_2O} = R_R \). The heat capacity of the moist offgas is modelled by (Perry and Green 1984), p. 12-3:

\[
c_p = 0.24 + 0.45 \omega
\]

where \( \omega = 0.622 \frac{p}{p_{H_2O}} \). Simplified schemes for \( R_R \) are found in Nath, Da Silva, and Chakraborti (1997) and Zou, Huang, Yang, and Chen (1995). The latent heat of evaporation is approximated by (Patisson et al. 1990)

\[
L_v(T_w) = 3.1563 \cdot 10^6 - 2396.6 \cdot T_w \cdot [J/kg]
\]

\( ^3 \)The present model is implemented with the Fe-coefficients.
2.3 Modeling

2.3.2 Modelling assumptions

In this section the main assumptions on which the global PDE model is based, are summarized.

i. The total pressure $p$ is assumed to drop linearly down through the bed. The gas velocity $v$ is considered as a control action and is assumed not to be distributed. I.e. all levels experience the same velocity at any given time instance.

ii. The manganese ore is treated as a single substance, i.e. various oxidation levels of manganese are not considered. Likewise other substances contained in the ore are neglected. More specifically, the various oxidation levels of manganese are treated as inerts, and only influence on the specific heat capacity of the ore.

iii. Complete coke combustion is assumed, hence CO is not generated. The gas $N_2$ is considered to be inert.

iv. Gas dynamics are assumed to be plug-flow. The gas dynamics are approximated by first order finite differences in the spatial dimension.

v. Radially homogeneous mixing is assumed. Adding another dimension should include Fourier’s law to allow conduction in the solid phase. Including radial conduction is not considered to be of major importance in a control relevant model. Channeling effects may have a significant influence on the sintering process, and taking this into account is a possible extension to the present model. The present model only considers this through the scaling of the Sherwood relation (2.10).

vi. Solid particles have homogeneous density and temperature. Coke particles are porous, but the void fraction of coke is considered as part of the gas phase. Small particle sizes gives uniform temperature inside particles, due to high thermal conductivity.

vii. Fusion (i.e. sintering) is modelled by a polynomial approximation. The polynomial was selected by adaption to measurements.

viii. Coke combustion and water evaporation/condensation are the only chemical reactions considered. Coke combustion generates the heat necessary for sintering/fusion to occur, and its kinetic parameters control especially the leading edge of the temperature front. A water evaporation model based on the literature is implemented. Other
reactions influence on the overall energy requirements, but are expected to have little influence on the dynamic characteristics. Decomposition of limestone is not modelled, but can be included without altering the structure.

ix. Thermodynamic relations are approximated by polynomials.

x. Slump and shrinkage are neglected. The sinter bed at Saouda is observed to shrink about 5 cm during a batch. This alters the heat exchange volume above the fusion zone, cf. figure 2.1. A small reduction in the cooling zone is expected to have minor influence on the conditions inside the fusion zone. Slump is only relevant for travelling grate sintering.

2.3.3 Comparison with existing models

There are three good models presented in the literature; (Hoislbauer and Jaquemar 1983), (Cumming and Thurlby 1990) and (Patisson, Bellot, Ablitzer, Marlière, Dulcy, and Steiler 1991). The model by Hoislbauer and Jaquemar (1983) has the best numerical qualities, while the model by Cumming and Thurlby (1990) is the most extensive. Note that the paper by Hoislbauer and Jaquemar (1983) focuses on numerical properties, and that the model is comparable in complexity to the one given by Patisson et al. (1991). Cumming’s model gives no data for the numerous chemical reactions considered. Hence, reproducing the results is hard. The numerical simulations are reasonable but seem to be based on simplifying assumptions not fully documented. The present model is based on Patisson et al. (1991). Their model includes the basic PDE model restated in section 2.3.1, the fusion, coke and water kinetics considered herein. Hence, the model by Patisson et al. (1991) includes the most important physical phenomena, and gives data for the water kinetics. The fusion data is not given, and the present model uses a simplified polynomial approximation. No models in the literature gives gas velocity simulations, and all use Ergun’s relation. Ergun’s relation is discussed in section 2.3.4 below.

2.3.4 Computation of the control input \( v \)

As discussed in section 2.2.2 the gas velocity is considered as a control input. The simplest approach, which is the method implemented in chapter 4, is to consider \( v \) directly as a control input. In an industrial implementation
the control actuator will typically be a valve disc in the outlet gas pipe. Manipulating the valve disc will alter the pressure drop across the bed which is a measured quantity. Therefore it is necessary to model the relationship between the pressure drop and gas velocity, and include gas velocity as a state in the model. The gas velocity model is derived below as

\[
\frac{dv}{dx} = \frac{RT_g}{p} \sum_{i,j} \hat{r}_{i,j} + \frac{v}{T_g} \cdot \frac{dT_g}{dx} - \frac{v}{p} \cdot \frac{dp}{dx} \tag{2.20}
\]

The ideal gas law with molar flow \( n_i \) in \([mol/m^2s]\) and apparent velocity \( v \) in \([m/s]\) is

\[
n_i = \frac{pv}{RT_g}
\]

Differentiation gives

\[
\frac{dn_i}{dx} = \frac{p_i}{RT_g} \cdot \frac{dv}{dx} + \frac{v}{RT_g} \cdot \frac{dp_i}{dx} - \frac{p_i}{p} \cdot \frac{v}{RT_g} \cdot \frac{dT_g}{dx}
\]

assuming \( v > 0 \) and reorganizing

\[
\frac{dp_i}{dx} = \frac{RT_g}{v} \cdot \frac{dn_i}{dx} - \frac{p_i}{v} \cdot \frac{dv}{dx} + \frac{p_i}{T_g} \cdot \frac{dT_g}{dx}
\]

Using

\[
\frac{dn_i}{dx} = s_i r_i
\]

where \( s_i \) is a stoichiometric constant gives

\[
\frac{dp_i}{dx} = \frac{RT_g}{v} \cdot s_i r_i - \frac{p_i}{v} \cdot \frac{dv}{dx} + \frac{p_i}{T_g} \cdot \frac{dT_g}{dx}
\]

The total molar flow is

\[
\frac{dn_t}{dx} = \sum_i s_i r_i
\]

and

\[
v = \frac{n_t RT_g}{p}
\]

differentiation and using the expression for \( n_t \) gives

\[
\frac{dv}{dx} = \frac{RT_g}{p} \cdot \frac{dn_t}{dx} + \frac{n_t R}{p} \cdot \frac{dT_g}{dx} - \frac{RT_g n_t}{p^2} \cdot \frac{dp}{dx}
\]

\[
= \frac{RT_g}{p} \cdot \sum_i s_i r_i + \frac{v}{T_g} \cdot \frac{dT_g}{dx} - \frac{v}{p} \cdot \frac{dp}{dx} \tag{2.21}
\]
The term $\sum_{i,j} \dot{\gamma}_{i,j}$ in equation (2.20) occurs from the matrix-vector product $S \cdot \dot{r}$ when there are more components present. Assuming infinite fast gas dynamics a mechanistic energy balance yields the pressure drop as the isothermal Ergun's relation:

$$\frac{dp}{dx} = 150 \frac{\mu \rho (1 - \varepsilon)^2}{(\phi_f d_s)^2 \varepsilon^3} + 1.75 \frac{\rho \nu^2 (1 - \varepsilon)}{\phi_f d_s \varepsilon^3}$$

(2.22)

For small particle sizes, low fluid velocity and high fluid viscosity, the flow will be laminar (viscous). For larger particle sizes, high fluid velocity and less viscous fluids, the flow will be turbulent. In grate sintering, the flow is a priori expected to vary continuously from laminar to turbulent flow as the sintering batch proceeds. The first term in Ergun's formula refers to the viscous and the second to the turbulent pressure drop.

Given the measured pressure drop across the bed the velocity is calculated by equation (2.21) under some simplifying hypotheses discussed next. Considering $dp/dx$ as a control input (i.e. a linear decay from top to bottom, the bottom pressure being a manipulated variable), assuming known (constants) $\varepsilon$ and $\phi_f d_p$, and computing $\mu$ by equation (2.14). Hence, all terms of equation (2.21) are defined and $dv/dx$ can be integrated to give the state $v$. However, assuming a linearly decaying pressure drop across the bed is not physical since it neither accounts for the distributed temperature profile, nor evaporation of water which produces additional gas molecules. In addition equation (2.22) is derived for isothermal conditions, while the temperature in the sintering bed is not constant. Since both the density and viscosity of the gas are temperature dependent, the extended Ergun relation of Wonchala and Ymnyckyj (1987) should be considered. Calculation of the pressure profile $dp/dx$ is also dependent upon the parameters $\varepsilon$ and $d_p = \phi_f d_s$, which are dependent on the degree of melting.

As outlined in Rosenqvist (1983), p. 146, Ergun's relation allows calculation of $\varepsilon$ and $d_p$ if two sets of measurements are available. Here $dp/dx$ is the pressure drop per unit height of the bed, $\mu$ and $\rho$ are viscosity and density of the fluid, and $v$ is the superficial velocity of the fluid, i.e. velocity referred to the empty bed. Laboratory tests for accurate measurement of $\varepsilon$ and $d_p$ are suggested in Hinkley, Waters, and Litster (1994) and Hinkley, Waters, O'Dea, and Litster (1994). Hinkley, Waters, and Litster (1994) also suggests that other constants should be utilized in the Ergun relation when wet charge is considered. The average particle diameter, $d_p$, will not have a physical interpretation once melting in the fusion zone has occurred, see the discussion on fusion in section 2.3.1. Still, all cited models utilize some equivalent particle diameter when melting has occurred.
Figure 2.6: Ergun’s relation. The figure shows Ergun’s relation for $\mu = 1.7e - 5 Pa \ s, \rho = 1.29 \ kg/m^2 \ s, L = 0.4 m, v = 1 m/s$. The nonlinearity in Ergun’s relation is considerable especially for small void fractions, $\varepsilon$, and small particle sizes, $d_p$. Noting that since the measurements presented in section 2.4 shows a typical pressure drop of 5kPa, the nominal values of $\varepsilon$ and $d_p$ cannot be too low. $\Delta p = 5kPa$ and $\varepsilon = 0.4$ implies a $d_p = 2.2 mm$, while $\varepsilon = 0.6$ implies a $d_p = 0.6 mm$.

Figure 2.6 shows the nonlinearity of Ergun’s isothermal relation as a function of $\varepsilon$ and $d_p$. As the discussion in the figure caption indicates the Ergun relation is moderately nonlinear in the region of interest. Using constant values for $\varepsilon$ and $d_p$ is reasonable as an initial approximation in a control relevant model. A model for $\varepsilon$ and $d_p$ should comply to the following heuristics (Olsen 1997)

- $\varepsilon_{ch}$ remains unchanged during the batch
- $\varepsilon_f$ is altered due to the particle growth caused by fusion. The fusion zone has the lowest permeability and thus has the lowest void fraction.
- $\varepsilon_{hex}$ is the largest.

where $\varepsilon_f < \varepsilon_{ch} < \varepsilon_{hex}$ are the void fractions in the fusion (zone 2 and 3), charge (zone 4 and 5) and heat exchange (zone 1) as referred to figure 2.1. The literature only give qualitative models for void fraction and particle growth (Cumming and Thurlby 1990).

A simplified approach compared to including $v$ as a state and applying Ergun’s relation is to compute $v$ directly from the quadratic equation
(2.22) in \( v \) for a specified \( dp/dx \). This approach should be validated against the complete model outlined above. Due to the added complexity of the extended Ergun relation and the uncertainty in modelling \( \varepsilon \) and \( dp \), the velocity \( v \) itself is considered as a control action in the following.

2.4 Experiments and measurement campaigns

Experiments conducted at the sintering plant in Sauda, Norway, were initially designed to collect data which could be used to obtain the following goals:

- Identification of an input-output model.
- Adaption and validation of the nonlinear PDE model.
- Verification of the connection between charge composition, process operation and product quality.
- Provide realistic feedback (process simulator) for testing nonlinear MPC.

In addition thorough knowledge of the sintering process was gained. The first goal was not achieved, since the unknown recycle led to large disturbances. Hence, the information content in the measured output was dominated by disturbances. The measurements allowed calculation of the recycle which showed that the recycle was much larger than expected. Initially the recycle was assumed to be in the order 20-30% with small variations. In section 2.6 the actual recycle is calculated to vary in the range 0-53%.

In addition the process output ”production rate” was not well-defined in terms of on-line measurements at the time the experiments were conducted. Model adaption and validation has been performed by visual comparison of the measurements against the simulations. This was an iterative procedure where model parameters were manually updated, the model simulated, and the result compared to the measurements, see figures 2.13 and 2.15 below. The relationship between in- and outputs has been verified by the experiments, and this motivated a mathematical formulation of a control objective suitable for use in nonlinear MPC. Nonlinear MPC is documented in chapter 4. The measurements were not used directly as process simulator, but the model was adapted to the data. Hence, the model is a realistic representation of the industrial process.

In section 2.4.1 follows a description of the experiment setup, including a more detailed description of the plant and the available instrumentation.
relevant for the experiments. The measurements conducted at the plant are documented in section 2.4.2. Data analysis is documented in section 2.6.

2.4.1 Plant and experiment description

The industrial sintering plant under investigation is located in Sauda, Norway and was owned by the Elkem ASA company at the time the experiments were conducted. It is now owned by Eramet Norway AS, a subsidiary of the Eramet Group. Two independent measurements campaigns were carried out. The first in March 1998, and the second during the Spring of 1999.

- The first campaign investigated the effect of altering the gasflow through the bed without altering the charge composition, see section 2.4.3.
- The second campaign investigated the effect of altering the charge composition without altering the gasflow. These experiments occupy the bulk of the remaining part of this chapter, in particular section 2.4.2. Note that some of the measurements documented in section 2.4.2 were available during the first measurement campaign as well.

The plant layout together with relevant instrumentation is described in figures 2.7 and 2.8. The sintering plant is part of a larger plant for electrical reduction to FeMn and SiMn, and the sintering plant is designed to provide suitable feed for the electrical furnaces at the plant. The sintering plant in Sauda is a batch-wise plant with six parallel Greenawalt-panns.

To allow the set-point change in coke composition to propagate into the pan, each experiment was designed as outlined in figure 2.9. Letting each experiment span three consecutive batches was based on the assumption of 20-30% recycle, i.e. accepting a bias in the coke composition, and compensating for this once the actual recycle has been calculated. Since each experiment spans 3 consecutive batches, it is relevant to investigate the relationship between any two consecutive batches. From the difference in fresh feed between two consecutive batches given in table 2.1, an empirical probability distribution function $F$ was calculated, see figure 2.10. Based on the third column of table 2.1 a bootstrap estimate (Efron and Tibshirani 1986) was computed. 1000 new observation series was generated. Note that since there are only 11 observations the variance estimates are uncertain. The expectation, standard deviation and BC (bias-corrected) confidence intervals are given in table 2.2.
Figure 2.7: Detailed sintering plant. The figure shows the details of the sintering plant that are important for the experiments, together with the available instrumentation. Starting from the upper left there are 12 feed bins containing coke, Mn-ore and various scrap from the plant. The mass-flow from each bin is measured automatically (FT). Added water is manually controlled (C) and the water flow is measured manually by a flotameter (L). The amount of recycle is unknown, as indicated by the irregular and unknown shape of the recycle bin. The recycle level is measured manually by lowering a mechanical device into the bin (L). The recycle output is controlled from the control room by adjusting the set-point of a vibrating device (C). The recycle temperature is measured automatically by a sensor attached to the outer wall (point-welding) of the recycle bin (TT). Inputs are mixed in a rotary mixer and stored in the charge bin. The feed is charged into the six sintering pans. The moisture content of the feed is measured manually by a drying test of a sample taken from a pan (A). Details of the instrumentation of the sintering pans inside the dotted box are shown in figure 2.8. After completion of the sintering process the produced sinter cake is crushed into manageable lumps by a mechanical crushing device. The sinter is then screened, and the fines ($d_p < 3mm$) are recycled, while coarser sinter is stored or fed to the furnace. Manual samples of the produced sinter are taken by shuffling approximately 40-50kg of sinter into containers before screening (A).

2.4.2 Measurements at plant: Campaign 2

This section summarizes the measurement campaign carried out at the sintering plant in Sanda during the Spring of 1999. The measurements logged during each experiment are shown for experiment 1 in figure 2.11 and A.1 in appendix A.2. The sampling period was 5 seconds. In addition to the
2.4 Experiments and measurement campaigns

Figure 2.8: *Instrumentation of sintering pan.* The figure shows the details of the instrumentation of the sintering pan that were available for the experiments. The figure shows the details of the block inside the dotted box in figure 2.7. The experiments were conducted in pan no. 1 of the six pans. Temperature measurements on the top and 15 cm down into the pan by K- and S-elements respectively, in addition to sensors (point-welding) on the outer wall at depths 15 cm and 30 cm were logged (TT). The offgas temperature and differential pressure were logged for both pan 1 and 2 (TT) and (PT). The offgas-flow is controlled from the control room by a choking valve (C). This is operated according to a prescribed recipe. The pressure after the cyclones was logged (PT), with a pitot-element (Pt-100) intended for flow-measurements. The gas flow must be compensated for temperature, measured by (TT) at the same location. Just below this point a thin pipe was inserted allowing for gas-samples to be taken (A). A fan was attached to this tube, and moisture and composition tests were taken by sucking out offgas.

Measurements shown in the figure mass-flows from the feed-bins and the and wall-temperature of the recycle bin were logged. Various manual samples such as the recycle level, the water content of the charge and offgas and sinter were also taken. Some details of the curves in figure 2.11 deserve special attention. In the first subfigure the solid temperature and ignition gas temperature in pan 1 are shown. The first batch starts at approximately 17 minutes as seen from the ignition gas temperature (dashed curve). Just before 20 minutes the ignition hood is removed and the S-element (cf. caption of figure 2.8) is inserted into a ceramic tube placed into the bed prior to ignition. At approximately 53 minutes the S-element is removed and pan 1 is fetched to be emptied into the crushing machinery. This pattern is repeated for each batch.
Figure 2.9: *Batchwise experiments*. The figure shows how the batchwise plant influences on the conducted experiments. The horizontal axis of the figure is time, and one batch lasts approximately one hour. To the left, experiment 1 starts by setting the feed set-point to the desired value. Due to the hold-up of the plant, the feed charged into the pans will not be influenced by the set-point change until approximately batch 2 or 3 (depending on the amount of recycle which is unknown). Note that each batch (labeled 1, 2, 3) consists of six pans as indicated on the figure by the six overlapping boxes. After batch 3 is finished, pan 1 is emptied into the crushing machinery and a sample is taken by shuffling a large amount of sinter into a container. Now experiment 1 is completed, and experiment 2 commences by setting the feed set-point to its desired value. Note that the set-point for experiment 2 may be altered earlier than indicated due to the plant hold-up. Since the recycle is unknown a degree of conservatism wrt. set-point alterations was introduced to guarantee that the feed composition in the pan in batch 3 actually was as desired.

In subfigure 2 it is observed that the batch in pan 2 starts about 5 minutes prior to the batch in pan 1. This is due to the sequential nature of the batch cycle at the plant, and was not altered during the experiments. The pressure does not vary substantially during the batch, despite the generation of gas molecules caused by evaporation. This indicates that the gas velocity increases during the batch. The pressure difference between pan 1 and 2 is discussed in the figure caption. No large leakages in the pipes were observed.

Towards the end of each batch the offgas temperature is expected to approach the gas temperature in the combustion zone. Subfigure 3 shows considerably lower offgas temperatures than the solid temperature shown in subfigure 1.

The slowly falling offgas temperature during the first part of a batch is attributed to a change from laminar to turbulent flow due to the lower differential pressure during the initial phase of the batch, combined with the large difference in heat-capacities between the solid and gas phase of the packed-bed system. I.e. initially the Reynolds-number is low giving poor heat-exchange and the hot ignition gas is transported through the pan without loosing to much heat to the solid phase. Once the pressure difference is increased, the Reynolds-number increases and the heat-exchange between the two phases is increased. Hence, the offgas temperature is expected to
### 2.4 Experiments and measurement campaigns

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<th>Experiment</th>
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<th>(s_2)</th>
<th>(s_3)</th>
<th>(\Delta s)</th>
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<td>17.3</td>
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<td>-</td>
<td>14.9</td>
<td>-</td>
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<td>-</td>
<td>16.5</td>
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Table 2.1: *Measured fresh feed from the feed bins.* The table shows measured fresh feed from the feed bins for series 2 and 3 for all experiments. The last column is used to estimate the variance between consecutive series shown in figure 2.10. Due to logging errors for the second series of experiment 4 and 10 they are not included in the variance estimates.

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<td>BC(_{lower})</td>
<td>-3.88</td>
<td>-3.74</td>
</tr>
<tr>
<td>BC(_{upper})</td>
<td>3.73</td>
<td>3.21</td>
</tr>
</tbody>
</table>

Table 2.2: *Bootstrap estimates.* The table gives the computed expectation, standard deviation and BC (bias corrected) confidence intervals for the bootstrap estimates shown in figure 2.10.

fall abruptly. As the figure shows it falls smoothly, and this is attributed to the difference in heat capacity.

### 2.4.3 Control action experiments: Campaign 1

This section contains a summary of an unpublished report (Martinsen 1998b) which summarizes measurements taken at the sintering plant at the Elkem (now owned by Eramet) plant in Sandefjord from 3rd to 5th of March 1998.

Air is sucked through the six sintering pans by means of three fans,
Figure 2.10: Bootstrap estimates. The figure shows the empirical distribution function (upper part) formed by sorting the data in the third column of Table 2.1. The estimates in the lower part show that the parametric (right part) normal distribution estimate is well suited for estimating the variance. This is concluded due to the similarity with the non-parametric estimate (left part). The normal distribution generated 1000 new datasets from the distribution \( X^* \sim N(\bar{X}_n, Y_n) \) where \( \bar{X}_n = \frac{1}{n} \sum_{i=1}^{n} X_i \), \( Y_n = \frac{1}{n} \sum_{i=1}^{n} X_i^2 \) and \( n = 11 \). The estimates show that the variance is considerable, and it cannot be expected that two consecutive batches are well correlated. I.e., large variations in fresh feed caused by large variations in recycle, makes it difficult to predict the charge composition in each batch.

Each fan being connected to two pans. This produces a differential pressure between atmosphere and the pipes connecting the pans to the fan inlet. Temperature and pressure are measured inside the pipes for each of the pans, hereafter denoted off-gas (bottom) temperature, \( T_{i, bot} \), and pressure, \( p_{i, bot} \) where \( i \) indexes pans 1 to 6, see figure 2.8. Gas-flow through the pans is controlled by means of valve discs for each pan. These valve discs were operated manually during the experiments to obtain increased gas-flow as compared to nominal operation. The effect of increased gas-flow on sintering time gives insight into how the disc valve should be operated if considered as an actuator. Possible negative side-effects of increased gas-flow are mainly the possibility of bed-collapse. The sampling period was preset to 5 seconds, and the sintering batch time was set to 38 minutes. The ignition time for each pan was set to 150 seconds. Figure 2.12 shows temperature measurements in pan 1 logged with two different pressure drops across the bed. As seen from the figure the batch with increased pressure
Figure 2.11: *Experiment 1: Measurements*. The figure shows the logged measurements during all three batches included in experiment 1. Subfigure 1 shows the temperature measured inside the pan 15\text{cm} down by a S-element (solid), and the temperature measured on top during ignition by a K-element (dashed). The dashed line at 1200\degree C indicates the fusion temperature $T_{fa}$. The dotted curves show the scaled value of the objective function $\phi(T)$. Subfigure 2 shows the differential pressure measured beneath pan 1 (solid) and pan 2 (dashed). The large difference in level between the two parallel pans can be due to instrumentation errors, valve malfunction, channeling inside the pans or leakages. The third subfigure shows the temperature measured beneath pan 1 (solid) and pan 2 (dashed).

... drop rises faster to its peak value, but due to measurement noise the results are uncertain. In these experiments temperature profiles were measured by K-elements inserted directly into the bed. K-elements are not designed for temperatures above 1250\degree C, and the measured values may deviate from the actual values. The non-smoothness of the solid temperature profile in figure 2.12 is attributed to breakage, since at approximately 41 minutes no further measured values were logged. The four "steps" towards the end of the measured $p_{1,bot}$ in figure 2.12 are caused by couplings between the different fans, possibly through the electric power supply or the common scrubber following the three fans. The four steps correspond to batch completion of pan 6, 5, 4 and 3 respectively. Pan 2 was not included in the batch cycle during this experiment. Such steps did not appear during the second measurement campaign carried out a year later, see section 2.4.2.
Figure 2.12: Control action experiments. The figure shows the logged measurements of one batch duration in pan 1 for two consecutive batches. Dashed-dotted lines in all three parts show measurements taken during the first batch with $p_{\text{bot}}$ at its nominal value. Solid lines in all three parts show measurements taken during the second batch with $p_{\text{bot}}$ at an increased value. The upper part shows the measured pressure drops across the bed. The spikes from approximately 10-12 minutes indicate that the actuator was manually adjusted to the desired value by trial and error. The middle part shows temperature profile measurements 20 cm down into the bed, while the lower part shows the ignition gas pressure. The lower part is included for synchronization issues: when $p_{\text{ign}}$ increases at approximately 9 minutes, the ignition is shut off and the K-elements are inserted into the charge. Ignition starts at approximately 6 minutes. The abrupt termination of the solid temperature profile indicates a broken K-element, and the remaining samples has been removed. The non-smooth corner in the dashed-dotted temperature profile at approximately 45 minutes was caused by manual removal of the K-element at the end of the batch.

Another run (not shown) in a neighboring pan showed that although the actuator was set at its maximum value, the pressure drop did not increase. Despite this, the difference in measured temperature profile were significant. Hence, the results reported from the experiments are not conclusive in the sense that it cannot be judged whether the differences in measured temperature profiles are caused by the pressure drops or by other factors. From figure 2.10 consecutive batches cannot be expected to be well correlated, mainly due to varying recycle and channeling effects. Further investigations into the relation between the pressure drop and temperature profile require
further experiments, preferably on laboratory equipment were disturbances are easier to handle.

Apart from the deviation case documented below and in figure 2.12, the plant was in nominal operation during the experiments. The production rate was logged to be above average with a low recycle, and a high production rate. As a consequence, the measurements are representative to the nominal operation mode. By nominal operation it is understood that the plant is operating without large deviations from the average operating conditions observed throughout a year. The measurements taken with increased suction have a larger air-flow through the pans (not nominal operating mode). These experiments were conducted in order to investigate whether increased gas-flow would lead to faster sintering batch times without collapsing of sintering beds or other undesired effects. The measurements are presented after filtering and interpolation to reduce measurement noise.

The results do show that increasing the nominal gasflow will not necessarily increase the sintering batch time. The present nominal value coincides with the maximum allowable value when all pans are operated simultaneously. This maximum value is upward limited by the fan capacity. Hence, pan 2 was excluded from the experiments shown in figure 2.12 to allow an increased pressure drop.

There are significant differences between pan-positions that should be investigated thoroughly. In practice the current actuators for adjusting the disk valve openings at the plant are not suited for automatic control. Hence, the actuators and possibly the disc valves must be replaced, and the fan capacity increased if automatic control of gas-flow is to be implemented.

2.5 Model adaption and validation

This section discusses implementation issues and documents how the model was adapted to data by comparing simulations and measurements. Two models are considered. In section 2.5.1 a full model is considered, where "full" indicates that all the states are included in the simulations. In section 2.5.2 a reduced order model is considered which includes a subset of the states of the full model. In section 2.5.3 some preliminary simulations illustrate the use of gas velocity as a control input to the reduced model. In section 2.5.4 the model is compared to data which it has not been adapted to.
2.5.1 Full PDE model

The model from section 2.3.1 was implemented in MATLAB and solved with \texttt{ode15s}, see figure 2.13. \texttt{ode15s} is an implicit solver of varying order using adaptive step lengths. It uses finite differences in solving the nonlinear equations. The spatial derivatives were approximated to the first order with 10 spatial elements. The simulated model was tuned by manually adapting the activation energy $E$ in equation (2.15) and visually comparing the boldface curves in the second subfigure of figure 2.13. Observe the "kink" in the temperature profiles caused by switching the fusion model from "melting" to "freezing". This kink is not desired, and future refinements of the model should include a more realistic model of fusion. The kink in the measured profile is caused by manual removal of the thermo-element from the sintering bed, see figure 2.11 for further details. Note that the velocity profile is spatially uniform in the sense that the velocity at any time instant was as shown in figure 2.13 in all spatial elements. Figure 2.13 shows that the solid temperature profiles in the upper layers are narrow, while the

![Figure 2.13: Simulation - full model.](image-url)
2.5 Model adaption and validation

Temperature profiles in the lower layers are wide. The figure also shows that the gas temperature profiles are almost equal to the solid temperature profiles. This does not comply with the measurements shown in figure 2.11, and further model refinements are needed. Towards the end of the batch, air passes through a bed almost completely converted to sinter with poor heat exchange properties, hence the air will not receive much heat from the sinter. The model does not reflect the different heat exchange capacities of wet charge and sintered material.

Since the model does not produce a physical gas temperature, the model must be refined if industrial implementation of model based control is to be considered. A physical gas temperature is essential for a control relevant model since the offgas temperature should be utilized for state estimation in an industrial implementation. If the gas temperature is considerably lower than the model temperature, other mechanisms may be important for transporting heat down through the bed, i.e. conduction by Fourier’s law and radiation. The adaption of the activation energy, together with the discrepancy in gas temperatures shows that further refinements are needed in an industrial implementation.

The models by Hoislbauer and Jaquemar (1983) and Patisson et al. (1991) are both simulated with finite element methods. Using the implicit solver ode15s resulted in acceptable simulation times but gave inexact gas concentrations (a "ripple" is introduced by the plug-flow assumption), see figure 2.14. I.e. the accuracy of the gas profiles was improved by increased spatial resolution, but this did not influence markedly on neither the temperature profiles nor the solid coke and water profiles. Hence, since the inaccuracy in gas concentrations has little influence on the important process states, water was excluded from the model and gas was considered as dry air in order to reduce the computational complexity.

2.5.2 Reduced model

The state vector after eliminating water and the gas components becomes

\[ x_{red} = [T_g, T_i, X_C] \]

The gas phase was lumped into dry air under the assumption that there is always excess air so that coke combustion is never limited by oxygen concentration. Water was excluded under the assumption that it does not have significant influence on the shape of the heat profile at elevated temperatures. The water does influence on the overall energy balance, and this influences on the temperature profiles in lower layers due to the distributed
Figure 2.14: *Gas concentrations - full model*. The figure shows simulations of the model with all states included (the full model). Subfigure 1 and 3 shows coke and water (respectively) concentration profiles reprinted from figure 2.13. Subfigure 2, 3 and 5 shows the ripple in the simulated gas profiles. Solid coke and water have units $kg/m^3$ while gas components have units $mol/m^3$. The ripple in gas composition is caused by limited spatial resolution combined with the plug-flow assumption.

nature of the process. Still the reduced model can be tuned to fit the measurements. The activation energy of the reduced model was tuned to be $E_r = 74 kJ/mol$, while the value for the full model is $E = 70.9 kJ/mol$. The activation energy is increased slightly to make coke combustion of the reduced model harder to start. This is as expected since no energy is needed to evaporate water. The resulting reduced model after tuning was simulated with `ode15s` as shown in figure 2.15.

The computational time on a COMPAQ Deskpro with a Pentium II processor and 128Mb memory for simulating the full model as shown in figure 2.13 was approximately 5 minutes, while it was approximately 20 seconds for the model shown in figure 2.15. The condition number of the Jacobian of the reduced model at the initial point $x_{red} = [14^o C, 14^o C, 18 kg/m^3]$ (with uniform spatial distribution) is in the order $10^{14}$, i.e. the system is very stiff. Attempts to solve both the full and reduced model with explicit and modified Euler, Runge-Kutta 4 and implicit Euler were unsuccessful. Due to the ill-conditioning and the limited accuracy of implicit Euler, very short step-lengths lead to excessive computational times. Simulating with the level 2 implicit Runge-Kutta method Lobatto IIIC allowed increasing the step
2.5 Model adaption and validation

Figure 2.15: Simulation - constant $v$. The figure shows simulations with the reduced model. The upper part shows gas temperatures (dashed-dotted) at depths 4, 8, 16 (solid) and 40cm, along with the ignition profile (dashed). The second part shows solid temperature profiles at the same depths along with the measured profile (dashed) at 15cm. The third part shows coke concentration profiles at the same depths, while the lower part shows the velocity (spatially uniform).

length to $h = 1s$. The total simulation time with Lobatto IIIC was approximately 10 hours. Adaptive step lengths did not reduce the simulation time for Lobatto IIIC. These issues influence on the MPC implementation and are revisited in chapter 4.

2.5.3 Introductory control action simulations

The suggested control scheme from section 2.2.2 is investigated by simulating the reduced model with two different velocity inputs as shown in figure 2.15 and 2.16. As is seen by comparison of figure 2.15 and 2.16, the temperature profiles are influenced by the velocity profile. The modified velocity profile gives a more evenly distributed temperature profile at different levels, but the sintering time is prolonged. I.e. a control objective should balance sintering time against a uniformly shaped temperature profile.

The full order model exhibited similar responses as the reduced model when exposed to the modified velocity profile. The spatial temperature profiles for the full model at selected time instances are shown in figure 2.17. Observe again the more even profile and prolonged sintering time in the lower part. Hence, maximizing $\phi$ alone from equation (2.5) may
lead to prolonged sintering times, and the control problem (2.6) should be augmented to penalize the batch duration time \( t_{\text{end}} \). The present model is implemented with a fixed batch time \( t_{\text{end}} \), which may lead to impaired solutions. If this turns out to be a problem, the objective can be augmented as discussed above as a remedy.

### 2.5.4 Model validation

The reduced model is compared to the measurements of the first campaign. In figure 2.18 the dashed pressure measurements from figure 2.12 are repeated (dashed). The model is seen to fit well to the new data. Observe that the measured pressure profile is used in the model to generate a spatial pressure profile as discussed in section 2.3.4. This pressure profile then allows direct calculation of the gas density \( \rho_g(T_g, p) \) by the ideal gas law. The velocity is scaled to reflect the level difference in the figure, since the pressure and velocity are not linked in the present model. Note that the scaling discussed in the figure caption can be done by using Ergun’s relation, equation (2.22). I.e. solving Ergun’s relation for \( p_1 = 5kPa \) and \( p_2 = 6kPa \) for a given set of parameters\(^4\) gives approximately the same ratio 6/5.

\(^4\mu = 1.7 \cdot 10^{-5} \text{kg/m s}, \ \rho_g = 1.29 \text{kg/m}^3, \ \phi_t = 2 \text{mm}, \ \varepsilon = 0.4 \) and \( \phi_f = 0.43 \).
Figure 2.17: *Simulation - $T_s$-profiles*. The figure shows simulations with the full model. The abscissa is position inside the bed with 0 cm being the top and 40 cm being the bottom. The figure shows solid temperature profiles at time instances 5.8, 10, 14.2, 18.3 (boldface), 22.5, 26.7, 30.8, 35 (boldface), 39.2, 43.3, 47.5, 51.7, 55.8, 60 and 64.2 minutes. The upper part shows profiles obtained with the nominal velocity profile from figure 2.15, while the lower part shows profiles obtained with the velocity profile shown in figure 2.16.

The simplified fusion model does not allow the simulated temperature to increase significantly above 1250°C. Validating against measurements for other experiments is hard since the temperature profile is poorly correlated with the coke input, see figure 2.23 in section 2.6 for details.

### 2.6 Data analysis

The data from the experiments documented in section 2.4 are analyzed in this section. The aim of this section is a verification of the control strategy suggested in section 2.2.2. In particular, the validity of the suggested control objective (2.6) is assessed. By conventional experiment planning methodology (Dougherty 1990), section 14, the input (feed composition) was perturbed in two dimensions (water and coke) and the output responses (quality and production rate) were measured. Since the perturbations were not conducted directly in the sintering pan, the hold-up of the recycle and charge bins forced a degree of conservatism in the experiment design, cf. figure 2.9.
Figure 2.18: Validation of model. The figure shows simulations with the reduced model and validation data. The upper part shows the ignition profile from figure 2.11, batch 3, and simulations of reduced model with this ignition profile. The measured profile (dashed-dotted boldface) is the one shown in figure 2.12. The lower curve shows the measured pressure drop for experiment 1, batch 3, (solid) which was used to tune the model along with the one from figure 2.12 (dashed). The approximate ratio between these is 6/5, hence, the simulated profile in the upper part was generated with the velocity profile from figure 2.15 scaled by 6/5, i.e. 0.42m/s. The solid simulated profile is plotted for the level corresponding to 20cm.

The coke content in the pan is not directly measurable. In particular, assuming a constant recycle will give a constant bias of coke content, while a varying recycle will give a varying bias. Figure 2.19 shows the set points and calculated real values of each experiment labeled 1 through 13. The figure clearly shows that the locations of the real operating points marked by (•) are not well correlated to the set-points labeled by (o), and identification of an input-output model based on the experiments was abandoned due to this. The experiments were designed to have ±2% deviation from normal operating values in coke and water concentrations. The water content in the pan was measured by drying a small sample of charge, and measuring the weight loss caused by evaporation. The coke content in the pan was calculated by calculating the recycle, see details in section 2.6.1.

The production rate is calculated by a mass balance in section 2.6.1, and the qualities reducibility and mechanical strength are analyzed in section 2.6.2. The objective function suggested in equation (2.6) is assessed in
2.6 Data analysis

Figure 2.19: Set-points for experiments. The figure shows the set-points (o) and real values (□) for coke and water concentrations for experiment 1-13. Note that a 2% bias is added to the real coke values. The real coke values were calculated by compensating for the recycle as described in the text, while the real water values are measured. The dashed circle only serves to emphasize the positions of the set-points at a circle with radius 2 and centered at the normal operating point.

section 2.6.3.

2.6.1 Productivity

A realistic measure of production rate should weight the recycle and mass gas-flow. The recycle is calculated from a stationary mass balance given by the difference between the measured output from the feed bins 1-12 in figure 2.7 and the calculated maximum production from the six Greenawalt-pans. An uncertainty is introduced by how the total mass of fresh feed (i.e. from the feed bins) is calculated from the measurements: The output from the feed bins is logged, but, due to the plant automation system, it is uncertain which parts of the logged time-series to include in the calculation. I.e. feed is added from the feed bins at irregular intervals based on level measurements and various time-stamps in the automation system. Close investigation of the batch-cycles was done to determine which parts to include in the calculation of the total mass of fresh feed. Then, the fresh feed was calculated by integrating the time-series from each feed bin. In addition to this, the calibration of the weights in the sintering plant was uncertain. Hence, the calculated real values for the set-points given in figure 2.19 are uncertain.
The total mass of the six pans is calculated by calculating $\rho_{ch}$ from the measured output from the feed-bins and multiplying by the volume:

$$m_{ch} = 6(1 - \varepsilon) \cdot \rho_{ch} \cdot L \cdot A$$

where $L = 0.4 \ [m]$ is the height and $A = 3^2 \ [m^2]$ is the cross-sectional area of each pan. The void fraction $\varepsilon$ is unknown, but can be measured if the density of solids is known. The bulk solid density $\rho_{ch}$ is computed from the logged feed-ratio and the measured moisture content. Since the coke and water fractions are small and do not vary much, assuming $\rho_{ch} \approx 3600 \ [kg/m^3]$ will not introduce large errors. The value $\varepsilon = 0.3$ was computed by assuming a 100\% production rate for the "best" experiment (no. 13), and computing the equivalent void fraction as $\varepsilon = 1 - m_{meas}/m_{max}$ where $m_{meas}$ is measured feed, and $m_{max}$ is the value achieved for $m_{ch}$ with $\varepsilon = 0$. Using $\varepsilon = 0.3$ in calculating the production rates gave the results shown in table 2.3. As can be seen from the table, the recycle is larger than expected and the variations are profound. Keeping in mind the large variance of consecutive batches from figure 2.10, the calculated productivity indicate that it is unlikely that the coke concentration in the pan will follow the set-point due to the large variations in the recycle.

### 2.6.2 Quality tests

The quality in terms of mechanical strength and reducibility was measured off-line by taking product samples from each of the thirteen experiments described in section 2.4.2. The mechanical strength was measured by the standard test equipment used at the plant. 12.50kg of sinter of fraction $d_p \in [10, 16] \ [mm]$ was tumbled according to a preset program. The weight fractions $\leq 10\text{mm}, 1-10\text{mm}$ and $\geq 1\text{mm}$ after tumbling were measured. The results are given in table 2.4. The reducibility of the sinter samples were measured by reduction in a $CO$-atmosphere in the laboratory scale retort shown in figure 2.20. Sinter lumps were loaded into the retort, and the retort was hung from a scale and placed in an electric heater. The retort was purged with the inert gas $N_2$ and preheated to $1000^\circ C$. Then $N_2$ was replaced by $CO$ and reactions similar to $Mn_{x_1}O_{y_1} + CO \rightarrow Mn_{x_2}O_{y_2} + CO_2$ gives a weight loss since oxygen from the charge is transported out of the retort. The weightloss for all 13 experiments were calculated in grams weight loss between 10\% and 90\% reduction from start to total weight loss. The reducibility experiments were conducted for both 10-16mm and 5-10mm fractions. The two different
Table 2.3: Production rates. The table gives the calculated production rates for the experiments. The table shows calculated production rates for experiments 1-13. The production rate varies between a maximum of 100% at experiment 13 and a minimum of 46.8% at experiment 4. The recycle, which is obtained by subtracting the production rate from 100 varies between 53.2% and 0%. Note that 100% production rate at experiment 13 was achieved under the hypothesis of a void fraction $\varepsilon = 0.3$. This void fraction is a lower bound on the void fraction for experiment 13. The actual void fractions were not measured. The coke concentration numbers were computed by a mass balance adding the measured feed and calculated recycle and assuming no coke in the recycle.

fractions gave almost equal reducibility measures. The reducibilities are summarized in table 2.5.

By assuming a linear dependence between the function $\tau_z$ from equation (2.4) and strength and reducibility, the MATLAB NAG toolbox function g02caf was used for linear regression. The heuristic rule that a certain minimum strength is required while simultaneously maintaining a high reducibility was implemented by weighting the two linear regression functions as shown in figure 2.21.

The computed quality model is conceptual since no data exists that allow verification, and there are no quantitative quality requirements given at the plant. Note that the choice of the weighting functions controls the shape of the quality model, hence different quality models can be formed by altering the weights. The quality model is founded on the arguable assumption that a linear regression is adequate. However, including heuristics by weighting
functions can still be applied even if the underlying functions are changed. The standard errors of the adapted parameters in the linear regressions allows assessment of the standard error of the quality model as is shown in figure 2.22.

The second column in table 2.6 gives the normalized values of \( \tau_z \) for all experiments. This figure gives a direct measure of the conditions inside the bed during sintering. As discussed in section 2.2 the quality of the produced sinter is governed by the temperature profile in the bed. The third column gives the values of the objective \( \psi_z \)\(^{5} \) from equation (2.6) as calculated from the data. The fourth and fifth column show the calculated integral of the sigmoid \( \int \sigma_z \, dt \) from equation (2.5) and \( T_{z,\text{max}} \) from the same data.

The identified quality model do show that the results from the experiments conform to the heuristics reported in the literature as discussed in section 2.2.1. The relation between the inputs coke and water and the outputs production rate, strength and reducibility are shown in figure 2.23.

The linear regression models shows that \( \tau_z \) increases (slightly) as expected with the coke content. The inverse proportionality towards water

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\(^{5}\text{The level } z \text{ being the position of the S-element, i.e. 15cm down into the bed.}\)
Figure 2.20: Retort used for reduction experiment. The figure shows the laboratory scale equipment used for reduction experiments. 350g of sinter lumps are loaded into the retort, and the retort with sinter is hung from a scale and pre-heated to 1000°C. During preheating the retort is purged with N₂. When the temperature reaches 1000°C N₂ is replaced by a CO gasflow. In the reducing CO atmosphere oxygen is removed from the sinter and transported out with the gas giving a weight loss which is logged on the scale. The internal diameter of the retort is 5.3cm, and the outer diameter is 5.7cm. The grate is placed 1 cm above the bottom, and the height from the bottom to the lid is 33cm. About 5cm charge is used. The retort is made of an FeCrAl-alloy and it is magnetic up to 950°C. At 1000°C the magnetic influence is low, but appears as noise on the logged measurements.

content is attributed to the competing properties of water: An optimal water content W* yields a higher permeability allowing the heat wave to travel faster through the bed, giving shorter sintering batch times. Increasing the water content beyond W* does not increase permeability, and additional energy is needed for evaporation, resulting in poorer sintering conditions. Hence a linear regression model is not well suited for analyzing water content with any output.

The production rate vs. coke content varies as expected, while strength and reducibility are almost flat. This is why the "intermediate" quality model based on τ₂ shown in figure 2.21 was suggested. "Intermediate" hints to the logical "chain" that a higher coke content implies a higher integral τ₂ yielding increased strength and decreased reducibility. The 90% confidence intervals are wide for all regression models, indicating that input-output identification cannot be expected to give good results. Nonlinear identification is not considered due to the known uncertainties in the experiments.
<table>
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<th>( \Delta m \ [g] )</th>
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Table 2.5: Reducibility of produced sinter. The table gives the measured reducibility of produced sinter for experiments 1-13. The quality reducibility is defined as the number \( \Delta m \) in the second column. The reducibility experiments were conducted on laboratory equipment located at the metallurgical department at NTNU in Trondheim, Norway.

### 2.6.3 Assessment of the objective function

From the discussion above, it is apparent that the validity of the objective function \( \phi \) suggested in equation (2.5) can be evaluated by comparing it to \( \tau_z \). The large variations in integrated sintering temperatures shown in the first column of table 2.6 suggest that a more detailed metallurgical analysis of the produced sinter can be used to verify the data on which the quality model from figure 2.21 is based on. Figure 2.25, 2.26 and 2.27 show microprobe images of sinter samples taken from experiment 1, 7 and 11 respectively. From the first column of table 2.6 these experiments correspond to the second smallest, maximum and (approximate) average of integrated sintering temperature. Experiment 1 was chosen in favor of experiment 5 (the minimum) since experiment 1 has been shown with in greater detail in the preceding sections. The pictures were taken by a scanning electron microscope (SEM) (EPMA - Electron Probe Micro Analyzer) with 4 wavelength-dispersive spectrometers and an energy-dispersive spectrometer, capable of taking both area and point measurements. The figures show (row-wise) a grey scale overview, \( Al \), \( Mn \), \( Ca \), \( O \), \( Si \), \( Fe \) and \( K \) plots for the same area of
Figure 2.21: Quality model. The figure shows the normalized reducibility ('o') and strength ('x') data along with the linear regression models (upper part). The weighting functions (middle part) were chosen somewhat arbitrarily, but according to the hypothesis in section 2.2.1. I.e. to balance the competing objectives that the temperature should be high to give good strength but not too high to give good reducibility. The quality model (lower part) is formed as the convex combination of the two linear regression models using the weighting functions. The dotted lines in the lower subfigure are reprints of the linear regression models from the upper subfigure.

Each of the three samples. The color coding along with the bars to the right gives the relative content of each component. Note the coarser resolution used for experiment 1.

The grey scale plots show that for experiment 1 the light gray phase (containing mainly Mn- and Fe-oxides) has sharp corners indicating that the amount of melting is minor. Similarly for experiment 7 the corners of the light gray phase are rounded and neighboring crystals grow together and extensive melting and recrystallization are prevailing. The average case in experiment 11 shows an intermediate stage where the smaller crystals in the light gray phase have rounded corners, while the larger crystals have sharp corners. Figures 2.25-2.27 support the calculated integral temperatures shown in table 2.5 and it can be concluded that the linear regression models in figure 2.21 are based on reasonable data. Observe that the results are based on point samples in a distributed media, and local effects such as
channeling, where when the sinter samples are taken etc. must be kept in mind. Despite these limitations, the results conform well to the hypothesis in section 2.2.1. I.e. the competing objectives that the temperature should be high to give good strength but not too high to give good reducibility are reproduced. Note that figure 2.25 and 2.26 corresponds to experiments 1 and 7 with coke content as shown in table 2.3. Along with the first subfigure in figure 2.23, this indicates that the calculated real setpoints as shown in figure 2.19 are wrong. I.e., since the locations of the calculated real set points are questionable, the hypothesis that increased coke content increases the sintering temperature cannot be assessed by the data.

From figures 2.25-2.27 and table 2.6 it is observed that $\tau_z$ is well suited as an objective. Since $\tau_z$ is non-smooth, the objective function $\psi_z$ from equation (2.6) was suggested. In figure 2.24 the correlation between $\psi_z$ and $\tau_z$ is shown. The objective function $\psi_z$ is seen to fit well to the integral. Observe from the lower part of figure 2.24 that the use $T_{max}$ gives an inappropriate objective function since it is not well correlated to $\tau_z$. Note that

Figure 2.22: Standard deviation of quality model. The figure shows the computed standard deviation of the quality model. The standard errors of the parameters of the linear regression models were used to generate 100 new models (upper part) from a normal distribution (Monte-Carlo simulation). 100 new quality models were formed by the same procedure as shown in figure 2.21. The 95% standard deviations were found by counting the points between 3 and 95 as shown by the solid lines. The bold face solid curves are reprints from figure 2.21.
2.6 Data analysis

<table>
<thead>
<tr>
<th>Experiment</th>
<th>(\tau_z) [(\text{s})]</th>
<th>(\psi_z = 15\text{cm}(T_z)/1000) [-]</th>
<th>(\int \sigma_z = 15\text{cm}(T_z)) [-]</th>
<th>(T_{\text{max}}) [(^\circ\text{C})]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.09</td>
<td>4.86</td>
<td>81.7</td>
<td>1300</td>
</tr>
<tr>
<td>2</td>
<td>0.32</td>
<td>17.21</td>
<td>121.0</td>
<td>1430</td>
</tr>
<tr>
<td>3</td>
<td>0.65</td>
<td>34.74</td>
<td>269.5</td>
<td>1410</td>
</tr>
<tr>
<td>4</td>
<td>0.44</td>
<td>23.61</td>
<td>139.3</td>
<td>1450</td>
</tr>
<tr>
<td>5</td>
<td>0.06</td>
<td>3.05</td>
<td>38.3</td>
<td>1330</td>
</tr>
<tr>
<td>6</td>
<td>0.44</td>
<td>23.46</td>
<td>154.0</td>
<td>1450</td>
</tr>
<tr>
<td>7</td>
<td>1.00</td>
<td>53.48</td>
<td>312.8</td>
<td>1450</td>
</tr>
<tr>
<td>8</td>
<td>0.11</td>
<td>6.04</td>
<td>100.3</td>
<td>1290</td>
</tr>
<tr>
<td>9</td>
<td>0.58</td>
<td>31.16</td>
<td>263.3</td>
<td>1340</td>
</tr>
<tr>
<td>10</td>
<td>0.67</td>
<td>35.74</td>
<td>245.8</td>
<td>1430</td>
</tr>
<tr>
<td>11</td>
<td>0.40</td>
<td>21.50</td>
<td>168.4</td>
<td>1420</td>
</tr>
<tr>
<td>12</td>
<td>0.45</td>
<td>21.50</td>
<td>168.4</td>
<td>1430</td>
</tr>
<tr>
<td>13</td>
<td>0.28</td>
<td>15.15</td>
<td>183.7</td>
<td>1390</td>
</tr>
</tbody>
</table>

Table 2.6: Assessment of the objective function. The table assesses the validity of the objective function for experiments 1-13. The first column shows the normalized integral of the measured temperature \(T_z > T_{\text{fz}}\) for all experiments. The second column shows the value of the objective function \(\phi(T_z)\) from equation (2.6) integrated over the time series for each experiment. The third column shows similar data for the integral of the sigmoid function \(\sigma(T_z)\) from equation (2.5). The last column shows the achieved maximum temperature for each experiment.

\(T_{\text{max}}\) was scaled to the interval \([0, 1]\) by choosing its lower value as the zero point and its upper value as one and scaling the intermediate values accordingly. Note also that using \(\int \sigma(T_z)\, dt\) alone as an objective is not as good as using \(\psi_z\), since \(\sigma\) doesn’t pay extra credit for solid temperature profiles with temperatures above, say \(1250\,^\circ\text{C}\), cf. figure 2.3.

It is concluded that \(\psi_z\) is well correlated to \(\tau_z\), and then the overall objective \(\phi\) from equation (2.6) is a valid objective since this is a weighted integral of \(\psi_z\) in the spatial dimension.

The parameter \(q\) from equation (2.6) can be selected by inspecting the second column of Table 2.6. The mean value \(q = \bar{\phi} = 22.42 \times 10^3\) may serve as an initial choice.\(^6\)

\(^6\)The actual value of \(q\) used in the implementation must be compensated for varying sampling period. The values in Table 2.6 were obtained by direct summation over the time series of the output from the \texttt{MATLAB} function \texttt{logsig}(\(T_z\)). Hence, the sampling periods of 5 seconds is inherent in Table 2.6.
Figure 2.23: *In- and output data.* The figure shows the datapoints ('x') along with linear regression models (solid lines) of various output variables plotted against the normalized calculated coke content (first column) and normalized measured water content (second column). The first row shows the normalized integral \( \int (T_s > T_{fw}) \) for all experiments. The second row shows the normalized calculated production rate, the third row shows the normalized measured quality strength and the last row shows the normalized measured quality reducibility. The standard errors of the parameters of the linear regression models were used to generate 100 new models from a normal distribution (Monte-Carlo simulation). The 90\% standard deviations (dotted lines) were found by counting the points between 10 and 90 (similar to figure 2.22).

2.7 Conclusions

A dynamic model of grate sintering is gathered from the literature, adapted to data, and simulated in MATLAB. A reduced order model including only the solid and gas temperatures and coke concentration was suggested to reduce the computational complexity. Extensive experiments were conducted to validate the model and the hypothesis on which the control strategy is founded. A control strategy was suggested, and simulations support the hypothesis discussed in sections 2.2.1 and 2.2.2.

The model is implemented using MATLAB's ode15s giving reasonable computational times, but inaccurate gas dynamics. The inaccurate gas dynamics has little influence on the temperature profiles. Since the gas dynamics has little influence on the temperature profiles, the gas states along with the
Figure 2.24: **Assessment of the objective function.** The figure shows the datapoints (‘x’) along with linear regression models (solid lines) of the normalized objective $\phi(T_s)$ from equation (2.6) plotted against the normalized temperature integral (lower left) and measured maximum temperature (lower left). The normalized sigmoid function $\sigma(T_s)$ from equation (2.5) is plotted against the normalized temperature integral (upper right). The normalized temperature integral is also plotted against the measured maximum temperature (lower right). The standard errors of the parameters of the linear regression models were used to generate 100 new models from a normal distribution (Monte-Carlo simulation). The 95% standard deviations (dotted lines) were found by counting the points between 5 and 95 (similar to figure 2.22).

Water is excluded from the model in the reduced model. The reduced order model is considerably faster to simulate; the simulation time drop from 5 minutes to approximately 20 seconds per batch. The reduced model maintains approximately the same level of accuracy as the full model. The gas temperature profiles do not comply with the measurements, and the activation energy of coke combustion has been extensively tuned to adapt the model to the data. The solid temperature profiles are satisfactory reproduced by the model. The model is good in the sense that it is intended as a control relevant model, and it is essentially the solid temperature profiles that govern the process outputs quality and production rate.

The gas velocity is suggested as a control input, and its viability has been documented by the experiments. However, an industrial implementa-
tion using pressure as control input must include the velocity as a state. In addition to correcting the erroneous gas temperature and activation energy, including velocity as a state and improving the fusion model are essential for an industrial implementation. This is left as future work. Despite these shortcomings, the principal properties are maintained and model based control with the present model is sound. An improved model is expected to fit into the same control framework as the present model.

The main contribution of this chapter is the reduced order model which along with the implementation gives short simulation times. The model is adapted to industrial data, and a control objective formally stated in equation (2.6) is proposed. Industrial experiments explore and support the viability of the proposed objective.
Figure 2.25: SEM exp. 1. The figure shows SEM (scanning electron microscope) plots for a sample taken from experiment 1.
Figure 2.26: *SEM exp. 7*. The figure shows SEM plots for a sample taken from experiment 7.
Figure 2.27: SEM exp. 10. The figure shows SEM plots for a sample taken from experiment 10.
Chapter 3

rFSQP - a feasible SQP method

This section considers nonlinear programming. By that we understand that we are seeking local solutions to smooth nonlinearly constrained optimization problems. We do not consider global, stochastic, or any form of discontinuous mathematical programming. Neither do we consider linear, quadratic or convex programming although quadratic programming is an important part in solving the subproblems occurring in nonlinear programming. Our main focus is on maintaining feasibility with respect to inequalities in reduced Hessian SQP methods. We start in section 3.1 with some general background relevant for comparison of various implementations of nonlinear programming codes. Then we continue with an introduction in section 3.2 pertaining to specific issues relevant to the suggested algorithm. In section 3.3 we suggest the algorithm rFSQP which is a feasible reduced Hessian SQP method. Then the convergence properties of rFSQP is analyzed in section 3.4, and we present some simulation results in section 3.5. We summarize this chapter in section 3.6.

Sections 3.2 through 3.4 and parts of section 3.5 have been submitted for possible publication in SIAM Journal on Optimization (Martinsen and Foss 2001).

3.1 Background

Our interest in nonlinear programming is due to our interest in nonlinear MPC which rely heavily on real-time optimization. Nominal stability results for nonlinear MPC relies on nominal feasibility of the model constraint and
feasibility of some other stabilizing inequality constraints at each iteration of the nonlinear MPC algorithm. Few results are available on robust stability of nonlinear MPC, but such results should not rely on nominal feasibility of the model constraint. The model constraint is an equality constraint, and currently the only efficient method available for maintaining feasibility with respect to equality constraints is by evolution. This is also known as the sequential method, single shooting or the Newton method. This method perform a simulation over the MPC horizon to find a solution to the nonlinear equalities, see chapter 4 for further discussions and references. See Ascher, Mattheij, and Russell (1995), sections 4.1 and 4.6.2, for an exposition of single shooting.

Simulating over the horizon to solve a nonlinear equality constraint like $f(x, u)$ where $x$ is dependent on $u$ results in an optimization problem in the reduced space of $u$ which typically is known as the control input. However, if there are nonlinear inequality constraints on the original nonlinear MPC problem, it is not trivial to resolve these in the reduced problem since they must be transformed through a nonlinear map from the space of $(x, u)$ into the reduced space of $u$. This chapter focus on optimization issues alone, and for now we leave the application issues until chapter 4.

This section continues by outlining some basic optimization principles needed to facilitate a comparison between various approaches to nonlinear programming. Then other work on reduced Hessian and feasible methods is summarized. We conclude this section with a summary of the most popular nonlinear programming codes with particular references to where numerical results can be found.

### 3.1.1 Background on optimization

This section contains brief descriptions of optimization methods used for nonlinear programming. Since this is mainly text-book material, we do not go into detail, but provide a few relevant references. The text-books by Gill, Murray, and Wright (1981) and Nocedal and Wright (1999) have been the main sources of information, but the books by Fletcher (1987) and Dennis and Schmabel (1996) have also been used to some extent.

#### General approaches

Note that the items below do not provide a mutually exclusive list. As an example an SQP method may be implemented with a reduced gradient method for step-computation. Likewise, the augmented Lagrangian method
is more a question of choice of merit function, which is listed below in the
section on low-level implementation issues. The list is therefore intended
as a compilation of "buzz-words" with a few comments and references to
further reading.

**Reduced gradient methods** There are a number of approaches that result
in variations of reduced gradient methods. These methods separate the
variables into dependent and independent variables. The dependent
are resolved from the equalities, while the independent ones are optim-
ized subject to remaining constraints. The original reduced gradient
method is GRG which seeks to remain feasible with respect to equalities,
but also reduced Hessian SQP methods are reduced gradient methods.
Reduced Hessian methods does not remain feasible with respect to
equalities. Also interior methods can use decomposition strategies for
step-computation. Even the sequential method frequently used in MPC
results in a reduced gradient method. See Gill et al. (1981) for an
introduction to reduced gradient methods.

**Augmented Lagrangian methods** replaced the earlier quadratic penalty meth-
ods by introducing explicit multiplier estimates in the merit function,
thereby reducing ill-conditioning. The multipliers of the subproblem
must converge to the optimal multipliers of the nonlinear program-
ing problem for the algorithm to converge. In particular, it cannot
converge faster than the multipliers, i.e. a first order estimate of the
multipliers is not sufficient for superlinear convergence which is needed
in practical algorithms. Elaborate multiplier schemes are therefore
needed, and with such schemes augmented Lagrangian methods show
excellent local convergence properties (noting that the merit function
is smooth and that the full Newton step will be accepted locally).
Global convergence is somewhat impaired by the strong dependence
on the multiplier estimates which may be poor far from the solution.
513-523, for introductions and Bertsekas (1982) for a deeper exposition
of augmented Lagrangian methods.

**Projected Lagrangian methods** uses a model of the nonlinear program
for step computation. Two variants SLC and SQP, exist of projected
Lagrangian methods. Sequential linearly constrained (SLC) program-
ing uses a nonlinear objective with linearized constraints. Sequen-
tial quadratic programming (SQP) uses a quadratic model of the La-
grangian with linearized constraints. The workload of each subproblem
is therefore lower in SQP, but at the expense of the need for a merit function to measure overall progress. Fewer function evaluations are typically observed in SQP than in SLC, since the subproblems in SLC must be solved to great accuracy. SQP methods may be implemented with incomplete solutions of the subproblems, see Murray and Prieto (1995).

Interior point methods for nonlinear programming typically use slacks for inequalities, and then put the slacks in a logarithmic barrier term. Then the slacks are kept positive, but since the inequalities are solved as equalities (with slacks), there is no feasibility guarantee for the inequalities. To avoid ill-conditioning, the slacks should not approach zero away from the solution, since this would make the barrier term exceedingly large. This is accomplished by computing a modified Newton direction, see Wright (1997b) and Nocedal and Wright (1999), pp. 510-512 for further details. Note that even though the iteration count usually is low for interior methods, the workload of each iteration may be high. Originally interior methods with barriers were suggested by Frisch (1954), section 12, and further investigated by Fiacco and McCormick (1990), but they were considered inferior to SQP methods due to the ill-conditioning until Karmarkar (1984) published his algorithm for linear programming. See Martinsen (1998a) for a historical overview of interior methods. Currently primal-dual interior methods for nonlinear programming are being implemented with considerable success, see the section on overview of existing methods below.

Feasibility

We illustrate the difference between infeasible and feasible steps by a conceptual example in figure 3.1:

The infeasible method to the left uses the usual decomposition into null- and range-space steps. The qp-subproblem generates a step $Z_k p Z_k$ in the null-space, while the range-space step $Y_k p Y_k$ is computed from the constraint linearizations at $x_k$. The vector sum $d_k = Z_k p Z_k + Y_k p Y_k$ gives the next trial-point $x_{k+1}$ indicated on the figure. To ensure convergence from remote starting points a line-search on an exact penalty function is performed along $d_k = x_{k+1} - x_k$ giving the actual next iterate as $x_{k+1} = x_k + \alpha d_k$. We observe that poor scaling and ill-conditioning may unbalance the null- and range-space steps which in turn alters the composite direction $d_k$ which in turn
3.1 Background

Figure 3.1: Conceptual comparison between an infeasible SQP (left) and a feasible GRG (right) method. The dotted line through $x_k$ is the null-space of the equality constraint $c(x)$ at $x_k$. The range-space is orthogonal to the null-space. The optimum of the constrained objective $f(x)$ is located at $x^*$.

may cause small steps in the line-search, especially far from the optimum $x^*$. Note that the line through $x_k$ is evaluated at an infeasible point, and that its slope need not be a "parallel" displacement of the tangent-plane through the point given by projecting $x_k$ onto $c$. It is even possible that the next iterate $x_{k+1}$ is located at a point where $c(x)$ is undefined. The feasible GRG method to the right alternates between solving a SLC-problem for the free variables (i.e. reduced gradient), and evaluating the model at trial points generated by a modification of the search direction to step back to the equality constraint. Note that the step back onto $c(x) = 0$ does not lie in the range-space in general.

Low level implementation issues

It is important to realize that the actual performance of an algorithm depends heavily on the implementation. That is, some successful codes do not have a sound theoretical foundation, and some that do have poor results. In general, even the very same code can lead to very different performance when compiled with different compilers (or options) or operating systems, due to small differences in rounding, orders in addition etc. For a code, there may be that for some examples, where on one machine the method works fine, and on another just fails; and in particular in ill-conditioned problems the number of iterations can easily differ\(^1\).

Step computation by solving the subproblems can be done in the full space of all variables, or by decomposition strategies where dependent variables are eliminated and a dense qp is solved for the dependent vari-

\(^1\)Personal communication from Andreas Wächter.
ables. Conjugate gradients, possibly projected, may also be considered. The time spent in the qp can be reduced if an incomplete solution can be incorporated in the overall algorithm, see Murray and Prieto (1995) for further details.

**Line search/trust-regions** The line search computes a direction in a subproblem and then determines step length by reducing the step length according to the Wolfe conditions applied to a penalty function. Usually only the first Wolfe condition is tested, and the BFGS update is skipped if the step length is too short. An implementation of the full Wolfe conditions is provided by Moré and Thuente (1994). Trust regions determine the step length first based on the relative success of previous iterations, and modifies the subproblem for step computation with the additional constraint \( \|dk\| \leq \Delta \) where \( dk \) is the step to be computed and \( \Delta \) is the (current) trust-region radius. The trust region approach is more involved than the line search, but is better suited to deal with indefiniteness of the model-Hessian. See Nocedal and Wright (1999), sections 3 and 4 for further details.

**Hessian** Exact second derivatives of the objective and constraint functions can be incorporated if the method is able to deal with indefinite Hessians. In favor of second derivatives are sparsity, accuracy and a speed-up due to improved curvature information, i.e., a quadratic convergence rate may be obtained. Counter-acting this is the need for handling a possibly indefinite Hessian, and the cost of producing second derivatives. Two major alternatives for dealing with indefiniteness exist; adding a multiple of the identity to the diagonal or using a trust-region that limits the step-size. Adding a multiple of the identity gives a convex model and can be done by perturbed Cholesky factorization. This gives a model-Hessian that deviates from the original Hessian. Trust-regions, on the other hand, limit the step-size in case of an unbounded solution which may occur with indefinite Hessians. A step to the boundary of the trust-region in the computed direction is then expected to "bypass" saddle points etc., and the iteration can proceed from the new point. Both approaches have been implemented with success in production codes. BFGS approximations, on the other hand, lead to a dense positive definite model-Hessian, but the convergence rate is only superlinear. In addition the quality of the model-Hessian may be poor during earlier iterations. In large-scale methods limited memory BFGS is used to reduce the storage requirement. See Murray
3.1 Background

(1997) for further details and references.

Penalty functions, or merit functions, are commonly used to provide global convergence results. Exact penalty functions have minimizers that coincide with the minimizers of the nonlinear program for finite values of the penalty weight. Inexact penalty functions like barrier-functions and the quadratic penalty function, which are smooth in relevant regions, does not have minimizers that coincide with the minimizers of the nonlinear program unless the penalty parameter is infinity. Infinite values of the penalty parameter give ill-conditioning, which is undesirable. Augmented Lagrangian methods are exact penalty functions that are smooth but depend strongly on the multiplier estimates as discussed above. The $l_1$-penalty function is exact but non-smooth like any norm-based penalty function would be. The $l_1$-function is less dependent upon the multiplier estimates, but needs complicated line search mechanisms (a watch-dog is frequently used) to accept the full Newton step locally. Hence, augmented Lagrangian methods have good local convergence properties, but global convergence is hard to establish. On the other hand, $l_1$-methods have better global convergence properties, but local convergence needs sophisticated line search mechanisms to be superlinearly convergent. See Fletcher (1987), chapters 12 and 14 for further details.

Numerical linear algebra is essential for the actual performance of any algorithm. On large-scale problems exploiting sparsity is essential. Avoiding unnecessary factorizations by directly updating the factorization itself is common. The choice of pivoting strategies is important for rank-deficient systems, see Golub and Van Loan (1996) for further details.

Other work on reduced Hessian methods

The method of Biegler et al. (1995) maintains a dense approximation of the reduced Hessian using quasi-Newton updates. In Tjoa and Biegler (1991) inequality constraints are slacked, and the slacks are resolved using a dense qp algorithm. These methods are designed for problems dominated by equality constraints with few degrees of freedom. Betts and Frank (1994) use second derivatives in combination with a sparse qp solver and sparse KKT factorizations and is not limited to problems with few degrees of freedom. Coleman and Conn (1982b), (1982a) consider inequalities, but need to resort to finite differences for the reduced Hessian to converge which can be costly. SNOPT
uses a full limited memory Hessian but computes the step by a null-space approach involving the reduced (i.e. projected) Hessian. A number of further references on reduced Hessian methods is given and discussed by Biegler et al. (1995).

Other work on feasible methods

By feasible methods we understand methods that remain feasible with respect to all inequalities at all intermediate iterates. These methods may still evaluate the problem functions outside the feasible region for example in the line search. We note that any method can easily be made feasible with respect to linear inequalities, so our discussion implicitly assumes the presence of nonlinear inequalities.

Mayne and Polak (1976) suggested a modification that would make any interior point method feasible. Their method were adapted to SQP methods by Tits and co-workers in a series of papers; Panier and Tits (1987), (1993), Lawrence and Tits (1996), (2000). Their algorithm FSQP has emerged as a reliable code which is commercially available. Interior methods can also be designed as feasible methods by including the inequalities and not the slacks in the barrier function. This approach has been pursued by Gay, Overton, and Wright (1998), but leads to complex algebraic manipulations in the derivation of the algorithm. Recently Byrd, Nocedal, and Waltz (2000) have suggested a feasible interior method using slack resetting with good results.

In optimal control feasibility of equality constraints has been approached by evolution of the dynamic model constraint over the relevant time-span. See Pytlak (1999) for further references. We return to these issues in chapter 4.

Overview of other large scale methods

The methods described in the following are a selection of established optimization codes. The selection is not exhaustive, and the description of each method is only of limited depth. The interested reader will need to resort to the cited references for a deeper presentation of each method.

GRG Until the mid-eighties generalized reduced-gradient (GRG) methods were recognized as the most successful methods for nonlinear programming. GRG methods try to remain feasible with respect to equalities by a feasibility restoration phase following the step computation. The feasibility restoration phase needs to evaluate the constraint functions at possibly
many trial points which can be costly. GRG methods therefore tend to perform poorly on problems with severe nonlinearities in the equality constraints, and when initialized far from the optimum. To remedy this practical implementations do not require feasibility at early iterations, and thus become more related to projected Lagrangian methods. For a description of a general GRG method see Gill et al. (1981), pp. 220-223. See Edgar and Himmelblau (1989), p. 362, for a comparison of GRG with other methods available in the mid-eighties. Further references are provided in the references above. Today the most successful GRG implementation is CONOPT by Drud (1985).

MINOS is a SLC method which solves a linearly constrained subproblem with a nonlinear objective. Although SLC methods are commonly agreed to be inferior to SQP methods due to the excessive number of function evaluations, MINOS by Murtagh and Saunders (1995) remains a successful implementation. For a description of a general SLC method see Gill et al. (1981), p.234-236, and Nocedal and Wright (1999), pp. 523-525. For an assessment of the performance of MINOS see Bondarenko et al. (1999). MINOS and CONOPT are designed for large problems with a modest number of degrees of freedom. MINOS does not implement globalization mechanisms like merit functions.

LANCELOT is a sequential augmented Lagrangian method. LANCELOT by Conn, Gould, and Toint (1992) is designed for large problems with many degrees of freedom. See Bondarenko et al. (1999) for numerical results.

SNOPT by Gill, Murray, and Saunders (1997) is an active-set SQP algorithm using a modified augmented Lagrangian merit function with line search. Global convergence results are difficult to establish because the merit function is treated as a function of the variables, slacks and multipliers and is not minimized by a solution point, i.e. it is not an exact penalty method. The convergence theory for SNOPT is similar to the properties of NPSOL addressed in Gill, Murray, Saunders, and Wright (1992). SNOPT uses a limited memory convex quasi-Newton approximation to the Hessian of the Lagrangian. It uses a reduced Hessian approach in solving the qp subproblems. See Gill et al. (1997), Bondarenko et al. (1999) and Morales et al. (2001) for numerical evaluations. SNOPT is expected to outperform MINOS on problems with highly nonlinear constraints.
filterSQP by Fletcher and Leyffer (1998) is a trust-region SQP method using second derivatives of the objective and constraints, and it solves the subproblem by an active-set method for indefinite quadratic programming. If a direction of negative curvature is detected it takes a step to the trust-region boundary in this direction. filterSQP uses a "filter" mechanism that eliminates the need for a merit function. See Morales et al. (2001) for numerical evaluations. Convergence results are ongoing research.

LOQO by Vanderbei and Shanno (1999) implements a line search primal-dual interior method. It uses second derivatives of the objective and constraint functions, and slacks for inequality constraints. It uses the quadratic inexact penalty function, hence global convergence results are difficult to obtain. It uses a variant of modified Cholesky factorization to handle indefinite subsystems. See Morales et al. (2001) for numerical evaluations.

KNITRO is a trust-region primal-dual interior-method using second derivatives. Unlike most interior methods it computes the steps in a SQP-like manor that approximately minimize the barrier function. It uses projected conjugate gradients (CG) to handle indefiniteness. I.e. when the CG-iteration breaks down due to indefiniteness, it takes a step to the trust-region boundary in the computed direction. It uses a non-differentiable merit function for global convergence. KNITRO is described in Byrd, Hribar, and Nocedal (1999), and analyzed in Byrd, Liu, and Nocedal (1998) and Byrd, Gilbert, and Nocedal (2000). See Morales et al. (2001) for numerical evaluations.

3.2 Introduction

In this section we suggest a feasible reduced Hessian SQP method. The method implements the $l_1$-merit function and BFGS updates for the reduced Hessian. The method is feasible with respect to inequality constraints. Since inequalities are the main problem in reduced Hessian methods, see Nocedal and Wright (1999) p.551, our method is aimed at continuous large-scale nonlinearly constrained optimization problems with few degrees of freedom. In particular we expect our method to be efficient for problems dominated by nonlinear equality constraints, with relatively few nonlinear inequalities. Note that any SQP method will be feasible with respect to affine inequalities and simple bounds. The method extends FSQP$^r$ of Tits and co-workers Panier
3.2 Introduction

and Tits (1987), (1993), Lawrence and Tits (1996), (2000) to the reduced Hessian setting. The work of Tits and co-workers extends the work of Mayne and Polak (1976).

The local convergence analysis for the present algorithm simply states that after the correct active set has been identified, the problem is equality constrained and two-step superlinear convergence follows as in Byrd and Nocedal (1991) or one-step superlinear convergence as in Biegler, Nocedal, and Schmid (1995).

In the following the NLP

\[
\min_{x_k} f(x_k) \\
\text{s.t. } c_E(x_k) = 0 \\
c_T(x_k) \leq 0
\] (3.1)

is considered with objective function \( f : \mathbb{R}^n \to \mathbb{R} \), equality constraints \( c_E : \mathbb{R} \to \mathbb{R}^{n_1} \) and inequality constraints \( c_T : \mathbb{R} \to \mathbb{R}^{n_2} \). \( n \) is the number of variables, \( n_1 \) is the number of nonlinear equality constraints and \( n_2 \) is the number of nonlinear inequality constraints. Subscript \( k \) refers to iteration index. We design our algorithm for the case \( n_1 \gg n_2 > 0 \), which corresponds to a large number of nonlinear equality constraints and few nonlinear inequality constraints. We associate two sets with the NLP (3.1):

\[
X = \{ x_k \in \mathbb{R}^n \mid c_E(x_k) = 0, \ c_T(x_k) \leq 0 \} \\
X_I = \{ x_k \in \mathbb{R}^n \mid c_T(x_k) \leq 0 \}
\]

with \( X \subseteq X_I \). A point \( x_k \in X_I \) satisfies the inequality constraints but not necessarily the equality constraints. Points in \( X \) are feasible, while points in \( X_I \) are (at least) feasible with respect to inequalities. We will generate iterates \( x_k \in X_I \) and a solution \( x^* \in X \). The Lagrangian \( L : \mathbb{R}^n \times \mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \to \mathbb{R} \) associated with (3.1) is defined by

\[
L(x_k, \lambda_E, \lambda_T) \triangleq f(x_k) + \sum_{i=1}^{n_1} \lambda_{E,k}^i c_E^i(x_k) + \sum_{i=1}^{n_2} \lambda_{T,k}^i c_T^i(x_k) \] (3.2)

where the real-valued vectors \( \lambda_{E,k} \) and \( \lambda_{T,k} \) are the Lagrange multipliers.

Practical experience with reduced Hessian methods indicate that they require a good starting point to converge. This is expressed in assumption 4.1 in Biegler et al. (1995), i.e. that the sequence of iterates \( \{x_k\} \) is contained in a convex set \( D \). In the present method this assumption can be satisfied by a suitable choice of the feasible set \( X_I \) with respect to the inequalities.
The prize to pay for this is the need for an initial point \( x_0 \in X_f \). Problems dominated by nonlinear equality constraints, possibly with nonlinear inequality constraints, occur in optimal control problems such as nonlinear MPC. Nonlinear inequalities may occur if there are quality-related constraints and quality is a nonlinear function of the problem variables, i.e. such as \( q = q(x^*) \) and \( q(x_k) \leq 0 \). Solving this with \( q \) as a slack variable cannot guarantee \( q(x_k) \leq 0 \) away from the solution \( x^* \). Initialization in nonlinear MPC may involve a shifted solution from the previous MPC-iteration, hence a feasible initial point is a reasonable assumption, see Allgöwer, Badgwell, Qin, Rawlings, and Wright (1999) and the references therein.

General benefits of feasible iterates are summarized in Lawrence and Tits (2000), and we restate them here with some comments pertaining to our algorithm.

- The qp subproblems may become infeasible if the constraint linearizations are inconsistent. This can happen since we include equality constraints in addition to inequalities.

- The objective cannot be used as merit function when equality constraints are present. We use the \( l_1 \)-merit function for global convergence.

- Keeping the iterates inside a feasible region can ensure that the problem functions always are evaluated at points where they are defined. If the feasible region is defined by linear constraints and simple bounds, this can be guaranteed for any SQP-method. In our method a Maratos correction term is computed by evaluating the constraint functions at the point \( x_k + d_k \), where the vector \( d_k \) is a step. The point \( x_k + d_k \) may lie outside the set \( X_f \) unless \( X_f \) is defined by linear constraints and simple bounds. See section 3.3.2, equation (3.32) for details. In addition the line search may evaluate the problem functions at points where inequality constraints are infeasible. These considerations applies to FSQP\(^2 \) as well.

- Meaningful exploration of trade-offs between design alternatives.

- The optimization algorithm will have iterates that are feasible with respect to inequalities. If terminated prior to convergence the non-optimal solution may be utilized.
3.2 Introduction

The usual SQP direction finding qp associated with (3.1) is

\[
\min_{d^0_k} \frac{1}{2} \langle d^0_k, W(x_k) d^0_k \rangle + \langle g_k, d^0_k \rangle \\
\text{s.t.} \quad c^1_k(x_k) + \langle \nabla c^1_k(x_k), d^0_k \rangle = 0 \quad i = \{1, \ldots, p_1\} \\
\quad c^2_k(x_k) + \langle \nabla c^2_k(x_k), d^0_k \rangle \leq 0 \quad i = \{1, \ldots, p_2\}
\]

(3.3)

where we introduce the objective gradient \( g_k = \nabla f_k \) and \( W(x_k) \) is the Hessian \( \nabla^2 \mathcal{L}_k \) of the Lagrangian or an approximation to it. The qp (3.3) produces the ordinary SQP direction \( d^0_k \). Superscript 0 refers to ordinary SQP directions throughout this chapter. The rFSQP algorithm tilts the ordinary SQP direction and produces a direction \( d_k \).

A feasible direction for \( x_k \in X_I \) is a direction \( d^0_k \in \mathbb{R}^n \) generated by (3.3) such that there exists an \( \overline{\alpha} > 0 \) satisfying

\[
(x_k + \alpha d^0_k) \in X_I \quad \forall \alpha \in [0, \overline{\alpha}]
\]

(3.4)

Define the index-set of \( \epsilon \)-active inequality constraints as

\[
\mathcal{J}^\epsilon(x_k) \triangleq \{ i \mid -\epsilon < c^1_k(x_k) \leq 0 \}
\]

(3.5)

for a small \( \epsilon > 0 \). Observe that (3.3) allows \( d^0_k \in \text{span} \{ \nabla c^i_k(x_k) \mid c^i_k(x_k) = 0 \} \perp \) which may violate (3.4). Define

\[
A(x_k) = \left[ \nabla c^i_k(x_k) \mid \forall i \in \{1, \ldots, p_1\}, \forall j \in \mathcal{J}^\epsilon(x_k) \right]
\]

(3.6)

To the best of our knowledge only Coleman and Conn (1982b), (1982a) give theoretical results for inequality constrained reduced Hessian methods. Tjoa and Biegler (1991) include simple bounds, and use slacks for the inequalities. In addition there exists a successful implementation, SNOPT, by Gill et al. (1997) with promising results (see Bondarenko et al. (1999) for results). We observe that varying dimension of the working set matrix will present additional challenges when inequality constraints are present in reduced Hessian methods, since BFGS updates do not generally allow varying dimensions. We discuss this issue as part of our implementation, but do not intend to resolve this issue since we take the view that since we are able to identify the correct active set at a finite but potentially large iteration index \( k_0 \) the problem is equality constrained thereafter. Hence, the tools of Byrd and Nocedal (1989) can be applied to handle the case of infinitely many BFGS updates.

This section continues with a description of the algorithm in section 3.3, then global and local convergence analysis are provided in section 3.4. Some implementation issues and numerical results are discussed in section 3.5, and some concluding remarks are provided in section 3.6.
3.3 The rFSQP algorithm

We adapt the feasibility mechanisms from FSQP' (Lawrence and Tits 2000) to the reduced Hessian setting. Observe that neither the equality constraints nor the reduced gradients we wish to investigate are present in FSQP'. We make the assumptions:

**Assumption 3.1** $X \neq \emptyset$.

**Assumption 3.2** The functions $f : \mathbb{R}^n \to \mathbb{R}$, $c^i_E : \mathbb{R}^n \to \mathbb{R}$ and $c^i_T : \mathbb{R}^n \to \mathbb{R}$ are continuously differentiable on $X_I$ for all $i$.

**Assumption 3.3** The set $\{ \nabla c^i_E(x^*) \mid \forall i \in \{1, \ldots, p_1\} \} \cup \{ \nabla c^i_T(x^*) \mid i \in J^{x,e} \}$ is linearly independent ( LICQ ).

**Assumption 3.4** Strict complementary slackness holds at $x^*$, i.e. $c^i_T(x^*)\lambda_T^{s,i} = 0$ for $i = \{1 \ldots p_2\}$ and if $c^i_T(x^*) = 0$ then $\lambda_T^{s,i} > 0$.

Under assumptions 3.1-3.4 and first and second order KKT-conditions, it is well known (see, for example Fiacco and McCormick (1990), Fletcher (1987)) that $x^*$ is an isolated local constrained minimizer of the NLP (3.1) with unique multipliers. We assume that at least one such isolated local constrained minimizer of (3.1) exists. The LICQ-assumption guarantees that the constraint linearizations are consistent at $x^*$. Note that we make a stronger assumption related to the LICQ-assumption in section 3.4.2, assumption 3.6. Recovering from infeasibility resulting from inconsistency is considered an implementation issue, see Marazzi and Nocedal (2000) for an exposition and Gill et al. (1997) for an example strategy.

3.3.1 The feasibility mechanism

We restate the essential features of FSQP' (Lawrence and Tits 2000). In FSQP' the qp (3.3) is perturbed as

$$\min_{d_k,\gamma_k} \frac{1}{2} \langle d_k, W_k d_k \rangle + \gamma_k$$

s.t.

$$\langle g_k, d_k \rangle \leq \gamma_k$$

$$c^i_E(x_k) + \langle \nabla c^i_E(x_k), d_k \rangle = 0 \quad i = \{1, \ldots, p_1\}$$

$$c^i_T(x_k) + \langle \nabla c^i_T(x_k), d_k \rangle \leq \gamma_k \eta_k \quad i = \{1, \ldots, p_2\}$$

with real scalars $\gamma_k$ and $\eta_k \geq 0$, and where we have added equality constraints. The tilting parameter $\eta_k$ controls the amount of tilting. Large values emphasize feasibility, while small values emphasize descent. Lawrence
and Tits (1996) handle equality constraints by rewriting them as doubly bounded inequalities, while we keep them as equalities. Problem (3.7) motivates the derivation of our reduced gradient mechanism in section 3.3.2. Note that \( \text{sign}(\gamma_k) = -\text{sign}(\eta_k) \) must be inferred to yield feasibility of the inequality constraints.

Lawrence and Tits (1996) update \( \eta_k \) based on the following least-squares problem. Given an estimate \( J_k^E \) of the active set, FSQP computes an estimate \( d_k^E \) of the SQP-direction \( d_k^0 \) by solving the qp (3.8).

\[
\begin{align*}
\min_{d_k^E} & \quad \frac{1}{2} \langle d_k^E, W_k d_k^E \rangle + \langle g_k, d_k^E \rangle \\
\text{s.t.} & \quad c_i^E(x_k) + \langle \nabla c_i^E(x_k), d_k^E \rangle = 0, \quad i = \{1, \ldots, p_1\} \\
& \quad c_i^E(x_k) + \langle \nabla c_i^E(x_k), d_k^E \rangle = 0, \quad i \in J_k^E 
\end{align*}
\]  

(3.8)

This estimate is used to update the parameter \( \eta_k \) to provide adequate tilting into the feasible set, and in FSQP this is cheaper to compute than \( d_k^0 \) itself since (3.8) is a least-squares problem.

The present algorithm solves qp's in the reduced space, so the need for the estimate \( d_k^E \) to reduce the computational workload is less important. Hence, we simply compute the SQP-direction. The notation \( d_k^E \) is retained for ease of exposition and to allow direct comparison between FSQP and rFSQP. Showing that \( d_k^E = d_k^0 \) for \( k \) sufficiently large is a simple observation, but it is still necessary to show that

\[
\eta_k = \mathcal{O}(\|d_k^E\|^2)
\]  

(3.9)

(with a suitable order constant \( C_k^E \)) is sufficient to guarantee global convergence and local superlinear convergence.

In FSQP a Maratos effect avoidance scheme is implemented near the solution by

\[
\begin{align*}
\min_{d_k^E} & \quad \frac{1}{2} \langle d_k^E + d_k^C, W_k (d_k^E + d_k^C) \rangle + \langle g_k, d_k^E + d_k^C \rangle \\
\text{s.t.} & \quad c_i^E(x_k + d_k^E + d_k^C) + \langle \nabla c_i^E(x_k + d_k^E + d_k^C), d_k^C \rangle = 0, \quad i = \{1, \ldots, p_1\} \\
& \quad c_i^E(x_k + d_k^E + d_k^C) + \langle \nabla c_i^E(x_k + d_k^E + d_k^C), d_k^C \rangle = -\|d_k^C\|^2, \quad i \in J_k^E 
\end{align*}
\]  

(3.10)

In (3.10) \( d_k^C \) denotes the correction to the direction \( d_k \), and \( \kappa \) is a scalar in the range \((2, 3)\). However, rFSQP is implemented with an \( l_1 \)-penalty function, and we do not expect (3.10) to remedy the well-known Maratos effect associated with this. Instead, to promote local convergence analysis, we assume that a step-length of one is accepted near the optimum, and work through the local analysis in view of this. This assumption is also made by Biegler
et al. (1995), and is motivated by that the Maratos effect can be handled
by implementing a non-monotone line-search like the watch-dog method of
Chamberlain, Powell, Lemarechal, and Pedersen (1982). Other alternatives
are listed in Nocedal and Wright (1999), section 18.11. Summarizing, the
correction $d_k^C$ from (3.10) is needed to guarantee that the feasibility condi-
tion $c^T_i(x_k + d_k + d_k^C) \leq 0$ with a unit step-length is satisfied. I.e. that
the watch-dog method can be implemented without interfering with feasibility
of inequality constraints.

We require that the sequence $\{d_k\}$ possesses the following properties:

**P1** $d_k = 0$ if $x_k$ is a KKT point for (3.1).

**P2** $D\phi_p(x_k, d_k) < 0$ if $x_k$ is not a KKT point for (3.1) (the $l_1$-merit function
$\phi_p$ is to be defined in (3.11)). The directional derivative operator $D$
is used due to the non-derivative property of $l_1$-merit functions.

**P3** $\langle \nabla_i^2(x_k), d_k \rangle < 0$ for all $i \in J_k^c$ if $x_k$ is not a KKT point for (3.1).

**P4** $d_k = d_k^0 + O(\|d_k^0\|^2)$.

Observe that P2 differs from P2 in Lawrence and Tits (2000) since we
need a descent in the $l_1$-merit function. Next the reduced gradient
method and the algorithm will be outlined.

### 3.3.2 The feasible reduced Hessian method (rFSQP)

The algorithm is essentially a restatement of algorithm II by Biegler et al.
(1995) with some extensions to allow for the additional inequality constraint
and the parameters $\gamma_k$ and $\eta_k$ in equation (3.7). Note that the dimension of
$A_k$ generally will change when the active set $J_k^c$ changes. The next iterate
is computed as $x_{k+1} = x_k + \alpha_k d_k + \gamma_k d_k^C$ where $\alpha_k$ is a step-length parameter
chosen to reduce the value of the constrained $l_1$-merit function

$$\phi_p(x_k) = f(x_k) + \nu_k \|c_\mathcal{C}(x_k)\|_1$$

s.t. $c_\mathcal{I}(x_k) \leq 0$

(3.11)

with penalty parameter $\nu_k$. Including a term $\nu_k \max \{0, c_\mathcal{I}^T(x_k)\}$ is oblivious
by a strictly feasible search direction. Observe that (3.11) differs from the
merit functions used in both Biegler et al. (1995) and Lawrence and Tits
(2000).

Define the nonsingular matrix $[Y_k, Z_k]$ where $Y_k \in \mathbb{R}^{n \times m_k}$ and $Z_k \in \mathbb{R}^{n \times (n-m_k)}$. $Y_k$ is a basis for the range space $\mathcal{R}(A_k^T)$ of the Jacobian $A_k$.
from equation (3.6), while \( Z_k \) is a basis for the null space \( \mathcal{N}(A_k^T) \). The dependence of \( m \) on \( k \) where \( m_k = p_1 + |J_k^e| \) allows adaption to varying size of the working set matrix \( A_k \). Here \( |J_k^e| \) denotes the length, i.e. number of elements in the vector \( J_k^e \). The null-space of \( A_k^T \) is the tangent space of the active constraints, and since \( Z_k \) is a basis for the null-space of \( A_k^T \) we have

\[
A_k^T Z_k = 0
\]  

(3.12)

We choose the variable-reduction factorization, see Gill et al. (1981), p.221, \( A(x_k)^T = [C(x_k) \quad N(x_k)] \) where

\[
Z(x_k) = \begin{bmatrix} -C(x_k)^{-1}N(x_k) \\ I \end{bmatrix}, \quad Y(x_k) = \begin{bmatrix} I \\ 0 \end{bmatrix}
\]  

(3.13)

More details on the factorization are found in Xie and Byrd (1999). The solution to (3.7) can then be separated as

\[
d_k = Y_k p_{Y,k} + Z_k p_{Z,k}
\]  

(3.14)

where the vectors \( p_{Y,k} \in \mathbb{R}^{m_k} \) and \( p_{Z,k} \in \mathbb{R}^{(n-m_k)} \). By (3.12), the range-space step becomes

\[
p_{Y,k} = -(A_k^T Y_k)^{-1} c_k
\]  

(3.15)

where

\[
c_k \triangleq \begin{bmatrix} c^e(x_k) \\ c^T(x_k) \end{bmatrix} \text{ and } \ c^T(x_k) \triangleq \{c^T_i(x_k) - \gamma_k^{-1} \eta_k \ | \ i \in J_k^e \}
\]  

(3.16)

Since \( \gamma_k \) is unavailable at this stage \( \gamma_{k-1} \) is used. Convergence of the sequence \( \{\gamma_k\} \) is established in section 3.4. Hence, using \( \gamma_{k-1} \) is sufficient. Then \( d_k = -Y_k(A_k^T Y_k)^{-1} c_k + Z_k p_{Z,k} \). Observe that \( Y_k(A_k^T Y_k)^{-1} \) is a right inverse of \( A_k^T \) and that (3.15) is a particular solution to the linearized equations. To compute \( d_k \), solve for \( p_{Z,k} \) and \( \gamma_k \) from (derived in section 3.4)

\[
B_k p_{Z,k} = -Z_k^T g_k - \zeta_k u_k \leq \gamma_k 
\]  

(3.17)

In (3.17) the cross-term approximation \( Z_k^T W_k Y_k p_{Y,k} = \zeta_k u_k \) is introduced where \( \zeta_k \) is a scalar damping parameter and \( u_k \) is an approximation to the rectangular matrix-vector product \( Z_k^T W_k Y_k p_{Y,k} \). Assuming positive definiteness of the reduced Hessian approximation \( B_k \), equation (3.17) gives a unique \( p_{Z,k} \) while there is freedom in choosing \( \gamma_k \). This might have been
anticipated, since augmenting the problem (3.7) with \( \gamma_k \) gives a semidefinite Hessian.

Since the inactive constraint linearizations are excluded, \( p_{Z,k} \) is computed by an EQP strategy, see Gill et al. (1981), p. 244, Fletcher (1987), sections 11.2 and 11.3, and Nocedal and Wright (1999), p. 534. The main motivation for choosing the EQP strategy is that it allows use of theorem 3.1 from Byrd and Nocedal (1989) restated below (note that \( Z_k^T \nabla^2 \ell_{I,k}^k \neq 0 \) when \( i \notin J_k^k \) in general). The active inequalities are treated as equalities and are included in \( c_k \) in (3.15).

The Lagrange multipliers are estimated from

\[
\lambda_k \triangleq [\lambda_{\ell,k} \lambda_{z,k}] = -(Y_k^T A_k)^{-1} Y_k^T g_k
\]

(3.18)

where \( \lambda_{z,k} = \{ \lambda_{z,k}^i \mid i \in J_k^k \} \). This is a first-order estimate of the form

\[
\min \| A_k \lambda_k + g_k \|
\]

obtained by observing that \( (Y_k^T A_k)^{-1} Y_k^T \) is a left-inverse to \( A_k \). I.e., any \( g_k \in \mathcal{R}(A_k) \) is compatible with (3.18), and we cannot assume that the estimated multipliers coincide with the NLP-multipliers away from a solution \( x^* \), see Gill et al. (1981), p. 248. By assumption 3.3 (LICQ), we have that \( \lambda^* \) exists and is unique. We choose the multipliers \( \lambda_{z,k}^i = 0, i \notin J_k^k \).

The update-rule for \( \zeta_k \) follows by solving

\[
\begin{align*}
\hat{\zeta}_k & = \min \left\{ 2 \cos \theta^{BFGS}_{k} (p_{Z,k}) \left| g_k^T Z_k w_k + w_k^T B_k^{-1} Z_k g_k + \hat{\zeta}_k w_k^T B_k^{-1} w_k \right| \right. \\
\zeta_k & = \min \left\{ 1, \hat{\zeta}_k \right\}
\end{align*}
\]

(3.19)

for a constant \( \rho > 0 \), \( \cos \theta^{BFGS}_k \) is defined in equation (3.38), and measures the angle between \( p_{Z,k} \) and \( B_k p_{Z,k} \). The null-space component \( Z_k p_{Z,k} \) must make an acute angle with the projection of \( -g_k \) onto the null-space to give descent. For the moment neglecting the cross-term \( w_k \), we have from (3.17) that \( B_k p_{Z,k} = -Z_k^T g_k \). Byrd and Nocedal (1991) derive the \( \cos \theta^{BFGS}_k \) relation for reduced Hessian methods. Note the dependence \( \zeta_k (p_{Z,k}) \) through \( \cos \theta^{BFGS}_k (p_{Z,k}) \), which is not available at this stage since \( \zeta_k \) must be computed before (3.17). Therefore the actual implementation is done as in Biegler et al. (2000). The update rules for the damping factor \( \zeta_k \in (0,1] \) and the penalty parameter \( \nu_k \)

\[
\nu_k = \begin{cases} 
\nu_{k-1} & \text{if } \nu_{k-1} \geq \| \lambda_k \|_\infty + 2 \rho \\
\| \lambda_k \|_\infty + 3 \rho & \text{otherwise}
\end{cases}
\]

(3.20)

are derived in lemma 3.3, section 3.4.2 and follows Biegler et al. (1995) closely.
3.3 The rFSQP algorithm

As in Biegler et al. (1995) we approximate the cross term $Z_k^T W_k Y_k$ by a rectangular matrix $S_k$. Since $W_{k+1} = \nabla_x^2 \mathcal{L}(x_{k+1}, \lambda_{k+1})$, the approximation

$$Z_k^T W_{k+1}(x_{k+1} - x_k) \approx Z_k^T \left[ \nabla_x \mathcal{L}(x_{k+1}, \lambda_{k+1}) - \nabla_x \mathcal{L}(x_k, \lambda_{k+1}) \right]$$

(3.21)

holds when $x_{k+1}$ is close to $x_k$. i.e., in section 3.4.3, lemma 3.11, we prove that $J_k^T = J^*$ for all $k$ sufficiently large. If $Z(x_k)$ is locally Lipschitz continuous the approximation (3.21) holds locally, and the comments in Nocedal and Wright (1999), p. 567, applies. This continuity assumption is also made in Biegler et al. (1995). The error in the approximation is of order $O(||d_k||^2)$. The matrix $S_{k+1}$ is required to satisfy the secant relation

$$S_{k+1} (x_{k+1} - x_k) = Z_k^T \left[ \nabla_x \mathcal{L}(x_{k+1}, \lambda_{k+1}) - \nabla_x \mathcal{L}(x_k, \lambda_{k+1}) \right]$$

and comparing with (3.21) we have $S_{k+1} \approx Z_k^T W_{k+1}$. Hence, computing the full matrix $Z_k^T W_k Y_k$ is avoided as in Biegler et al. (1995) by approximating $S_k$ by Broyden’s method, (see Dennis and Schnabel (1996), p. 170):

$$S_{k+1} = S_k + \frac{(\tilde{y}_k - S_k \tilde{s}_k) \tilde{s}_k^T}{\tilde{s}_k^T \tilde{s}_k}$$

(3.22)

where

$$\tilde{y}_k = Z_k^T \left[ \nabla_x \mathcal{L}(x_{k+1}, \lambda_{k+1}) - \nabla_x \mathcal{L}(x_k, \lambda_{k+1}) \right]$$

$$\tilde{s}_k = x_{k+1} - x_k$$

(3.23)

and computing

$$w_k = \alpha_k S_k Y_k p_{v,k}$$

$$\tilde{w}_k = \alpha_k S_k Y_k p_{v,k}$$

(3.24)

Since the Broyden approximations may become unbounded they are safeguarded as in Biegler et al. (1995). I.e. choose a constant $\Gamma$ and define

$$w_k = \begin{cases} w_k & \text{if } ||w_k|| \leq \frac{\Gamma}{\|p_{v,k}\|^{1/2}} ||p_{v,k}|| \\ \frac{\Gamma}{\|p_{v,k}\|^{1/2}} ||w_k|| & \text{otherwise} \end{cases}$$

(3.25)

Choose a sequence of positive numbers $\{\gamma_k\}$ such that $\sum_{k=1}^{\infty} \gamma_k < \infty$, and set

$$\tilde{w}_k = \begin{cases} \tilde{w}_k & \text{if } ||\tilde{w}_k|| \leq \frac{\alpha_k}{\gamma_k} ||p_{v,k}|| \\ \frac{\alpha_k}{\gamma_k} ||p_{v,k}|| & \text{otherwise} \end{cases}$$

(3.26)
However, if the BFGS update criterion (to be discussed) is not satisfied, $w_k$ is recalculated by finite differences:

$$\begin{align*}
  w_k &= Z_k^T \left[ \nabla_x \mathcal{L}(x_k + Y_k p_{Y_k}, \lambda_k) - \nabla_x \mathcal{L}(x_k, \lambda_k) \right] \\
  \bar{w}_k &= Z_k^T \left[ \nabla_x \mathcal{L}(x_k + \alpha_k Y_k p_{Y_k}, \lambda_{k+1}) - \nabla_x \mathcal{L}(x_k, \lambda_{k+1}) \right]
\end{align*}
$$

(3.27)

which require reevaluation of the constraint gradients at two extra points. Biegler et al. (1995) argues that finite difference updating of $w_k$ and $\bar{w}_k$ does not occur too often. However, with inequality constraints and changes in the active set finite difference updating is likely to be required more often since the conditions for application of the Broyden-update, see (3.36) below, may be harder to satisfy when adding constraints to the active set. The cross term approximations $w_k$ and $\bar{w}_k$ does not influence on the global convergence properties. Hence, an efficient implementation may only calculate them if the algorithm seems to approach a solution to speed up the local convergence rate.

The auxiliary subproblems (3.8) and (3.10) from FSQP must be adopted before the algorithm is summarized. Since $d_k^C$ is computed with $J_k^r$ and $d_k^E$ is computed with $J_{k+1}^r$, no extra factorizations of $A_k$ is needed to compute $d_k^C$ and $d_k^E$. (Since the algorithm can compute $d_k^E$ after the new updates $f_{k+1}$, $g_{k+1}$, $c_{k+1}$, $A_{k+1}$, $Y_{k+1}$, $Z_{k+1}$ and $B_{k+1}$ are available, the next active set is available to us at this stage, so we can actually compute the SQP-direction directly (without estimating $J_k^E$ as in FSQP')).

Consider the null-space approach for (3.8)

$$d_{k+1}^E = Y_{k+1} p_{Y_{k+1}}^E + Z_{k+1} p_{Z_{k+1}}^E$$

(3.28)

where $p_{Y_{k+1}}^E \in \mathbb{R}^{m_{k+1}}$ and $p_{Z_{k+1}}^E \in \mathbb{R}^{n-m_{k+1}}$ are computed from

$$p_{Y_{k+1}}^E = -(A_{k+1}^T Y_{k+1})^{-1} c_{k+1}^E$$

(3.29)

where $c_{k+1}^E \triangleq \begin{bmatrix} c_c(x_{k+1}) \\ c_T(x_{k+1}) \end{bmatrix}$ with $c_T(x_{k+1}) \triangleq \{c_T^i(x_{k+1}) \mid i \in J_{k+1}^r \}$, and the unconstrained (observe that (3.8) only has equality constraints)

$$\min_{p_{Z_{k+1}}^E} \left\langle Z_{k+1}^T(g_{k+1} + \xi_{k+1} w_{k+1}, p_{Z_{k+1}}^E) + \frac{1}{2} \left\langle p_{Z_{k+1}}^E, B_{k+1} p_{Z_{k+1}}^E \right\rangle \right.$$  

The approximation $c_{k+1}^E w_{k+1}$ is computed in the same manner as $\xi_{k+1} w_{k+1}$. Assuming a positive definite $B_{k+1}$ this gives

$$B_{k+1} p_{Z_{k+1}}^E = - \left( Z_{k+1}^T g_{k+1} + \xi_{k+1} w_{k+1} \right)$$

(3.30)
3.3 The rFSQP algorithm

The Maratos correction term $d_{k+1}^C$ has a similar decomposition, observing that only equality constraints are present in (3.10). Construct the right-hand side $c_k^C = \left[ \frac{c^T(y_k + d_k)}{\delta_k} \right]$ with $\delta_k = \{ c^T(y_k + d_k) + ||d_k||^2 | i \in J^e_k \}$. Compute

$$d_k^C = Y_k p_{Y,k}^C + Z_k p_{Z,k}^C$$

(3.31)

where $p_{Y,k}^C \in \mathbb{R}^{m_k}$ and $p_{Z,k}^C \in \mathbb{R}^{(n-m_k)}$,

$$p_{Y,k}^C = -(A_k^T Y_k)^{-1} e_k^C$$

(3.32)

and the unconstrained

$$\min_{p_{Z,k}^C} \left\{ Z_k^T g_k + \zeta_k (w_k + w_k^C) + B_k p_{Z,k}^C, p_{Z,k}^C \right\} + \frac{1}{2} \left\langle p_{Z,k}^C, B_k p_{Z,k}^C \right\rangle$$

giving (assuming $B_k$ positive definite)

$$B_k p_{Z,k}^C = - \left( Z_k^T g_k + \zeta_k (w_k + w_k^C) + B_k p_{Z,k}^C \right)$$

(3.33)

The approximation $u_k^C$ is computed by the same method as $u_k$ was computed (Broyden or finite differences). Note that equations (3.15, 3.29, 3.32) requires solving a set of linear equations with changing right-hand sides which can be done efficiently, since the same factorizations apply. However, this strategy requires evaluation of the constraint functions at three different points in addition to the finite difference updates for $u_k$ and $\bar{u}_k$ above, which may be costly.

3.3.3 The BFGS update scheme

An updating scheme for the reduced Hessian $B_k = Z_k^T W_k Z_k$ allowing for changes in the active set is discussed next. It is well known that the BFGS formula

$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k}$$

(3.34)

will give a positive definite update $B_{k+1} \in \mathbb{R}^{m \times m}$ provided that $B_k$ is positive definite and that $s_k^T y_k > 0$. Define

$$s_k = \alpha_k p_{Z,k}$$

$$y_k = Z_k^T [\nabla_x \mathcal{L}(x_{k+1}, \lambda_{k+1}) - \nabla_x \mathcal{L}(x_k, \lambda_{k+1})] - \bar{w}_k$$

(3.35)
When the working-set changes from iteration \( k \) to \( k + 1 \) the dimensions of the secant vectors \( s_k \) and \( y_k \) will not be compatible with the dimension of \( B_k \). In \( rFSQP \) \( B_{k+1} \) is re-initialized to \( I \) when the working set changes. To the best of our knowledge, BFGS updates for reduced Hessian methods with inequality constraints are not available in the literature. (The updating scheme in SNOPT by Gill et al. (1997) updates the sparse but full Hessian \( W_k \), but applies LUSOL by Gill, Murray, Saunders, and Wright (1987) to allow for adding and deletion of rows and columns in the working-set matrix \( A_k \), from which \( Z_k \) is formed. Then the reduced Hessian can be produced by computing \( B_k = Z_k^T W_k Z_k \).) This topic is also addressed in MINOS (Murtagh and Saunders 1995).

A similar scheme allows varying dimensions in the Broyden update (3.22).

In addition the BFGS update criterion I of Biegler et al. (1995) is implemented. i.e. choose a constant \( \gamma_{fd} > 0 \) and a sequence of positive numbers \( \{ \gamma_k^{\infty} \} \) such that \( \sum_{k=1}^\infty \gamma_k^{\infty} < \infty \) (this is the same sequence as in (3.26)). Compute \( s_k \) and \( y_k \) by the secant relation (3.35).

- If \( \tilde{y}_k \) is computed by Broyden's method (3.24, 3.26), and if both \( s_k^T y_k > 0 \)
  \[
  \| p_{Y,k} \| \leq (\gamma_k^{\infty})^2 \| p_{Z,k} \| \tag{3.36}
  \]
  hold at iteration \( k \), then update \( B_k \) by the BFGS formula (3.34). Otherwise, set \( B_{k+1} = B_k \).

- If \( \tilde{a}_k \) is computed by finite differences (3.27), and if both \( s_k^T y_k > 0 \)
  \[
  \| p_{Y,k} \| \leq \gamma_{fd} \| p_{Z,k} \| / \sigma_k^{1/2} \tag{3.37}
  \]
  hold at iteration \( k \) where \( \sigma_k = \max \{ \| e_k \|, \| e_{k+1} \| \} \), \( e_k = x_k - x^* \). Then update \( B_k \) by the BFGS formula (3.34). Otherwise, set \( B_{k+1} = B_k \).

The dependence \( \sigma(x^*) \) is circumvented as in Biegler et al. (1995), noting that the KKT condition measure must be modified as in equation (3.44) defined in section 3.4. The main benefit of the scheme is that it allows application of the following theorem from Byrd and Nocedal (1989). Define

\[
\cos \theta_k^{BFGS} = \frac{s_k^T B_k s_k}{\| s_k \| \| B_k s_k \|} \tag{3.38}
\]
3.3 The rFSQP algorithm

**Theorem 3.1** Byrd and Nocedal (1989): Let \( \{B_k\} \) be generated by the BFGS scheme above, where for all \( k \geq 1 \), \( s_k \neq 0 \) and

\[
\frac{y_k^T s_k}{s_k^T s_k} \geq m_1 > 0 \\
\frac{\|y_k\|}{y_k^T s_k} \leq M
\]

Then there exist constants \( \beta_1, \beta_2 \) and \( \beta_3 > 0 \) such that, for any \( k \geq 1 \), the relations

\[
\cos \theta_j^{BFGS} \geq \beta_1 \\
\beta_2 \leq \frac{\|B_j s_j\|}{\|s_j\|} \leq \beta_3
\]

hold for at least \( \left\lceil \frac{k}{2} \right\rceil \) values of \( j \in [1, k] \).

Since the updates are skipped for the remaining iterates; \( B_{k+1} = B_k \), all matrices in \( \{B_k\} \) are characterized by the theorem. This theorem applies to the present update scheme since we are able to identify the correct active set at a finite index \( k_0 \), see section 3.4.3, lemma 3.11.

Since adding rows and columns will only take place a finite number of times, the condition number will be finite at index \( k_0 \). After \( k_0 \) theorem 3.1 applies directly. In practice, finite precision numerics can impair the finite conditioning, and some testing and/or restarting procedure must be implemented. The definition of good iterates follow as in Biegler et al. (1995).

3.3.4 The rFSQP algorithm

This is based on algorithm FSQP’ in Lawrence and Tits (2000) and algorithm \( \Pi \) in Biegler et al. (1995).

**Algorithm 3.1 rFSQP**

1. Choose constants \( \theta \in (0, \frac{1}{2}) \), \( \kappa \in (2, 3) \), \( \epsilon_l > 0 \), \( 0 < C_0^\mu < \tilde{C}_0^\mu \), \( \tilde{D} > 0 \), \( 0 < \tau < \tau' < 1 \), \( \Gamma > 0 \), \( \rho > 0 \), \( \gamma_{ld} > 0 \) for (3.25, 3.37), \( \gamma_{-1} < 0 \) for (3.15), \( \eta_0 > 0 \) for (3.16) and \( C_0^\mu \in \left[ C_0^\mu, \tilde{C}_0^\mu \right] \) for (3.9). Select a summable sequence of positive numbers \( \{\gamma_k^w\} \) for (3.26, 3.36). Choose a bound \( \epsilon > 0 \) for the active set identification.
Set $k = 0$ and select a starting point $x_0 \in X_I$, set the initial active set $J_0 = \{i \mid \epsilon < c^2_i(x_0) \leq 0\}$. Choose the initial penalty parameter $\nu_0$, a $(n - m) \times (n - m)$ symmetric and positive definite matrix $B_0$ and a $(n - m) \times n$ starting matrix $S_0$ for the Broyden approximation.

ii. Evaluate $f_0$, $g_0$, $c_0$ and $A_0$. Compute $Y_0$ and $Z_0$ from (3.13).

iii. Set findiff=false. Solve for the range space step $p_{Y,0}$ from (3.15).

iv. Compute an approximation $\nu_0$ by Broyden’s method (3.24,3.25)

v. Compute the damping parameter $\zeta_0 \in (0,1]$ from (3.19) and compute the tilted null-space step $p_{Z,0}$ and $\gamma_0$ from (3.17).

vi. If (3.37) is satisfied, but (3.36) is not satisfied, set findiff=true and recompute $\nu_0$ by finite differences (3.27), with $\sigma_0$ replaced by $\|\text{KKT}\|$ from (3.44). Further, recompute $\zeta_0$ from (3.19) and recompute $p_{Z,0}$ and $\gamma_0$ from (3.47).

vii. MAIN LOOP: Define the tilted SQP direction by $d_k = Y_k p_{Y,k} + Z_k p_{Z,k}$ from (3.14). If $d_k = 0$ STOP.

viii. Compute the Maratos correction term $d^C_k$ from (3.31,3.32,3.33) if it exists and satisfies $\|d^C_k\| \leq \|d_k\|$. Otherwise set $d^C_k = 0$. Set $\alpha_k = 1$.

ix. Armijo search. Test the constrained Armijo condition

\[ \phi_{\nu_k} (x_k + \alpha_k d_k + \alpha^2_k d^C_k) \leq \phi_{\nu_k} (x_k) + \theta \alpha_k D \phi_{\nu_k} (x_k, d_k) \]
\[ \text{s.t. } c^2_i(x_k + \alpha_k d_k + \alpha^2_k d^C_k) \leq 0, \; i = 1, \ldots, p_2 \]  

(3.40)

x. If (3.40) is not satisfied, choose a new $\alpha_k \in [\tau \alpha_k, \tau' \alpha_k]$ and go to step (ix), otherwise set $x_{k+1} = x_k + \alpha_k d_k + \alpha^2_k d^C_k$, and define $J^c_{k+1} = \{i \mid \epsilon < c^2_i(x_{k+1}) \leq 0\}$ from the last evaluation of $c_I$ in (3.40).

xi. Evaluate $f_{k+1}$, $g_{k+1}$, $c_{k+1}$ and $A_{k+1}$. Compute $Y_{k+1}$ and $Z_{k+1}$ from (3.13).

xii. Compute the Lagrange multiplier estimates from (3.18) for $i \in J^c_{k+1}$, set $\lambda^c_{I,k+1} = 0$ for $i \notin J^c_{k+1}$. Update the weight $\nu_{k+1}$ of the merit function from (3.20).

xiii. Update $S_{k+1}$ from (3.22, 3.23). If findiff=false, calculate $\bar{\nu}_k$ by Broyden’s method (3.24, 3.26), otherwise calculate $\bar{\nu}_k$ by finite differences (3.27).
xiv. Compute $s_k$ and $y_k$ from (3.35). If $s_k^T y_k \leq 0$ or if [findiff=true and (3.37) is not satisfied] or if [findiff=false and (3.36) is not satisfied] set $B_{k+1} = B_k$. Otherwise compute $B_{k+1}$ by the BFGS update scheme in section 3.3.3.

xv. Set findiff=false. Compute $p_k^E$ from (3.29). Compute an approximation $w_{k+1}$ by Broyden’s method (3.24,3.25), and $\zeta_{k+1} \in (0,1]$ from (3.19). Compute $p_k^Z$ from (3.30).

xvi. If (3.37) is satisfied, but (3.36) is not satisfied, set findiff=true and recompute $w_{k+1}$ by finite differences (3.27), with $\sigma_{k+1}$ replaced by $||KKT||$ from (3.44). Further, recompute $\zeta_{k+1}$ from (3.19) and recompute $p_k^Z$ from (3.30).

xvii. Select $C_{k+1}^n \in [C_n^q, \bar{C}_n^q]$.

If ($\|d_k\| < \epsilon_l$) then, compute $d_{k+1}^E$ from (3.28). Then

if $\|d_{k+1}^E\| \leq \bar{D}$ then set $\eta_{k+1} = C_{k+1}^n \|d_{k+1}^E\|^2$
else set $\eta_{k+1} = C_{k+1}^n \|d_k\|^2$

else set $\eta_{k+1} = C_{k+1}^n \|d_k\|^2$

xviii. Compute $p_{Z,k+1}$ from (3.15). Compute $p_{Z,k+1}$ and $\gamma_{k+1}$ from (3.17) with $w_{k+1}$ and $\zeta_{k+1}$ computed in step (xv, xvi). If findiff=false and if (3.37) is satisfied, but (3.36) is not satisfied, set findiff=true and recompute $w_{k+1}$ by finite differences (3.27), with $\sigma_{k+1}$ replaced by $||KKT||$ from (3.44). Further, recompute $\zeta_{k+1}$ from (3.19) and recompute $p_{Z,k+1}$ and $\gamma_{k+1}$ from (3.17) with the new $w_{k+1}$.

xix. Set $k \leftarrow k + 1$ and go to step (vi)

### 3.4 Global and local convergence

This section is based on Lawrence and Tits (2000) and Biegler et al. (1995). The first subsection summarizes KKT conditions. Subsection 3.4.2 and 3.4.3 are concerned with global convergence, i.e. that the algorithm will converge from any starting point $x_0 \in X_I$, and local convergence, i.e. the convergence rate when initialized within a sufficiently small neighborhood of a local minimizer $x^*$. Global convergence is based on descent, while local convergence is based on Newton’s method.

Previous work on inequality constrained reduced Hessian SQP methods include Coleman and Conn (1982b), (1982a), and Fletcher and co-workers,
see Fletcher (1987), p. 317. In particular Byrd and Nocedal (1991) and Biegler et al. (1995) only consider equality constraints, while SNOPT by Gill et al. (1997) includes nonlinear inequality constraints. The convergence properties of SNOPT are similar to the properties of NPSOL addressed in Gill, Murray, Saunders, and Wright (1992).

The local convergence analysis in section 3.4.3 is based on Biegler et al. (1995). I.e. by proving that the optimal active set is identified, i.e. $J_k^* = J^{*,e}$ for all $k$ sufficiently large. A complicating factor is the updating rule for the reduced Hessian $Z_k^T W_k Z_k$ with varying dimension of $Z_k$, see section 3.3.3. Still, our main focus remains on feasibility mechanisms and not on approximations to the reduced Hessian. Changes in the active set might be handled if we accept refactorization of the null-space matrix $Z_k$ of the working set matrix $A_k$ ($\neq A_{k-1}$) at each major iteration. The effort needed for this can be reduced by application of LUSOL, see Gill et al. (1997), Gill et al. (1987) for further comments. In the present algorithm the choice of the parameter $\epsilon$ in equation (3.5) has significant influence on the practical performance. Choosing a large value for $\epsilon$ causes the algorithm to stay well away from inequalities, hence refactorizations are less frequent than what could be anticipated. On the other hand, a large $\epsilon$ value causes the algorithm to approach inequalities conservatively. Large $\epsilon$-values therefore seem to give the algorithm a practical behavior more related to interior methods than to conventional SQP methods.

Observe that eliminating variables, by considering the equality constraints only, cannot lead to superlinear convergence, since the Hessian of the Lagrangian

$$\nabla^2 \mathcal{L} = \nabla^2 f(x^*) + \sum_{i=1}^{p_1} \lambda_i^* \nabla^2 c_i^*(x^*) + \sum_{i \in J^{*,e}} \lambda_i^* \nabla^2 c_i^*(x^*) \quad (3.41)$$

also depends on the active inequality constraints (note the influence of strict complementary slackness, assumption 3.4). Superlinear convergence can only be achieved if the reduced Hessian approximation scheme $B_k$ converges to the projection of $\nabla^2 \mathcal{L}^*$ in the tangent space of active constraints at $x^*$.

Define the projection onto the tangent space of equality constraints and active inequality constraints by

$$\mathcal{P}(x_k) = I - A(x_k) \left( A(x_k)^T A(x_k) \right)^{-1} A(x_k)^T$$

The corresponding projection onto the range space of $A(x_k)$ is written

$$\mathcal{Q}(x_k) = I - \mathcal{P}(x_k)$$
Denote \( P(x_k) = P_k \) and \( Q(x_k) = Q_k \). From Boggs and Tolle (1995), theorem 3.5, two-step superlinear convergence of \( x_k \to x^* \) requires

\[
limit_{k \to \infty} \frac{\| P_k \left( W_k - \nabla^2 L^* \right) P_k (x_{k+1} - x_k) \|}{\| x_{k+1} - x_k \|} = 0
\]

with superlinear convergence occurring for tangential convergence, i.e. if

\[
limit_{k \to \infty} \frac{Q_k (x_{k+1} - x_k)}{\| x_{k+1} - x_k \|} = 0
\]

i.e. if there are active inequality constraints at \( x^* \) we will not be able to achieve superlinear two-step convergence by excluding inequality constraints in the matrix \( A(x_k) \). In addition, the conditions for theorem 3.5 in Boggs and Tolle (1995) in the reduced Hessian case requires that the null-space matrices \( Z_k \) are smooth, i.e. that

\[
\| Z(x_k) - Z(x^*) \| = \mathcal{O}(\| x_k - x^* \|)
\]  

(3.42)

We prove in the following that for \( k \) large enough that \( J_k^* = J_{k+1}^* \), hence (3.42) can be achieved near the solution \( x^* \) by using the QR-factorization or updating the factors of this, see Nocedal and Wright (1999), p. 567, for further comments. Alternative implementations from Biegler et al. (2000) and Xie and Byrd (1999) for the decomposition (3.13) below have not been shown to satisfy (3.42). Note that close to the solution refactorization is rarely needed once the optimal active set has been identified. Hence, this may not be an important issue in practice.

### 3.4.1 KKT conditions

The KKT-conditions of the original NLP (3.1) are

\[
g(x^*) + \sum_{i=1}^{p_1} \lambda^{s,i}_c \nabla c^i_c(x^*) + \sum_{i=1}^{p_2} \lambda^{s,i}_T \nabla c^i_T(x^*) = 0
\]

\[
c^i_c(x^*) = 0, \quad i = \{1, \ldots, p_1\}
\]

\[
c^i_T(x^*) \leq 0, \quad i = \{1, \ldots, p_2\}
\]

\[
\lambda^{s,i}_c \geq 0, \quad i = \{1, \ldots, p_2\}
\]

A measure of the error \( \sigma_k = \max \{ \| \epsilon_k \|, \| \epsilon_{k+1} \| \} \), \( \epsilon_k = x_k - x^* \) used in equation (3.37) must be specified without knowledge of \( x^* \) to be practical. Denote the pseudo-inverse of \( Z^T \) as \( Z^+T \), then \( Z^+T Z^T = I \). The first line of the KKT conditions (3.43) is restated as

\[
Z^+T Z^T (g_s + A_s \lambda_s) = Z^+T Z^T g_s = 0
\]
implying $Z_k^T g_k = 0$. Then a distance measure of (3.43) can be stated as

$$\| K T \| \triangleq \| Z_k^T g_k \| + \| c_{\mathcal{E},k} \| + \| \lambda_{\mathcal{I},k} c_{\mathcal{I},k} \| + \| \max \{ 0, c_{\mathcal{I},k} \} \| + \| \min \{ 0, \lambda_{\mathcal{I},k} \} \|$$  \hspace{1cm} (3.44)

We need to establish the relationship between the SQP direction $d_k^0$ from (3.3) and the feasible direction $d_k = Y_{P_k} + Z_{P_k}$ from (3.15, 3.47), when implemented as a reduced gradient method. It is well known that when $W_k$ is positive definite and $X \neq \emptyset$ that $d_k^0$ (unique due to convexity) is a KKT point for (3.3) iff $\exists (\lambda_{\mathcal{E},k}^0, \lambda_{\mathcal{I},k}^0)$ such that

$$W_k d_k^0 + g_k + \sum_{i=1}^{p_1} \lambda_{\mathcal{E},k}^{0,i} \nabla c_{\mathcal{E},i}(x_k) + \sum_{i=1}^{p_2} \lambda_{\mathcal{I},k}^{0,i} \nabla c_{\mathcal{I},i}(x_k) = 0$$

$$c_{\mathcal{E},i}(x_k) + \left\langle \nabla c_{\mathcal{E},i}^T, d_k^0 \right\rangle = 0, \quad i = \{1, \ldots, p_1\}$$

$$c_{\mathcal{I},i}(x_k) + \left\langle \nabla c_{\mathcal{I},i}^T, d_k^0 \right\rangle \leq 0, \quad i = \{1, \ldots, p_2\}$$

$$\lambda_{\mathcal{I},k}^{0,i} \left( c_{\mathcal{I},i}^T(x_k) + \left\langle \nabla c_{\mathcal{I},i}^T, d_k^0 \right\rangle \right) = 0 \quad \text{and} \quad \lambda_{\mathcal{I},k}^{0,i} \geq 0, \quad i = \{1, \ldots, p_2\}$$  \hspace{1cm} (3.45)

The KKT-conditions for the reduced gradient problem in Biegler et al. (1995) subject to inequality constraints and treated as an EQP are

$$Z_k^T W_k Z_k p_{Z,k}^0 + (Z_k^T g_k + \zeta_k w_k) = 0$$  \hspace{1cm} (3.46)

The $p_{Z,k}$ and $\gamma_k$ relations in (3.17) are motivated by considering the following reduced qp

$$\min_{p_{Z,k}, \gamma_k} \frac{1}{2} \langle p_{Z,k}, B_k p_{Z,k} \rangle + \gamma_k$$

$$s.t. \quad (Z_k^T g_k + \zeta_k w_k, p_{Z,k}) \leq \gamma_k$$  \hspace{1cm} (3.47)

The KKT-conditions for this are

$$Z_k^T W_k Z_k p_{Z,k} + \mu_k (Z_k^T g_k + \zeta_k w_k) = 0$$

$$\mu_k = 1$$

$$\langle Z_k^T g_k + \zeta_k w_k, p_{Z,k} \rangle \leq \gamma_k$$

$$\mu_k \left( (Z_k^T g_k + \zeta_k w_k, p_{Z,k}) - \gamma_k \right) = 0 \quad \text{and} \quad \mu_k \geq 0$$  \hspace{1cm} (3.48)

These conditions are always consistent since $(p_{Z,k}, \gamma_k) = (0, 0)$ satisfies the constraints, and always gives a unique solution due to convexity, see lemma 3.1 below. This guarantees the existence of the associated qp-multiplier $\mu_k$. Assuming $Z_k^T W_k Z_k$ positive definite, bounded $\mu_k$, and assumption 3.2, $p_{Z,k}$ and $\gamma_k$ can be computed from (3.17) directly with $Z_k^T W_k Z_k = B_k$. 

3.4.2 Global convergence

It is established in the following that a sequence \( \{x_k\} \) generated by the algorithm has accumulation points that are KKT points of the original NLP. We start with some modifications of some of the lemmas in Lawrence and Tits (2000) to incorporate the equality constraints, range-null space decomposition and reduced Hessian. These lemmas state that solving the problem (3.15, 3.47) resemble solving the original NLP with \( x_k \in X_I \ \forall k \) and \( x^* \in X \). Note that most of the results in the following represent minor modifications to the results in Lawrence and Tits (2000), but that the multipliers are handled differently since we use the estimate (3.18) and not the qp-multipliers.

We maintain the same structure as in Lawrence and Tits (2000) to facilitate comparison.

Assume in the sequel a positive definite and bounded reduced Hessian approximation \( B_k = Z_k^T W_k Z_k \);

**Assumption 3.5** \( K_1 \| p_{Z,k} \|^2 \leq \langle p_{Z,k}, B_k p_{Z,k} \rangle \leq K_2 \| p_{Z,k} \|^2, \ \forall p_{Z,k} \in \mathbb{R}^{(n-m)}, K_1 \) and \( K_2 \) strictly positive.

This assumption is introduced for ease of exposition, since it is satisfied for the BFGS update rule we use, see discussion in section 3.3.3 in conjunction with theorem 5.6 in Biegler et al. (1995).

**Assumption 3.6** Assume that there exists positive constants \( \gamma_a \) and \( \beta_0 \) such that

\[
\left\| Y(x_k) \left( A^T(x_k) Y(x_k) \right)^{-1} \right\| \leq \gamma_a, \quad \| Z(x_k) \| \leq \beta_0
\]

for all \( x_k \in X_I \). This implies \( \| Y_k p Y_k \| \leq \gamma_a \| c_k \| \). Assume also that (3.39) holds for all \( k \geq 1 \) when \( B_k \) is updated, and that there exist a constant \( \kappa_c > 0 \) such that for all \( k \)

\[
\| w_k \| \leq \kappa_c \| c_k \|^{1/2}
\]

This is satisfied for both finite differences and Broyden updating, see Biegler et al. (1995), section 4, for a discussion. Note that assumption 3.6 is related to assumption 3.3 (LICQ) since \( A_k^T Y_k \) must have linearly independent columns to be invertible. The implementation of rFSQP handles this by using a feature of the LU-decomposition routine MA28AD. I.e. linearly dependent rows are included into the null-space which guarantees full rank of \( A_k^T Y_k \).
Lemma 3.1 Suppose assumptions 3.1-3.6 hold. Then, since $B_k$ is symmetric positive definite, if $x_k \in X_I$, then $p_{Z,k}$ is well-defined and $(p_{Z,k}, \gamma_k)$ is the unique KKT point of (3.47). Furthermore, $p_{Z,k}$ is bounded over compact subsets of $X_I \times \mathcal{P} \times \mathbb{R}^+$, where $\mathcal{P}$ is the set of symmetric positive definite $n - m_k \times n - m_k$ matrices and $\mathbb{R}^+$ the set of nonnegative reals. In addition $d_k = Y_k p_{V,k} + Z_k p_{Z,k}$ exists and is unique and bounded over $X_I \times \mathcal{R} \times \mathcal{P} \times \mathbb{R}^+$ where $\mathcal{R}$ is the set of nonsingular $m_k \times m_k$ matrices defined by $A_k^T Y_k$ and the decomposition of $A_k$ in (3.13).

Proof: Observe that $(p_{Z,k}, \gamma_k) = (0,0)$ always satisfies the inequality constraint of (3.47). Boundedness of $p_{Z,k}$ and $\gamma_k$ is a consequence of the Frank-Wolfe theorem (Frank and Wolfe 1956), (Perold 1980) and assumption 5: "Every quadratic program whose objective function is bounded below on the feasible set has a finite global minimizer." Uniqueness follows from assumption 3.5 (convexity). I.e. $(p_{Z,k}, \gamma_k)$ is well-defined. By theorem 6 in Fiacco and McCormick (1990) the solution is continuous. The multiplier $\mu_k$ is obviously bounded. Due to non-singularity of $(A_k^T Y_k)$ the range-space step $p_{V,k}$ is well-defined, unique, continous and bounded for all bounded $c_k$ which are bounded on the compact the set $X_I$ by assumption 3.2. Then $d_k = Y_k p_{V,k} + Z_k p_{Z,k}$ exists and is continous, unique and bounded as well. \(\square\)

This extends lemma 1 of Lawrence and Tits (2000) to include equality constraints, partitioning of $d_k$ in (3.14) and the reduced Hessian $B_k$ and establishes existence, uniqueness, continuity and boundedness of $d_k = Y_k p_{V,k} + Z_k p_{Z,k}$. The lemma characterizes the solution of the problem (3.47), which is utilized to characterize the solution of (3.17) in lemma 3.2.

Lemma 3.2 Suppose assumptions 3.1-3.6 hold. Then, given $B_k$ symmetric positive definite and $\eta_k \geq 0$

1) $\gamma_k \leq 0 \forall x_k \in X_I$. Moreover, $\gamma_k = 0$ iff $p_{Z,k} = 0$

2) $d_k = Y_k p_{V,k} + Z_k p_{Z,k} = 0$ iff $x_k$ is a KKT point for the NLP (3.1), where $\gamma_k$ and $p_{Z,k}$ are defined by equation (3.47), $p_{V,k}$ is defined by (3.15) and $d_k$ by (3.14).

Proof: To prove i) observe that since $(p_{Z,k}, \gamma_k) = (0,0)$ is always feasible for (3.47) the optimal value is non-positive. Since $B_k$ is positive definite we have $(p_{Z,k}, B_k p_{Z,k}) \geq 0$, i.e. $\gamma_k \leq 0$. If $p_{Z,k} = 0$ the inequality of (3.47) gives $\gamma_k = 0$ by squeezing. Finally suppose $\gamma_k = 0$, then for $x_k \in X_I$, $B_k \succeq 0$ we observe that since $p_{Z,k} = 0$ is feasible it is also optimal due to the
3.4 Global and local convergence

non-negativeness of the objective. Convexity gives uniqueness of \( p_{Z,k} = 0 \). To prove \( ii) \) suppose that \( d_k = 0 \), from (3.14) this solution is satisfied by choosing \( Y_k p_{\gamma,k} = -Z_k p_{Z,k} \). In detail, (3.13) gives

\[
\begin{bmatrix}
I \\
0
\end{bmatrix} p_{\gamma,k} = -
\begin{bmatrix}
-C^{-1}_k N_k \\
I
\end{bmatrix} p_{Z,k}
\]

The last \( n - m_k \) rows implies \( p_{Z,k} = 0 \), which inserted in the first \( m_k \) rows implies \( p_{\gamma,k} = 0 \). We have

\[ d_k = 0 \iff (p_{\gamma,k}, p_{Z,k}) = (0, 0) \] (3.51)

If \( A_k \) is factorized by QR-factorization the relation (3.51) follows from the direct sum \( \text{span}(A_k) = \mathcal{R}(A_k^T) \oplus \mathcal{N}(A_k) \). When \( (p_{\gamma,k}, p_{Z,k}, \gamma_k) = (0, 0, 0) \) then by (3.48) there exist a scalar multiplier \( \mu_k \geq 0 \) such that

\[
\mu_k \left( Z_k^T g_k + \zeta_k w_k \right) = 0 \quad \mu_k = 1
\] (3.52)

Thus, since by the selection in step (x) of algorithm rFSQP \( c^i_k(x_k) = 0 \) \( \forall i \in J^*_k \), the last line of the optimality conditions (3.52) become \( \lambda^T_{i,k} c_i(x_k) = 0 \) since \( \lambda_k \)’s estimated by (3.18) are bounded, and we choose \( \lambda^T_{i,k} = 0 \), \( \forall i \notin J^*_k \). Also \( p_{\gamma,k} = 0 \) implies \( w_k = 0 \) if either Broyden’s method or finite differences is used. The first line of (3.52) then becomes \( Z_k^T g_k = 0 \). We have

\[ \| Z_k^T g_k \| = \| Z_k^T (g_k + A_k \lambda_k) \| = 0 \] Hence, the KKT-conditions (3.43) are satisfied by following the derivation of (3.44). To prove the converse part of \( ii) \) note that if \( x_k \) is a KKT point for the NLP, then the NLP’s KKT-conditions (3.43) and (3.48) show that \( (p_{\gamma,k}, p_{Z,k}, \gamma_k) = (0, 0, 0) \) is a KKT point of the reduced gradient problem. Assumption 3.3 implies uniqueness of \( \lambda^* \). □

This adapts lemma 2 of Lawrence and Tits (2000) to our setting. The lemma is concerned with problem (3.47). We observe that the KKT-conditions (3.48) imply (3.17), hence statements about the solution to (3.47), are equally valid for \( p_{Z,k} \) and \( \gamma_k \) computed by (3.17).

The next two lemmas establish that the line search is well defined.

**Lemma 3.3** Suppose assumptions 3.1-3.6 hold. Suppose \( x_k \in X_k \) is not a KKT point for the NLP, \( B_k \) is symmetric positive definite and \( \eta_k > 0 \). Then

\begin{enumerate}
  \item[i)] \( D\phi_h(x_k, d_k) < 0 \), and
  \item[ii)] \( \langle \nabla c^i_T(x_k), d_k \rangle < 0 \), for all \( i \in J^*_k \)
\end{enumerate}
iii) \( \phi_{\nu}(x_j) - \phi_{\nu}(x_{j+1}) \geq \gamma_{\nu} \left[ \left\| Z_j^T g_j \right\|^2 + \|c_j\|_1 \right] \) for the good iterates \( j \) and constant \( \nu_j \) in (3.11).

This lemma is modeled after section 3.4 and lemma 4.1 of Biegler et al. (1995), and replaces lemma 3 in Lawrence and Tits (2000). The proof is almost identical to the proof in Biegler et al. (1995), and is given in appendix B for completeness. Item iii) guarantees the existence of a non-zero steplength for non-stationary points. The use of Taylor’s theorem for the continuous non-differentiable merit function locally is justified by observing that existence of the directional derivative in a point implies existence in a small "neighbourhood" in the relevant direction of the point by continuity. This is also assumed implicitly in Biegler et al. (1995). A related alternative to this is to apply the mean-value theorem locally. The lemma allows direct application of theorem 4.2 in Biegler et al. (1995).

From the proof in appendix B we get the usual update rule for the penalty parameter \( \nu_k \)

\[
\nu_k = \begin{cases} 
\nu_{k-1} & \text{if } \nu_{k-1} \geq \|\lambda_k\|_\infty + 2\rho \\
\lambda_k\|_\infty + 3\rho & \text{otherwise}
\end{cases}
\]  

(3.53)

The update-rule for \( \hat{\zeta}_k \) follows by choosing \( \zeta_k = \min \{1, \hat{\zeta}_k\} \) where \( \hat{\zeta}_k \) is defined by solving equation (B.4) with equality.

**Lemma 3.4** Suppose assumptions 3.1-3.6 hold. Then, if \( \eta_k = 0 \), \( x_k \) is a KKT point for the MILP (3.1) and the algorithm will stop in step (vii) at iteration \( k \). On the other hand, whenever the algorithm does not stop in step (vii), the line search is well defined, i.e. step (ix) is satisfied for a step \( \alpha_{k_j} > 0 \) for some finite \( k_j \).

**Proof:** Suppose that \( \eta_k = 0 \). Then \( k > 0 \) and by step (xviii), either \( d_k^E = 0 \), or \( d_{k-1} = 0 \). The latter cannot hold due to step (vii). If \( d_k^E = 0 \) equation (3.30) with \( (p_{Y,k}, p_{Z,k}^E) = (0,0) \) implies \( \|Z_k^T g_k\| = 0 \). Lemma 3.3 iii) gives feasibility of \( c_k^E(x_k) \). For all \( i \in J_k^E \) we have \( c_k^E(x_k) = 0 \), and for \( i \notin J_k^E \) we are free to choose \( \lambda_{k,i}^E = 0 \), hence \( \lambda_{k,i}^E c_k^E(x_k) = 0 \). We have \( c_k^E(x_k) = 0 \) from (3.29) whenever \( p_{Y,k}^E = 0 \). Since the KKT measure (3.44) is zero we have that \( x_k \) is a KKT point for the NLP with multipliers \( \lambda^{*,i} \) from (3.18) for \( i \in J_k^E \) and \( \lambda^{*,i} = 0 \) for \( i \notin J_k^E \). By lemma 3.2 item iii) \( d_{k+1} = 0 \) and the algorithm will stop in step (vii). The first claim is proved. Also, we have established that \( \eta_k > 0 \) whenever step (ix) is reached. Lemma 3.3 (descent and feasibility) and assumption 3.2 (continuity) gives the second claim. \( \square \)
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This is equivalent to lemma 4 in Lawrence and Tits (2000). Lemma 3.3 and 3.4 show that the algorithm is well defined, Lemma 3.2 shows that if the algorithm generates a finite sequence terminating at a point $x_N$, then $x_N$ is a KKT point for the NLP (3.1). We now turn to consider infinite sequences $\{x_k\}$, i.e. that $\eta_k > 0$ for all $k$ by lemma 3.4.

**Lemma 3.5** Suppose assumptions 3.1-3.6 hold. Then the sequence $\{\eta_k\}$ generated by algorithm rFSQP is bounded. Further, the sequence $\{d_k\}$ is bounded on subsequences on which $\{x_k\}$ is bounded.

**Proof:** The first claim follows from step (xvii) of algorithm rFSQP. When $\eta_k$ is bounded, so is $d_k$ by lemma 3.1 under assumption 3.5 on compact subsets $X_I \times R \times R^+$. □

This is lemma 5 of Lawrence and Tits (2000), and neither the lemma nor the proof is affected by the reduced gradient approach. We restate proof since it is very short.

**Lemma 3.6** Suppose assumptions 3.1-3.6 hold. Suppose $\mathcal{K}$ is an infinite index set such that $x_k \xrightarrow{k \in \mathcal{K}} x^* \in X$, $\{\eta_k\}$ is bounded on $\mathcal{K}$, and $d_k \xrightarrow{k \in \mathcal{K}} 0$. Then $J_k^e \subseteq J^{*e}$, for all $k \in \mathcal{K}$, $k$ sufficiently large and the multiplier sequence $\{\lambda_k\}$ is bounded on $\mathcal{K}$. Further, given any accumulation point $\eta^* \geq 0$ of $\{\eta_k\}_{k \in \mathcal{K}'}$, $(0, 0)$ is the unique solution of (3.17) when $p_{y, k} = 0$.

**Proof:** From (3.51) $p_{y, k} \xrightarrow{k \in \mathcal{K}} 0$, $p_{z, k} \xrightarrow{k \in \mathcal{K}} 0$. We have $\gamma_k \xrightarrow{k \in \mathcal{K}} 0$ by squeezing in (3.17). Arguing as in Lawrence and Tits (2000) we have for an $i' \notin J^{*e}$ and a $\delta_{i'} > 0$ that

$$c^{i'}_R(x_k) + \left< Y_k^T \nabla c^{i'}_{L,k}, p_{y,k} \right> - \gamma_{k-1} \eta_k \leq -\frac{\delta_{i'}}{2} < 0$$

i.e. $i' \notin J^e_k$ for all $k \in \mathcal{K}$ and $k$ sufficiently large, hence $J^e_k \subseteq J^{*e}$ is proved. Boundedness of $\{\lambda_k\}$ follows from (3.18). The third claim follows by taking limits in (3.17) with $p_{y, k} = 0$ proving that $(0, 0)$ is the unique solution. □

This is equivalent to lemma 6 of Lawrence and Tits (2000).

**Lemma 3.7** Suppose assumptions 3.1-3.6 hold. Then, if $\mathcal{K}$ is an infinite index set such that $d_k \xrightarrow{k \in \mathcal{K}} 0$, all accumulation points of $\{x_k\}_{k \in \mathcal{K}}$ are KKT points for the NLP (3.1).

**Proof:** Suppose $\mathcal{K}' \subseteq \mathcal{K}$ is an infinite index set on which $x_k \xrightarrow{k \in \mathcal{K}'} x^* \in X$. In view of assumption 3.5 and lemma 3.5, assume, without loss of generality
that $B_k^{-1} \eta_k \rightarrow Z^* W^* Z^*$, a positive definite matrix, and $\eta_k \rightarrow \eta^*$ \geq 0$. In view of lemma 3.6, $(p_{\nu,k}, p_{Z,k}, \gamma_k) = (0,0,0)$ is the unique solution to (3.15, 3.47), which is a KKT point satisfying $\|KKT\| = 0$ in (3.44) by lemma 3.2. □

This is equivalent to lemma 7 of Lawrence and Tits (2000). The proof is unaltered and follows from lemma 3.2 and 3.6 herein. Note that requiring $B_k^{-1} \eta_k \rightarrow Z^* W^* Z^*$ is less strict than requiring $W_k^{-1} \eta_k \rightarrow W^*$.

**Theorem 3.2** Under assumptions 3.1-3.6, algorithm rFSQP generates a sequence $\{x_k\}$ for which all accumulation points are KKT points for the NLP (3.1).

**Proof:** Suppose $K$ is an infinite index set on which $x_{k} \rightarrow x^*$. In view of lemma 3.5 and assumption 3.5 we may assume without loss of generality that $d_k \rightarrow 0$, $\eta_k \rightarrow \eta^* \geq 0$ and $B_k^{-1} \eta_k \rightarrow Z^* W^* Z^*$. If $\eta^* = 0$ step (xvii) of algorithm rFSQP implies the existence of an infinite index set $K' \subseteq K$ such that either $d_k \rightarrow 0$ for all $k \in K'$, or $d_{k-1} \rightarrow 0$. If $d_{k-1} \rightarrow 0$, $x_{k-1} \rightarrow x^*$, since $|x_k - x_{k-1}| \leq 2 |d_{k-1} \rightarrow 0$. Lemma 3.7 implies that $x^*$ is a KKT point. When $d_k \rightarrow 0$ from step (xvii) and $J_k \subseteq J^x$ for all $k \in K'$ from lemma 3.6. Boundedness of $\{\lambda^E_k\}$ follows since we are free to choose them as the estimates (3.18). Taking limits in (3.29, 3.30) we conclude from $\|Z_k^T \eta_k\| \rightarrow 0$, $|c_k| \rightarrow 0$ and (3.44), that $x^*$ is a KKT point for the NLP.

For $\eta^* > 0$ lemma 3.3 applies and the claim follows from theorem 4.2 in Biegler et al. (1995). I.e. bounded $\{\|\lambda_k\|\}_{k \in K}$ implies that there exist a $k_0$ such that $\nu_k$ is constant for $k > k_0$ by the update rule (3.53). Consider $k > k_0$ and using lemma 3.3 iii)

$$\phi_\nu(x_{k_0}) - \phi_\nu(x_{k+1}) = \sum_{j=k_0}^{k} (\phi_\nu(x_j) - \phi_\nu(x_{j+1})) \geq \gamma_\nu \sum_{j \in J \cap [k_0,k]} \left[ \|Z_j^T \eta_j\|^2 + |c_j| \right]$$

where $J$ is the set of good iterates as defined by Biegler et al. (1995). By descent from lemma 3.3 i) and assumption 3.2 $\nu_k$ is bounded below and the sum is finite. The multiplier estimate (3.18) at $x^*$ and assumption 3.3 implies $\|KKT\| = 0$ in (3.44). □

This is equivalent to theorem 1 of Lawrence and Tits (2000), and the first part concerning the case $\eta^* = 0$ is restated for the sake of completeness.
3.4.3 Local convergence

The local convergence section in Lawrence and Tits (2000) is mainly concerned with restating global convergence under stronger 2nd order conditions, and proving that the FSQP direction $d_k^2 + d_k^p$ converges to the SQP direction $d_k^0$. Once this is established a step-length of 1 is accepted locally and 2-step superlinear convergence follows by a standard result. On the other hand, the local convergence analysis of Biegler et al. (1995) is mainly concerned with establishing 1-step superlinear convergence. This is possible due to the approximation terms $w_k$ and $\tilde{w}_k$, and a detailed order analysis. Note that the Maratos correction term $d_k^0$ in FSQP does not handle the Maratos effect for the $l_1$-merit function used in the present algorithm. As in Biegler et al. (1995) we implement a standard watch-dog strategy to handle the Maratos effect, and prove in proposition 3.1 that the constraint in (3.40) does not prevent a step-size of one to be accepted for a large enough $k$.

The regularity assumptions are strengthened:

**Assumption 3.7** The functions $f, c^i_E, c^i_T : \mathbb{R}^n \to \mathbb{R}$, for all $i$ are three times continuously differentiable on $X_I$, and their Hessians are Lipschitz continuous in a neighborhood of $x^*.$

**Definition 3.1** A point $x^*$ satisfies second order sufficiency conditions with strict complementary slackness for the MLP (3.1) if there exist a multiplier vector $\lambda^* \in \mathbb{R}^{n + w}$ such that:

- The pair $(x^*, \lambda^*)$ satisfies (3.43), i.e. $x^*$ is a KKT point for the MLP (3.1).
- $\lambda^{*,i} > 0 \ \forall i \in J^{*,e}$
- $Z_k^T \nabla^2_{xx} \mathcal{L}(x^*, \lambda^*) Z_k$ is positive definite on the subspace

$$\{ \nabla c^i_E(x^*) \mid \forall i \in \{1, \ldots, p_1\} \} \cup \{ \nabla c^i_T(x) \mid i \in J^{*,e} \}$$

In section 3.4.2, we proved that every accumulation point of $\{x_k\}$ is a KKT point of the MLP (3.1). We define the reduced Hessian of the Lagrangian function

$$G_k = Z_k^T \nabla^2_{xx} \mathcal{L}(x_k, \lambda_k) Z_k$$

To prove that the sequence $\{x_k\}$ converges to a KKT point $x^*$, we need the following assumptions.

**Assumption 3.8** The sequence $\{x_k\}$ has an accumulation point $x^*$ which satisfies the second order sufficiency conditions with strict complementary slackness.
**Assumption 3.9** Biegler et al. (1995) (assumption 5.1): The point \( x^* \) is a local minimizer for the NLP (3.1), at which the following conditions hold:

i) For all \( q \in \mathbb{R}^{m-m} \), \( q \neq 0 \), we have \( q^T G^* q > 0 \).

ii) There exist constants \( \gamma_0 \), \( \beta_0 \) and \( \gamma_c \) such that, for all \( x_k \) in a neighborhood of \( x^* \),

\[
\begin{align*}
\| Y(x_k) \left[ A(x_k)^T Y(x_k) \right]^{-1} \| & \leq \gamma_a \\
\| Z(x_k) \| & \leq \beta_0 \\
\left\| \left[ Y(x_k) Z(x_k) \right]^{-1} \right\| & \leq \gamma_c
\end{align*}
\]

(see assumption 3.6 as well)

iii) \( Z(x_k) \) and \( \lambda(x_k) \) are Lipschitz continuous in a neighborhood of \( x^* \), i.e. there exist constants \( \gamma_\lambda \) and \( \gamma_Z \) such that

\[
\begin{align*}
\| \lambda(x) - \lambda(z) \| & \leq \gamma_\lambda \| x - z \| \\
\| Z(x) - Z(z) \| & \leq \gamma_Z \| x - z \|
\end{align*}
\]

for all \( x, z \) near \( x^* \).

Item numbers i)-iii) follow item numbers iii)-v) in Biegler et al. (1995). Assumption 3.9 v) requires that we are able to identify the correct active set \( J^{*c} \) for a finite \( k_0 \). Then, for a \( k_1 \geq k_0 \), for all \( k \geq k_1 \) the assumption requires that any possible refactorization of \( A(x_k) \) will result in a continuous \( Z(x_k) \). This assumption can be satisfied if no further factorizations are needed for all \( k \geq k_1 \). This holds locally by continuity, i.e. a finite condition number of \( A(x^*) \) will give a finite condition number of \( A^T_k \bar{Y}_k \) in a neighborhood of \( x^* \). Then there is no need to refactorize \( A(x_k) \). If the algorithm is implemented with refactorization at each iteration, the assumption is violated unless QR-factorizations are employed.

**Assumption 3.10** Biegler et al. (1995) (assumption 5.2): The line search has the property that, for all large \( k \), \( \phi_\vartheta((1 - \vartheta)x_k - \vartheta x_{k+1}) \leq \phi_\vartheta(x_k) \) for all \( \vartheta \in [0, 1] \). In other words, \( x_{k+1} \) is in the connected component of the level set \( \{ x \mid \phi_\vartheta(x) \leq \phi_\vartheta(x_k) \} \) that contains \( x_k \).

As in Biegler et al. (1995) assumption 3.10 is only likely to hold locally with practical line search methods. The presence of inequalities does not influence on assumption 3.10 since we are always feasible with respect to them in algorithm \texttt{rFSQP}. Thus assumption 3.10 applies for all \( k \geq k_1 \), and we can assume that lemma 4.1 and 4.2 of Byrd and Nocedal (1991) (lemma 4.1 in Xie and Byrd (1999)) hold in the level sets defined by assumption 3.10.
Lemma 3.8 Suppose assumptions 3.1 and 3.3-3.10 hold. Then the entire sequence generated by algorithm rFSQP converges to a point \( x^* \) satisfying definition 3.1.

Proof: Note that points \( x^* \) satisfying definition 3.1 are isolated by theorem 2.1 in Robinson (1974) under assumption 3.3. I.e., there exists a ball \( B(x^*, \varepsilon) \) containing \( x^* \) in its interior as the only KKT point. From assumption 3.8 the sequence has such an accumulation point \( x^* \). By descent from lemma 3.3 i) and assumption 3.7 \( \phi_k \) is bounded below, then we have that the sequence \( \{ \phi_k \} \) is bounded below. By the Armijo condition (3.40) we have that \( \{ \alpha_k \phi_k(x_k, d_k) \} \to 0 \), giving

\[
\{ \alpha_k \langle g_k, d_k \rangle - \alpha_k \nu_k \| c_k \| \} \to 0
\]

where \( \nu_k > 0 \) by (3.53). If \( g_k = 0 \) and \( c_k = 0 \), we are at a KKT point according to (3.43) and there is nothing to prove. Assume \( g_k \neq 0 \), then since \( c_k \neq 0 \) implies \( d_k \neq 0 \) by (3.15), it suffices to consider the first part, i.e., we have \( \{ \alpha_k \langle g_k, d_k \rangle \} \to 0 \), implying \( \{ \alpha_k d_k \} \to 0 \) since \( g_k \neq 0 \). We have

\[
| x_{k+1} - x_k | = \left| \alpha_k d_k + \alpha_k^2 d_k^2 \right| \\
\leq 2 \alpha_k | d_k |
\]

by step (viii) and \( 0 < \alpha_k \leq 1 \). Obviously \( | x_{k+1} - x_k | \to 0 \) for large enough \( k \). I.e., \( | x_{k+1} - x_k | = \| x_{k+1} - x^* + x^* - x_k \| \leq \| x_{k+1} - x^* \| + \| x_k - x^* \| < \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = \varepsilon \), and we cannot leave \( B(x^*, \varepsilon) \) without creating another cluster point and hence another KKT point in \( B(x^*, \varepsilon) \). □

This is equivalent to lemma 8 of Lawrence and Tits (2000). Observe that the lemma is concerned with the case where the algorithm rFSQP never stops in step (vii). The proof follows Panier and Tits (1987), (1993).

The next lemmas guarantee that the sequence \( \{ d_k + d_k^C \} \) approach the sequence \( \{ d_k^0 \} \) of ordinary SQP directions sufficiently fast, where \( d_k^0 = (p_{N,k}, p_{Z,k}) \) is the solution to the unperturbed problem (3.46) with \( p_{Z,k} = p_{Z,k} \).

Lemma 3.9 Suppose assumptions 3.1 and 3.3-3.10 hold. Assume that the sequence \( \{ x_k \} \) converges to a KKT point \( x^* \). Then \( d_k^0 \to 0 \) and \( \lambda_k^0 \to \lambda^* \).

Proof: At \( x^* \) we have from (3.43) that \( Z^T_x g_* = 0, c_i^T(x^*) \leq 0, \) and \( \lambda_{i,x}^* \geq 0, i = \{ 1, \ldots, p_2 \}. \) Since \( c_{\varepsilon}^T(x^*) = 0 \) and \( c_{\varepsilon}^T(x_k) = 0 \) \( \forall \varepsilon \in J^*_k \) continuity and (3.15) with \( c_k \triangleq \begin{bmatrix} c_{\varepsilon}^T(x_k) & c_{T}^T(x_k) \end{bmatrix}^T \) and \( \tilde{c}_k(x_k) \triangleq \{ c_i^T(x_k) \mid i \in J^*_k \} \) imply \( p_{N,k}^0 \to 0 \) implying \( w_k \to 0 \). Assumptions 3.2, 3.5
and 3.6 gives strict convexity and boundedness of (3.46), implying \( p_{Z,k}^0 \to 0 \) by (3.44). Evidently all multipliers estimated by (3.18) will converge since \((Y_k^T A_k)^{-1} y_k^*\) is a left-inverse of \( A_k \), and \( g^* = -A^* \lambda^* \) by (3.43), then assumption 3.3 and 3.8 gives a unique \( \lambda^* \) satisfying strict complementary slackness. Assumption 3.2 implies that LICQ holds in a small neighborhood of \( x^* \), and \( \lambda_k^0 \to \lambda^* \) follows. \( \square \)

This is equivalent to lemma 9 of Lawrence and Tits (2000) modified to allow for the decomposition. The proof partly follows Panier and Tits (1987). If \( \| d_{k+1}^E \| > 0 \) and \( \| d_k \| > 0 \), then we know from step (xvii) that \( \eta_k > 0 \). If \( \| d_k \| = 0 \) the algorithm will stop in step (vii). Comparing (3.29), (3.30) with (3.44), we observe that \( \| d_{k+1}^E \| = 0 \) can only occur at KKT points, and by lemma 3.2, the algorithm would have stopped at step (vii). Hence, \( \eta_k > 0 \) can be assumed for all \( x_k \neq x^* \).

**Lemma 3.10** Suppose assumptions 3.1 and 3.3-3.10 hold. Then, if \( K \) is a subsequence on which \( \{ \eta_k \} \) converges, say to \( \eta^* \geq 0 \), then \( d_k \to 0 \) and \( \gamma_k \to 0 \).

**Proof:** We prove that \( (d_k, \gamma_k)_{k \in K} \to (0,0) \) by contradiction. I.e. suppose that on some infinite index set \( K' \subseteq K \) that \( (d_k, \gamma_k) \) is bounded away from zero. Assumption 3.5 allows the assumption \( B_k \to B^* \) without loss of generality. When assumption 3.8 holds at \( x^* \) (lemma 3.2 ii) and (3.51) imply \((\bar{p}_k^*, p_k^*) = (0,0)\). Assumption 3.7 implies for any \( x_k \to x^* \) that \( p_{Z,k} \to 0 \), \( \gamma_k \to 0 \). Clearly \( p_{Y,k} \to 0 \) by (3.15) since \( \| c(x_k) - c(x^*) \| \to 0 \) by continuity, and the contradiction proves the claim.

Now suppose \( p_{Z,k} \to 0 \). Since \( \{ B_k \} \) and \( \{ \eta_k \} \) are bounded, there exists an infinite index-set \( K \) on which \( \{ B_k \} \) and \( \{ \eta_k \} \) converge and \( p_{Z,k} \) is bounded away from zero. This contradicts \( p_{Z,k} \to 0 \) established above, i.e. \( p_{Z,k} \to 0 \). Then \( \gamma_k \to 0 \) by squeezing in (3.47). A similar argument gives \( p_{Y,k} \to 0 \), hence \( d_k \to 0 \) by (3.14). \( \square \)

This is equivalent to lemma 12 of Lawrence and Tits (2000) modified to allow for the decomposition. This lemma is included to show that assumption 3.8 does not inhibit convergence. The next lemma shows that we eventually identify the correct active set.

**Lemma 3.11** Suppose assumptions 3.1 and 3.3-3.10 hold. Then, for all \( k \) sufficiently large \( J_k^* = J^{*\prec} \).

**Proof:** Since \( \{ \eta_k \} \) is bounded and lemma 3.10 implies \( (d_k, \gamma_k) \to (0,0) \), lemma 3.6 implies \( J_k^* \subseteq J^{*\prec} \) for all \( k \) sufficiently large. Choose an \( \mathcal{U} \in J^{*\prec} \). 
By assumption 3.7 we have \( c'_{I,k}^j \rightarrow c'_{I,s}^j \). Hence \( J_k^* \rightarrow J^{*,*} \) asymptotically. Then for any \( \epsilon > 0 \) we will have \( \left| c_{I,k}^j \right| > -\epsilon \) for all \( k \) large enough. Then, since \( x_k \in X_I \) \( \forall k \) and \( j' \) was arbitrarily, \( J_k^* = J^{*,*} \) for all \( k \) large enough. □

This is equivalent to lemma 13 of Lawrence and Tits (2000) modified to allow for the decomposition. In FSQ, the \( \rho \)-multipliers are used to identify the correct active set as done by Powell (1978). In rFSQ we use \( \epsilon \)-active constraints \( J_k^* \), and prove by continuity of \( c_k \) that asymptotically \( J_k^* \rightarrow J^{*,*} \). Then \( J_k^* \) will be stable for all large enough \( k \). Note that the complementary slackness assumption was not utilized in the proof. Since there exists a finite \( k_0 \) such that \( J_k^* = J^{*,*} \) for all \( k \geq k_0 \) we have an equality constrained problem. Identification of the optimal active set allows us to treat the problem as equality constrained locally (see Powell (1978)), and the local analysis will follow directly from Biegler et al. (1995) and Byrd and Nocedal (1991), provided that our tilted direction approach the ordinary SQP direction \( d_0^* \) sufficiently fast, and that the constrained line-search accepts a unit step-length. These provisions are proved in the following.

Identification of the correct active set in full-space methods is important since it says that the \( \rho \)-multiplier actually solves the problem in the correct tangent space. When we solve for \( P_{I,k} \) from (3.15) we always satisfy this, provided that we pick the correct active set in step (x) of algorithm rFSQ. Thus, a pre-assigned active set strategy depends on accurate identification of the correct active set near the solution. Choosing the \( \epsilon \)-active set \( J_{k+1}^* \) from (3.5) in step (x) of algorithm rFSQ, identification of the optimal active set occurs when the algorithm converges to a KKT point. The bound \( \epsilon > 0 \) can be chosen as the nonlinear inequality feasibility tolerance \( \epsilon_{intol} \) and is typically a small number.

**Lemma 3.12** Suppose assumptions 3.1 and 3.3-3.10 hold. For all \( k \) sufficiently large, \( \delta_k^E \) is uniquely defined and \( d_k^E = d_k^0 \).

**Proof:** Since (3.29) with the associated \( c_k^E \) equals equation (12) in Biegler et al. (1995), augmented with the additional active inequalities, \( P_{Z,k}^E = P_{Y,k}^0 \) follows. The estimate \( P_{Z,k}^E \) is defined as the unique solution of (3.30), where uniqueness follows from assumption 3.5. Then \( P_{Z,k}^E = P_{Y,k}^0 \) follows since (3.30) is identical to (3.46). Note that \( \zeta_{k+1}^E \) and \( w_{k+1}^E \) are computed by the same relations as \( \zeta_{k+1} \) and \( w_{k+1} \), see steps (xv,xvi) in algorithm rFSQ. Uniqueness and \( d_k^E = d_k^0 \) then follow from (3.28). □

This is equivalent to lemma 15 of Lawrence and Tits (2000) modified to allow for the equality constraints. The lemma shows that \( d_k^E \) is a "good"
estimate of the SQP direction $d^0_k$, which is obvious since in fact it is the
SQP-direction.

**Lemma 3.13** Suppose assumptions 3.1 and 3.3-3.10 hold. Then, $\eta_k \to 0$.

**Proof:** This follows from step xvii of algorithm \texttt{rFSQP} since by lemma 3.10
and 3.12 \{d_k\} and \{d^E_k\} both converge to 0. □

This is lemma 16 of Lawrence and Tits (2000). The proof is unchanged.
Note that the lemma establishes that $\eta_k$ actually converges, a property that
has been assumed so far.

We now consider the approximation error between $d_k$, $d^E_k$ and $d^0_k$.

**Lemma 3.14** Suppose assumptions 3.1 and 3.3-3.10 hold. Then,
\begin{enumerate}
  \item $\eta_k = \mathcal{O}\left(\|d^0_k\|^2\right)$
  \item $p_{Y,k} = p_{Y,k}^0 + \mathcal{O}\left(\|d^0_k\|^2\right)$ and $p_{Z,k} = p_{Z,k}^0$
  \item $d_k = d^0_k + \mathcal{O}\left(\|d^0_k\|^2\right)$
  \item $\gamma_k = \mathcal{O}\left(\|d^0_k\|^2\right)$
\end{enumerate}

**Proof:** $\eta_k = \mathcal{O}\left(\|d^0_k\|^2\right)$ follows without modifications from Lawrence and
Tits (2000), i.e. by step (xvii) of algorithm \texttt{rFSQP}. Lemma 3.12 gives exist-
ence and uniqueness of $d^E_k = d^0_k$. Lemma 3.10 and 3.9 ensure that step
(xvii) of algorithm \texttt{rFSQP} chooses $\eta_k = C^0_k \|d^E_k\|^2$ for all $k$ sufficiently large,
thus item i) follows.

From equation (3.17) and (3.46) $p_{Z,k} = p_{Z,k}^0$. From (3.15) and the asso-
ciated $c_k$ we have

\[
(A^T_k Y_k)p_{Y,k} = -c_k = -\left[
\begin{array}{c}
c_{\xi,k} \\
c_{\tau,k}
\end{array}
\right]
- \left[
\begin{array}{c}
0 \\
\gamma_{k-1}\eta_k e^{}_{|J_k|}
\end{array}
\right]
= -c_k^0 - \left[
\begin{array}{c}
0 \\
\gamma_{k-1}\eta_k e^{}_{|J_k|}
\end{array}
\right]
\]

where $e_{|J_k|}$ is a vector of ones of length $|J_k|$. We have $p_{Y,k} = p_{Y,k}^0 + \mathcal{O}(\|d^0_k\|^2)$,
since $\gamma_{k-1} < 0$ away from KKT points by lemma 3.2. By item i) $d_k =
Y_k p_{Y,k} + Z_k p_{Z,k} + \mathcal{O}(\|d^0_k\|^2) = d^0_k + \mathcal{O}(\|d^0_k\|^2)$ for all $k$ sufficiently large.
From inequality (3.47) we have $\langle Z_k^T y_k + \zeta_k w_k, p_{Z,k} \rangle \leq \gamma_k \leq 0$. By lemma
5.8 in Biegler et al. (1995), $w_k = \mathcal{O}(p_{Y,k})$, $\gamma_k \leq 0$, assumption 3.2, and using

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\[ c \| d_k^\ell \|^2 \leq \alpha \left( \| p_{Y,k}^0 \|^2 + \| p_{Y,k}^0 \| \| p_{Y,k}^0 \| + \| p_{Y,k}^0 \|^2 \right) \], we have from item ii) that

\[ |\gamma_k| \leq c_1 \| p_{Z,k} \| + c_2 \| p_{Z,k} \| \| p_{Y,k} \| \]
\[ \leq c_1 \| p_{Z,k}^0 \| + c_3 \| p_{Z,k}^0 \| \left( \| p_{Y,k}^0 \|^2 + \| p_{Y,k}^0 \| + \| p_{Y,k}^0 \|^2 \right) \]
\[ = c_1 \| p_{Z,k}^0 \| + c_3 \| p_{Z,k}^0 \| \| p_{Y,k}^0 \| + c_3 \| p_{Z,k}^0 \| ^2 + c_3 \| p_{Y,k}^0 \| ^3 \]

Now, since for \( a, b \geq 0 \)

\[ (a + b)^2 \geq a \]
\[ (a + b)^3 \geq 2ab \]
\[ (a + b)^3 \geq a^2b + ab^2 + b^3 \]

we have, writing \( (a + b) = \left( \| p_{Z,k}^0 \| + \| p_{Y,k}^0 \| \right) \)

\[ |\gamma_k| \leq c_1 \left( \| p_{Z,k}^0 \| + \| p_{Y,k}^0 \| \right) + c_4 \left( \| p_{Z,k}^0 \| + \| p_{Y,k}^0 \| \right)^2 + c_5 \left( \| p_{Z,k}^0 \| + \| p_{Y,k}^0 \| \right)^3 \]

then \( \gamma_k = \mathcal{O} \left( \| d_k^0 \| \right) \) by (3.51). \( \square \)

This is equivalent to lemma 17 of Lawrence and Tis (2000) modified to allow for the decomposition.

**Lemma 3.15** Suppose assumptions 3.1 and 3.3-3.10 hold. Then \( \| d_k^C \| = \mathcal{O} \left( \| d_k^0 \|^2 \right) \).

**Proof:** Let \( \tilde{c}_{I,k} = \left( c^i_I(x_k + d_k) + \| d_k \|^\gamma_i \mid i \in J^{\star \epsilon} \right)^T \). Then, for \( t^i \in (0,1) \)

\[ \tilde{c}_{I,k} = c^i_I(x_k) + \langle \nabla c^i_I(x_k), d_k \rangle + \frac{1}{2} \langle d_k, \nabla^2 c^i_I(x_k + t^i d_k) d_k \rangle + \| d_k \|^\gamma_i \]

when \( d_k = Y_k p_{Y,k} + Z_k p_{Z,k} \), we have by (3.15), (3.16), \( Z_k^T \nabla c^i_{I,k} = 0 \), \( \forall i \in J_k \) and lemma 3.11 for \( i \in J^{\star \epsilon} \) and \( k \) sufficiently large

\[ = \gamma_k \gamma_{k-1} + \mathcal{O}(\| d_k \|^2) + \| d_k \|^\gamma_i \]

and from lemma 3.14

\[ = \mathcal{O}(\| d_k^0 \| ^2) \mathcal{O}(\| d_k^0 \| ^2) + \mathcal{O}(\| d_k \|^\gamma_i) \]
\[ = \mathcal{O}(\| d_k^0 \| ^2) \]
since $\kappa > 2$. We have from (3.32), assumption 3.6 and the Broyden safeguards (3.25, 3.26) (see also lemma 5.8 in Biegler et al. (1995)) that $p^{C}_{Z,k} = O(\|c_E(x_k + d_k) - \tilde{c}(x_k)\|_2) = O(\|d_k\|^2)$. We have from (3.33) that $B_k \left(p^{C}_{Z,k} + p_{Z,k}\right) = -(Z_k^T g_k + \tilde{g}_k (w_k + u^C_k))$, using (3.17)

$$B_k p^{C}_{Z,k} = -\tilde{g}_k u^C_k$$

We have by assumption 3.5

$$p^{C}_{Z,k} = O(p^{C}_{Y,k}) = O(\|d_k\|^2)$$

and the claim follows from (3.31). $\Box$

This is equivalent to lemma 18 of Lawrence and Tits (2000) modified to allow for the decomposition.

**Proposition 3.1** Suppose assumptions 3.1 and 3.3-3.10 hold. Then a step-length $\alpha_k = 1$ satisfies the feasibility requirement in the line-search (3.40) of algorithm rFSQP for all $k$ sufficiently large.

**Proof:** Consider $\alpha_k = 1$, then $x_{k+1} = x_k + d_k + d^C_k$. We need to prove $c^T(x_{k+1}) \leq 0$. The definitions

$$c(x_k) = \begin{bmatrix} c^T(x_k) \forall i \in \{1, \ldots, p_1\} \\ c^T(x_k) - \gamma_{k-1}\eta_k, i \in J^k \end{bmatrix}, \quad c^C(x_k) = \begin{bmatrix} c^T(x_k + d_k) \forall i \in \{1, \ldots, p_1\} \\ c^T(x_k + d_k) + \|d_k\|^\kappa, i \in J^k \end{bmatrix}$$

allows

$$c(x_{k+1}) = c(x_k + d_k) + \langle A(x_k + d_k), d^C_k \rangle + O(\|d^C_k\|^2)$$

expanding and using lemma 3.15 gives

$$= c(x_k + d_k) + \langle A(x_k), d^C_k \rangle + \langle d_k, \nabla^2 c(x_k) d^C_k \rangle + O(\|d_k\|^2)\|d^C_k\|^2 + O(\|d^C_k\|^4)$$

denoting $A(x_k) = A_k$ and using lemmas 3.14 and 3.15 give

$$= c(x_k + d_k) + \langle A_k, Y_k p^C_{Y,k} \rangle + \langle A_k, Z_k p^C_{Z,k} \rangle + O(\|d_k\|^3)$$

inserting $p^C_{Y,k} = -(A_k^T Y_k)^{-1}c_k^C$ from (3.32) and using $A_k^T Z_k = 0$ gives

$$= c(x_k + d_k) - A_k^T Y_k (A_k^T Y_k)^{-1}c^C(x_k) + O(\|d_k\|^3)$$
finally the above definitions of \( c(x_k) \) and \( c^C(x_k) \) result in

\[
- \gamma_k \eta_k - \frac{\partial k}{k} + \eta_k \| d_k \|^2_k + O(\|d_k\|^3)
\]

By lemma 3.14 \( \gamma_k \eta_k = O(\|d_k\|^3) \), then \( \kappa < 3 \) gives \( c^i_T(x_{k+1}) < 0 \), \( i \in J_k \).

This is equivalent to the first part of proposition 1 of Lawrence and Tits (2000). Note that we do not prove descent, since we are working with a \( l_1 \)-penalty function. We observe by \( A_k^T Z_k = 0 \) in the proof above that \( p_{Z,k}^C \)
only serves to minimize \( \| d_k + d_k^C \|_B \) i.e. that the correction \( d_k^C \) does not tilt the overall step \( d_k \) unnecessarily away from the SQP direction.

**Theorem 3.3** Suppose assumptions 3.1 and 3.3.1.10 hold. Then algorithm \( rFSQP \) generates a sequence \( \{x_k\} \) which converges 1-step superlinearly to \( x^* \).

**Proof:** The proof follows from Biegler et al. (1995) since the algorithm produces a convergent sequence of iterates satisfying

\[
x_{k+1} - x_k = \frac{\partial k}{k} + O(\|d_k\|^3)
\]

Note that by lemma 3.11 the local analysis is an equality constrained problem and then lemma 3.3 and assumption 3.9 and 3.10 gives theorem 5.4 of Biegler et al. (1995). Then theorem 5.6 of Biegler et al. (1995) follows and assumption 3.5 is satisfied by our Hessian update scheme. \( \zeta_k = 1 \) is allowed in equation (3.19) for large \( k \) since

\[
\hat{\zeta}_k \left[ 2 \cos \theta_k^{RFGS} \left[ g_k^T Z_k w_k \right] + w_k^T B_k^{-1} Z_k^T g_k + \hat{\zeta}_k w_k^T B_k^{-1} w_k \right] \leq \rho \| c_k \|_1
\]

The last inequality will be satisfied with \( \zeta_k = 1 \) for large enough \( k \) (see Biegler et al. (1995), section 6). Lemma 6.2 and 6.3 in Biegler et al. (1995) then gives the claim. \( \Box \)

As in Biegler et al. (1995) removing the approximation term \( w_k \) will give a two-step superlinearly convergent algorithm. This will reduce the workload of each iteration, and may therefore give a better algorithm in practice. See Biegler et al. (2000) for numerical comparisons of this issue.

### 3.5 Implementation and results

We discuss implementation and test the algorithm on selected problems from the Hock-Schittkowski (Hock and Schittkowski 1981) test-set. The results
presented in this section illustrate some of the properties of rFSQP, but do not expose it to its intended use; large-scale optimization of problems dominated by equality constraints with a few nonlinear inequality constraints. Two such cases are investigated in chapter 4.

3.5.1 Implementation details

Some essential details are discussed next. The algorithm was implemented in MATLAB 6.0 (R12) and Visual FORTRAN 6.5\(^2\) developing studio, with mex-gateways to some FORTRAN routines.

Most implementation issues follow the same strategy as described in Biegler et al. (2000) and Lawrence and Tits (2000), but are somewhat simplified by vectorization in MATLAB. We treat linear constraints \(A_{L,L} x_k \leq b_{L,L} \) and \(A_{L,E} x_k = b_{E,L} \) and simple bounds, \(L \leq x_k \leq U\), by solving a \(\text{qp}\) for \(p_{Z,k}\) and \(\gamma_k\). This requires an explicit \(Z_k\). Hence, the "adjoint" approach for computing products like \(Z_k^T g_k\) without forming an explicit \(Z_k\) is not implemented. Note that simple bounds and linear constraints are not included in the Jacobian matrix \(A_k\) in equation (3.6) which defines the matrix \(Z_k\). The \(\text{qp}\) solved when utilizing the specific form of \(Z_k\) and \(Y_k\) is

\[
\begin{align*}
\min_{p_{Z,k}, \gamma_k} \quad & \frac{1}{2} \langle p_{Z,k}, B_k p_{Z,k} \rangle + \gamma_k \\
\text{s.t.} \quad & \langle Z_k^T g_k + \xi_k u_k, p_{Z,k} \rangle \leq \gamma_k \\
& \left\langle Z_k^T A_{L,L}^T, p_{Z,k} \right\rangle \leq b_{L,L} - A_{L,L} x_k - C_k p_{Y,k} \\
& \left\langle Z_k^T A_{E,L}^T, p_{Z,k} \right\rangle \leq b_{E,L} - A_{E,L} x_k - C_k p_{Y,k} \\
& L - x_k - Y_k p_{Y,k} \leq Z_k p_{Z,k} \leq U - x_k - Y_k p_{Y,k} \\
& \left\langle Z_k^T \nabla c_{i,k}^T, p_{Z} \right\rangle - \gamma_k \eta_k \leq -c_{i,k}^2(x_k) - \left\langle Y^T \nabla c_{i,k}^T, p_{Y,k} \right\rangle, \quad i \notin \mathcal{J}_k \\
\end{align*}
\]

where the last line includes the inactive inequality constraints not included in the computation of \(p_{Y,k}\). i.e. we do not implement the EQP strategy which was assumed during the analysis to facilitate use of theorem 3.1.

Similar \(\text{qp}\)'s, but without \(\gamma_k\), are solved for \(p_{Z,k}^E\) and \(p_{Z,k}^C\) as well, i.e. 3 reduced size \(\text{qp}\)'s are solved at each iteration. The clipping of \(d_k^C\) and \(d_k^E\) occurring in Lawrence and Tits (2000) is not needed, since all bounds are accounted for in the \(\text{qp}\)'s. If a \(\text{qp}\) was declared infeasible, we set \(p_{Z,k}\) to zero and cut \(d_k = Y_k p_{Y,k}\) so as to satisfy bounds. This is only introduced to

\(^2\)MATLAB is a licensed product from The Mathworks Ltd. Visual FORTRAN 6.5 is a licensed product from COMPAC.
3.5 Implementation and results

recover from inconsistent constraint linearizations away from the solution. Alternatives are described by Gill et al. (1997) (elastic programming). We use the qp-solver e04naa from the NAG toolbox. The NAG-solver only accepts dense Jacobians, and should be replaced by a sparse solver in a production code\(^3\).

The update rule for \(\eta_k\) is vectorized, and the update rule for \(C_k^n\) is as in FSQP:

1. If the full step \(\alpha_k = 1\) was accepted set \(C_{k+1}^n = C_k^n\).
2. If \(\alpha_k < 1\) and no constraints were infeasible at any trial points, set \(C_{k+1}^n = \max \left\{ \frac{C_{k}^n}{\delta}, C_k^n \right\} \) (decrease \(C_{k+1}^n\)).
3. If \(\alpha_k < 1\) and some constraints were infeasible at some trial points, set \(C_{k+1}^n = \min \left\{ \delta C_{k}^n, C_k^n \right\} \) (increase \(C_{k+1}^n\) ) for the constraints that were infeasible at some trial points, and set \(C_{k+1}^n = C_k^n\) for the rest.

All parameter values are as given in Biegler et al. (2000), and Lawrence and Tits (2000) except for the tolerance \(\epsilon_f\) controlling the \(\eta_k\)-updates. We use the default value \(\epsilon_f = 1e-3\). The parameter \(\epsilon\) controlling the inclusion in the active set \(J_k\) is critical for the performance of rFSQP. We use the default value \(\epsilon = 1\). To speed up the algorithm, it may be advantageous to start with a large value, say \(\epsilon = 1\), and decrease it down to \(k \times \text{featlol}\), where \(\text{featlol}\) is the feasibility tolerance for the nonlinear inequalities and \(k > 1\), during the progress of the algorithm. This is problem dependent though, and the results reported are for constant values of \(\epsilon\). The value \(\epsilon = 1\) was found by trial and error. A large value of \(\epsilon\) is beneficial for problems where the solution \(x^*\) does not lie on active inequality constraints. For problems where the solution does lie on active inequality constraints, large values of \(\epsilon\) can cause slow convergence, since the algorithm may approach the solution conservatively.

Basis selection in MATLAB can be done by LU-decomposition using partial pivoting given \(n > m_k\) provided \(\text{rank}(A_k) = m_k\). If \(\text{rank}(A_k) < m_k\) the system is not guaranteed to have a solution, and this can cause numerical problems. To deal with rank-deficient problems row and column pivoting are necessary, and we use the Harwell routine MA28 (Harwell Laboratory

\(^3\)In the present implementation of rFSQP the constraint Jacobian is converted to a dense matrix by issuing the MATLAB command full just before the call to e04naa. Still this works better than using MATLAB’s quadprog which accepts sparse Jacobians, but does not handle poorly conditioned Jacobians appropriately.
1995) through a mex-gateway for this purpose. This routine allows reuse of a previous pivoting sequence provided the same non-zero structure is maintained. Hence, complete refactorization is rarely needed (this is similar to the approach of Biegler et al. (2000)), except when a change in the active set occurs.

To assess the relative level of sophistication of our implementation we implemented the algorithm of Biegler et al. (2000) which we term rSQP for brevity. In fact rFSQP is implemented as an extension to this algorithm with some important modifications. Our implementation of the algorithm by Biegler and co-workers was sensitive to the results from the qp-solver on some of the harder problems. Since the MATLAB qp-solver seems to produce inaccurate solutions for badly conditioned problems, we implemented rSQP with the qp-solver QPKWIK obtained with kind permission from Professor Lorenz T. Biegler. QPKWIK is also used in Biegler’s implementation. Since QPKWIK needs the inverse Cholesky-factors of the Hessian as input, we also replaced the BFGS-updating scheme with Biegler’s updating scheme for the inverse Cholesky-factors (which makes use of the qp-multipliers). Since the Hessian of the implemented qp (3.54) is semi-definite, the inverse Cholesky factors are undefined and use of QPKWIK in rFSQP is therefore not trivial. However, since rFSQP worked well with both MATLAB’s quadprog and NAG’s e04naf in combination with a standard BFGS updating scheme we did not consider using QPKWIK in rFSQP. Clearly this puts a bias on the comparison of the two algorithms, and we only include the results on rSQP to give an idea of the level of sophistication of rFSQP. Some of the results reported below give unexpectedly poor results for rSQP and we expect that this is a result of our implementation.

The line search is identical in both implementations apart from the feasibility check in rFSQP, and follows as in Dennis and Schnabel (1996) modified to allow for checking of constraint violations. The constrained line search tests for feasibility prior to descent, but does not re-order constraints as in Lawrence and Tits (2000). I.e. vectorization in MATLAB allows a simultaneous test, while a FORTRAN program must perform this test in a loop. In the present version of rFSQP the qp-multipliers are not used other than for updating the penalty parameter $\nu$.

When constraints are removed from the active set, we re-initialize the corresponding reduced Hessian to $I$. The current implementation does not implement a watch-dog strategy, and we do not handle a rank-deficient Jacobian. The algorithm detects this and stops, but this does not occur on any of the test-problems. From table 4 in Biegler et al. (2000) we note that the cross-terms $u_k$ and $\bar{w}_k$ have relatively little influence on the
3.5 Implementation and results

iteration counts for the selected problems from the Hock-Schiittkowski test-set. Therefore we implemented both algorithms with Broyden corrections only. Then, since we never resort to finite differences the iteration counts and gradient evaluation counts reported below are identical for both rSQP and rFSQP.

3.5.2 Results

We give preliminary test results for a selection from the Hock-Schiittkowski test set for our implementation of rSQP by Biegler et al. (2000), and rFSQP in table 3.1. The results for rSQP are included to illustrate the level of sophistication of the implementation of rFSQP. In rSQP nonlinear inequalities were implemented as equalities with slacks.

On hs33 both implementations converge to $\bar{x}^* = (0, 0, 2)$ with objective value $f^* = -4$ (which is also reported in table 6.4 of Gill et al. (1997)). The value $\bar{x}^*$ is the same value as returned by the NAG routine e04ucf. On hs34 rFSQP performs poorly, and needs $\epsilon = 0.1$ to converge. On hs93 rFSQP attracts very slowly to $x^*$, and no BFGS-updates occurs. On hs111 both algorithms converge to a point $\bar{x}^* \neq x^*$ given by Hock and Schiittkowski (1981). The value $\bar{x}^*$ is the same value as returned by the NAG routine e04ucf. In hs112 there is an error in the problem, and the problem was solved with the modification stated in the CUTE (Bongartz, Conn, Gould, and Toint 1995) test set. We expect that the difference between rSQP and rFSQP on hs111 is caused by the different choices of Hessian update schemes in combination with different qp-solvers.

The rSQP-results indicate the inadequate level sophistication of the code which we based rFSQP on. I.e. it solves the simpler problems with iteration and function evaluation counts comparable to Biegler et al. (2000), but experiences problems especially on hs100 and hs111 and fails on hs84 and hs117. The rFSQP-results show that on some problems the iteration count increases (as expected), when the SQP-direction is tilted. In other cases the performance is improved, since feasible iterates may remain in a “nicer” region than the pure SQP iterates. This may be beneficial during later iterations. Observe that the workload of each iteration of rFSQP is larger than for rSQP since 3 subproblems must be solved instead of one.

Comparing to the results reported for FSQP’ by Lawrence and Tits (1996), Lawrence and Tits (2000) show that FSQP’ performs better on most of the problems reported in table 3.1. In particular, rFSQP performs poorly on hs12, hs34, hs43, hs84, hs93 and hs117. Comparing with SNOPT it is observed that rFSQP experiences problems on hs34, hs43, hs66, hs80, hs84, hs93,
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Table 3.1: *rFSQP on the Hock-Schittkowski test set.* The table gives the results on the Hock-Schittkowski (Hock and Schittkowski 1981) test set. rSQP=our implementation of the algorithm of Biegler et al. (2000), rFSQP=the present algorithm. IT=iterations, NF=function evaluations, NG=gradient evaluations, NO=objective evaluations, and NC=constraint evaluations. For rSQP NO=NC=NF. Since finite differences are turned off we have IT=NG. $\epsilon$ is the active set tolerance for rFSQP. The default value $\epsilon=1$ is marked with (def). For equality constrained problems $\epsilon$ is irrelevant and marked with (-).
3.5 Implementation and results

hs100 and hs117. Hence, further testing is necessary to evaluate the possible advantages of the rFSQP algorithm over the algorithms of Lawrence and Tits (2000), Biegler, Nocedal, and Schmid (1995) and Gill, Murray, and Saunders (1997). It may be that the reported results can be improved by improving the implementation of rFSQP. Hence, the poor results need not necessarily be a result of the method rFSQP, but rather a consequence of the implementation.

We experienced that the rFSQP algorithm is sensitive to the threshold value $\epsilon$ for $J_k$ on certain problems. On equality constrained problems $\epsilon$ is irrelevant. A large value like $\epsilon = 1$ causes the algorithm to stay well inside the interior of the feasible region, and this reduces the number of changes in the active set, which reduces the frequency of complete re-factorization of the constraint Jacobian to find a new pivoting strategy. However, this causes the algorithm to approach inequalities conservatively, which may cause slow convergence on problems where the optimum is located on active nonlinear inequalities. The observed behavior of the algorithm is thus more related to interior methods\(^4\) than to "working set" SQP methods. Still it is implemented and analyzed as a SQP method, and in particular larger counts for function evaluations are expected on large scale problems, as is usual for SQP methods.

There are a number of issues to be addressed to improve the present implementation. It should be tested on large-scale problems, the Hessian updates should be improved, possibly by exploiting the $\mathbf{qp}$-multipliers. 2nd derivative Hessians may be introduced, for example by partial separability of the Lagrangian combined with perturbed Cholesky factorization or with trust-regions combined with conjugate-gradient steps. Other line searches and mechanisms for global convergence should be implemented, in particular how to implement a watch-dog in combination with the constrained line search. Finite differences and rank-deficient Jacobians should be handled. Hot-starting the $\mathbf{qp}$-solver by re-use of the last active set, and sparse linear algebra $\mathbf{qp}$-solvers could be used. A production code should also be independent of the interpreted MATLAB environment.

To illustrate the workings of rFSQP we compare it with the iterations of rSQP on hs12 from the Hock-Schittkowski test-set and a modification of hi3 in Himmelblau (1972), p. 394. The modification is that we multiply the objective by 1000 and alter the second constraint. Note that hi3 is quite

\(^4\)Some feasible interior methods for nonlinear programming has appeared recently; Forsgren and Gill (1998) and Byrd, Nocedal, and Waltz (2000).
similar to hs59. We restate these problems for completeness.

\[
\begin{align*}
\min_x & \quad 0.5x_1^2 + x_2^2 - x_1x_2 - 7x_1 - 7x_2 \\
\text{s.t.} & \quad 25 - 4x_1^2 - x_2^2 \geq 0
\end{align*}
\] (3.55)

\[
\begin{align*}
\min_x & \quad 1000 \cdot f(a, x, x^2, x^3, x^4, \exp(x)) \\
\text{s.t.} & \quad 700 - x_1x_2 \leq 0 \\
& \quad \frac{x_1^2}{125} - x_2 \leq 0 \\
& \quad 5(x_1 - 55) - (x_2 - 50)^2 \leq 0 \\
& \quad 0 \leq x_1 \leq 75 \\
& \quad 0 \leq x_2 \leq 65
\end{align*}
\] (3.56)

In hs12, equation (3.55), the initial point is \( x_0 = (0, 0) \) while the solution is \( x^* = (2, 3) \). In hi3, equation (3.56), the original initial point is infeasible, so we start from \( x_0 = (70, 40) \) instead. The solution is \( x^* = (75, 65) \). The iterations are plotted with objective contours and constraints as equalities in figures 3.2 and 3.3. The feasible regions are evident from the bold face lines which are the borders of the inequalities. The iteration sequences for

![Figure 3.2](image)

**Figure 3.2:** Iterations for rSQP (o) and rFSQP (×) on hs12 from the Hock-Schittkowski test set.

rSQP and rFSQP on hs12 are given in table 3.2. The iteration sequences for rSQP and rFSQP on hi3 are given in table 3.3.
3.5 Implementation and results

We observe from figure 3.2 that rSQP produces infeasible iterates, while rFSQP remain feasible. The effect of the constrained line search is observed in iteration 1 where both methods generated the same step $d_1 = (3.5, 3.5)$. In rSQP the full step was accepted since this gives a reduction in the merit function, but in rFSQP the full step gives infeasibility and the next trial value $\alpha = 0.5$ is tested. $\alpha = 0.5$ is accepted since it is feasible and gives a decrease in the merit function. In Biegler et al. (1995) one-step superlinear convergence was proved with finite differences for the correction terms $w_k$ and $\tilde{w}_k$. Since we only implement Broyden corrections we expect 2-step superlinear convergence, i.e. that we get one extra correct figure every 2nd iteration (for large $k$). The results for hs12 shows that this is nearly obtained for both algorithms. We have $\alpha_{k, rSQP} = 1$ for all $k$ and $\alpha_{k, rFSQP} = 0.5$ for all $k$ on hs12. Improvements in performance can be expected by implementing a watch-dog for rFSQP to allow unit step-lengths for large $k$ and including finite differences. The quality of finite difference corrections depends on good multiplier estimates, and using the qp multipliers should be considered.

On hs12 one could anticipate that reducing $\epsilon = 1$ down towards $\text{featol} = 10^{-5}$ would improve the result for rFSQP. It turned out that rFSQP was

---

**Figure 3.3:** Iterations for rSQP ($\circ$) and rFSQP ($\times$) on h3 from Himmelblau (1972).
<table>
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<th>Iteration no.</th>
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Table 3.2: rFSQP on hs12. The table gives the iterations for rSQP and rFSQP on hs12 from the Hock-Schittkowski test set.

Insensitive to $\epsilon$ on hs12, and the same result was achieved for all trial values $\epsilon \in [10^{-5}, 10]$. However, increasing the parameter $\delta$ used in updating the parameter $c_{k}^{n}$ has an effect. $C_{k}^{n}$ in turn influence on the updating of $\gamma_{k}$ through step xvii in the rFSQP algorithm. Increasing $\delta$ from 2 to $> 2.5$ reduced the iteration count from 15 to 12 iterations on hs12.

Figure 3.3 illustrates the practical performance of rFSQP in the face of a nonconvex feasible region. Observe that rFSQP tends to stay far away from the inequality boundary during the early iterations, which in this case is beneficial. In hs12 where the optimum is located on a nonlinear inequality boundary, rFSQP is seen to be somewhat conservative. On hi3 rSQP also
Table 3.3: $rFSQP$ on hi3. The table gives the iterations for $rSQP$ and $rFSQP$ on hi3 from Himmelblau (1972).

walks round the third inequality constraint in equation (3.56). The first direction for $(x_1, x_2) = (70, 40)$ is $d_1 = (-0.4160, 1.3540)$. (The direction for the third slack is zero, with $s_3(0) = 0$.) The full step is accepted, but does not enter or cross the feasible region in this case. Note that not all $\alpha_k$’s are equal to one for $rSQP$ in this example. The number of function evaluations $NF$ is 32 for $rSQP$ and NO/NC is 5/10 for $rFSQP$. For hi3 we have $\alpha_k = rFSQP = 1$ for all $k$.

3.6 Conclusions

$rFSQP$ is a reduced Hessian SQP method that remains feasible with respect to inequality constraints at all iterates. $rFSQP$ is designed for large scale problems dominated by equality constraints, but with a few nonlinear inequality constraints of which we wish to remain feasible. It can be argued that feasibility of inequalities can give general benefits as discussed in section 3.2, which motivate the extension to large scale methods like reduced Hess-
sian methods. The benefit of feasible iterates must be traded off against the main benefit of SQP methods; the iterates need not be feasible, see Boggs and Tolle (1995) (feasibility can be very expensive to achieve in the presence of nonlinear constraints). However, we are only concerned with feasibility of inequalities, and the trade-off is thus shifted in favor of rFSQP, although of course no general recommendation can be provided.

The preliminary results in section 3.5.2, show that on some problems rSQP performs better, while on other problems rFSQP perform better. As could have been anticipated there is no general recommendation to be made about the method of choice for a given problem. Comparing the results of rSQP with the results of Biegler et al. (2000) shows that there is a significant potential for improvements in rFSQP as well. Hence, the testing is not conclusive. Given the complexity of the algorithm, further testing and refinements are needed to show any clear advantages of the proposed algorithm.

Acknowledgement 3.1 The author expresses his gratitude to Professor Lorenz T. Biegler and Andreas Wächter at Carnegie Mellon University for their insightful comments concerning various implementation issues and for providing access to their implementation of the algorithm published in Biegler et al. (2000).
Chapter 4

NMPC

Nonlinear model predictive control (NMPC) is a control strategy where application of nonlinear optimization methods is essential. The motivation for this chapter is to combine the model from chapter 2 and the optimization algorithm from chapter 3 in a NMPC framework. This chapter is application oriented, and contributes to the practical knowledge of implementation of NMPC. Parts of this chapter has been submitted for possible publication to the 15th IFAC World Congress on Automatic Control (Martinsen and Biegler 2002).

Optimal control problems generally lead to boundary value problems (BVP), since the adjoint equations must be integrated backwards in time (Vinter 2000), (Lewis and Syrmos 1995). Since NMPC is a special case of optimal control problems, it is expected that numerical methods suitable for BVP’s should be adapted in NMPC as well. The most popular numerical methods for solving BVP’s are (finite) element methods, possibly in combination with orthogonal collocation (Finlayson 1980). Multiple shooting has also been applied to BVP’s with success, see Ascher, Mattheij, and Russell (1995) for details on multiple shooting and orthogonal collocation. However, it is important to observe that batch-processes may be formulated as initial value problems (IVP), since stabilizing end-point constraints are irrelevant.

The chapter focuses on application of SQP optimization algorithms in NMPC, but emphasizes that appropriate model discretization is essential for the performance. A rule of thumb is that if it is impossible to integrate a model with a certain method, the method cannot be used in NMPC. In particular, since the sinter model from chapter 2 could not be integrated by explicit methods, it should not be represented with explicit methods in NMPC.
We discuss the differences and similarities between feasible and infeasible path methods, sequential and simultaneous methods and reduced and full space methods. We informally assess the suitable choices between these various strategies by applying them to two cases of different complexity.

The chapter starts with some background in section 4.1. In section 4.2 a conceptual comparison between single shooting and reduced Hessian methods is provided. Simulation results follow in section 4.3. Discussion and conclusions to the chapter follow in sections 4.4 and 4.5.

4.1 Introduction

This chapter is concerned with practical issues related to optimization within nonlinear model predictive control (NMPC), which is one of the major obstacles to be overcome in industrial applications of NMPC (Qin and Badgwell 2000). We consider different approaches to optimization, such as feasible vs. infeasible methods, sequential vs. simultaneous methods, reduced vs. full space methods and dense vs. sparse algebra methods, and apply these methods to two cases; a CSTR with first order reaction and to the grate sintering from chapter 2.

The theory of optimization algorithms is not dependent on how the equality constraints are formed. For instance in optimal control, and in particular in the special case of nonlinear model predictive control (NMPC), much concern is put into discretization schemes for the nonlinear equality constraints. These equality constraints result from a continuous-time nonlinear dynamical system repeated over a time horizon $P$. Three major variants are usually considered to handle unstable modes; orthogonal collocation, multiple shooting and single shooting (possibly with a variable grid). Ascher, Mattheij, and Russell (1995) discuss the general benefits of these approaches, and Barclay, Gill, and Rosen (1998) discuss this in conjunction with SQP algorithms. Vassiliadis (1993) addresses the dynamic optimization of general DAE systems. These approaches seek to find formulations of the equality constraints that are less hard to satisfy, while simultaneously reducing the discretization error.

Nonlinear inequality constraints may be introduced for stability purposes in NMPC (Scokaert, Mayne, and Rawlings 1999), (Chen and Allgöwer 1998b), (1998a). These references extend earlier work (Li and Biegler 1988), (Li and Biegler 1989), (Li, Biegler, Economou, and Morari 1990), (de Oliveira and Biegler 1995). These references are concerned with nominal stability. Hence, termination prior to convergence of the optimizer cannot guarantee
4.1 Introduction

stability unless the equality constraints are satisfied.

The immediate answer to this is single shooting; i.e. always solving the model. Single shooting algorithms progress towards a solution by iterating between solving the model and solving a reduced size optimization problem. Due to this, single shooting is said to be a sequential method. Single shooting produces a reduced gradient problem in the free variables to be solved at each NMPC iteration. Maintaining feasibility of nonlinear inequalities involving dependent variables can then be obtained by use of \textit{rFSQP} from chapter 3 or \textit{FSQP} of Lawrence and Tits (2000). This may be costly if evaluation of the problem functions is costly, e.g. if an implicit discretization scheme must be applied. In addition, according to Ascher et al. (1995), section 4.1 and 4.6.2, single shooting lacks robustness when applied to unstable systems. This problem can be somewhat alleviated by using an adaptive step length (Baker and Polak 1994), (Pytlak and Vinter 1998), (Pytlak and Vinter 1999), (Pytlak 1999).

To solve optimization problems with stabilizing endpoint constraints simultaneous methods must be applied. End-point constraints make the problem a two-point boundary value problem (TPBVP) which in general cannot be resolved with single shooting. Simultaneous methods do not solve the model at each iteration. Instead a simultaneous search for a model solution and optimal point is carried out. Multiple-shooting and orthogonal collocation, possibly on finite elements (Finlayson 1980), are the most widely used simultaneous methods. Since simultaneous methods do not solve the model at each iteration, they cannot guarantee stability in the nominal stability setting of dual-mode or quasi-infinite horizon NMPC if terminated prior to convergence. Note that the results reported in Bock, Diehl, Schlöder, Allgöwer, Findeisen, and Nagy (2000) show that termination prior to convergence in multiple shooting may be viable for some applications. Decomposition strategies for orthogonal collocation on finite elements have been considered by Cervantes and Biegler (2000) and Biegler, Cervantes, and Wächter (2001).

Initialization near the optimal point can happen frequently in real-time applications like model predictive control and receding horizon estimation (see Allgöwer et al. (1999)). In NMPC an optimization problem is solved repeatedly with (usually) small changes from one problem to the next. These are real-time applications where termination prior to convergence may be necessary, and an improved but non-optimal feasible solution is favorable if early termination is required. The only method that can be terminated prior to convergence is single shooting. As shown in section 4.3 below, choosing an appropriate optimization algorithm may have significant influence on
the overall computation time, in particular for processes where implicit discretization schemes are necessary.

Observe that for finite time batch-processes stability in the sense of Lyapunov\(^1\) is irrelevant, provided the process does not have finite escape time. Hence, the grate sintering case is formulated as a NMPC problem without endpoint constraints, and it is not established that the objective is a Lyapunov function for the NMPC problem. As a consequence, TPBVP techniques are not needed to solve this problem. Due to the stiffness of the model the implicit Lobatto IIIa scheme was adapted in the solution.

The choice between active set vs. interior-point methods is also important in NMPC. Bartlett, Wächter, and Biegler (2000) discuss this issue both on the NLP and the qp level. The results in section 4.3 were achieved with the qp solver e04nfaf from the MATLAB NAG toolbox. This is an active set solver, whereas the constraint Jacobian must be presented as a dense matrix.

Define the superscript notation \( z^k = \{ z_k \}_{k \in \mathbb{N}} \) for an entity \( z \) indexed by \( k \). The nonlinear MPC problem with \( \dim(u_k) = n_u \) and \( \dim(x_k) = n_x \)

\[
\min_{x,u^k} \quad \frac{1}{2} \left( \sum_{k=0}^{P-1} \| x_{k+1} \|^2_Q + \sum_{k=0}^{M} \| u_k \|^2_R \right) \\
\text{s.t.} \quad c_{\mathcal{K}} = c_{\mathcal{L}}(x_k, u_k) = f(x_k, u_k) - x_{k+1} = 0, \quad k = 0, \cdots, P - 1 \\
x^k \in \mathcal{X} \times \cdots \times \mathcal{X} \\
u^k \in \mathcal{U} \times \cdots \times \mathcal{U}
\]

(4.1)

with \( M < P \) is considered in this paper. The equality constraints in (4.1) have been formed by assuming an explicit discretization scheme. Endpoint constraints or augmentation of the objective may be included to guarantee nominal stability of the MPC algorithm, see Mayne, Rawlings, Rao, and Scokaert (2000). Observe that reference tracking and non-zero set-points can be handled in this framework with minor modifications. We assume sufficiently smooth 1st principles state-space models with measured states, analytic 1st order derivatives and that

\[ (\mathcal{X}, \mathcal{U}) = (\mathcal{X} \times \cdots \times \mathcal{X}, \mathcal{U} \times \cdots \times \mathcal{U}) \]

can be described by bounds.

\(^1\)For example, cf. Khalil (1996), theorem 3.1.
4.2 Optimization methods

First we consider SQP in general. The MPC problem (4.1) can be restated as a general nonlinear programming (NLP) problem:

\[
\begin{align*}
\min_{x} & \quad f(x) \\
\text{s.t.} & \quad c^E(x) = 0 \\
& \quad c^T(x) \leq 0
\end{align*}
\]  

(4.2)

where \( f : \mathbb{R}^n \to \mathbb{R} \), \( c^E : \mathbb{R}^n \to \mathbb{R}^m \) and \( c^T : \mathbb{R}^n \to \mathbb{R}^p \) where \( n = n_xP + n_uM, m = n_x(P + 1) \) and \( p = 2n \) (assuming upper and lower bounds on \( (x_k, u_k) \) over the horizons \( P \) and \( M \)). The Jacobian matrix of the equality constraints is denoted \( A_k^E = A(x_k)^T = [\nabla c^1_E(x_k), \nabla c^2_E(x_k), \cdots, \nabla c^m_E(x_k)] \) where \( c^i_E(x_k) \) is the \( i \)-th component of the vector \( c(x_k) \). The matrix \( G(x_k) \) made up of \( A_k^E \) and the gradients of the active inequality constraints is assumed to have full column rank. The null-space of \( G(x_k)^T \) defines the tangent space to the equality and active inequality constraints at \( x_k \). Denote \( H\mathcal{L}_k \) the Hessian of the Lagrangian function \( \mathcal{L}(x_k, \lambda^E_k, \lambda^T_k) = f(x_k) + \lambda^E_k c^E(x_k) + \lambda^T_k c^T(x_k) \) where \( \lambda^E_k \) and \( \lambda^T_k \) are the multiplier vectors. We assume strong second order sufficient conditions, i.e. that \( x^* \) is an isolated minimum of the NLP (4.2) and that \( \lambda^*_E \) and \( \lambda^*_T \) are unique. The strong second order conditions are:

A1 The 1st order necessary conditions hold, i.e. \( \exists \lambda^*_T \geq 0, \lambda^*_E \) (optimal multipliers) s.t. \( \nabla \mathcal{L}^* = \nabla f(x^*) + \nabla c^E(x^*) \lambda^*_E + \nabla c^T(x^*) \lambda^*_T = 0 \).

A2 The columns of \( G(x^*) \) are linearly independent.

A3 Strict complementary slackness hold, i.e. \( c^i_E(x^*) \lambda^i_T = 0, i = 1, \cdots, p \) and if \( c^i_E(x^*) = 0 \) then \( \lambda^i_T > 0 \).

A4 The Hessian of the Lagrangian function with respect to \( x \) is positive definite on the null space of \( G(x^*)^T \), i.e. \( d^T H\mathcal{L}^* d > 0 \forall d \neq 0 \) s.t. \( G(x^*)^T d = 0 \).

The quadratic subproblem to be solved at each iteration of the SQP algorithm becomes:

\[
\begin{align*}
\min_{d_k} & \quad \nabla f(x_k)^T d_k + \frac{1}{2} d_k^T B_k d_k \\
\text{s.t.} & \quad \nabla c^E(x_k)^T d_k + c^E(x_k) = 0 \\
& \quad \nabla c^T(x_k)^T d_k + c^T(x_k) \leq 0
\end{align*}
\]  

(4.3)
where $B_k > 0$ usually is an approximation to $H\mathcal{L}_k$. The inequality constraints of this qp can be resolved either by an active-set strategy or an interior-point strategy. Interior-point methods usually introduce slacks $s \geq 0$ to the inequality constraints s.t. $c_T(x) + s = 0$, and augment the objective; $f(x) + \sigma \sum_{i=1}^{p} \log s_i$. This leads to ill-conditioning when $s \to 0$ and consequently modified Newton methods must be applied to ensure rapid convergence, see Wright (1997b) for further details. Both active-set and interior-point methods can be implemented with sparse matrix solvers, but this seems to be easier to implement for the latter approach (Wright 1997a).

If $B_k$ is uniformly positive definite on the null space $\mathcal{N}(G_k^T)$, then the solution $d_k$ of problem (4.3) forms a strong descent direction for an exact penalty function $\phi_\nu$. The minimum of $\phi_\nu$ corresponds to a solution of problem (4.2) (Fletcher 1987). Therefore a step size $\alpha_k$ along $d_k$ can be found which is bounded away from zero yielding convergence. Convergence from remote starting points is not guaranteed by this since the linearized constraints might lead to infeasible subproblems. This can be resolved by resorting to elastic programming giving ”good” infeasible points, see e.g. Gill, Murray, and Saunders (1997). We have argued that the basic SQP-method will converge to stationary (KKT) points, but special provisions must be made to avoid convergence to maximum and saddle points. This usually involve exact second order derivatives and trust-region methods, see Biegler (2000) for an introduction. Further details on SQP can be found in Boggs and Tolle (1995). The basic SQP-algorithm with quasi-Newton updates is summarized as:

**Algorithm 4.1 SQP**

i. Guess $x_0$, set $B_0 = I$.

ii. At $x_k$ evaluate $f(x_k), c_\varepsilon(x_k), c_T(x_k), \nabla f(x_k), \nabla c_\varepsilon(x_k)$ and $\nabla c_T(x_k)$.

iii. If a certain curvature condition is satisfied update $B_k$ by a BFGS formula.

iv. Solve (4.3) for $d_k$.

v. Test for convergence.

vi. Find a step-size $\alpha_k$ s.t. $0 < \alpha_k \leq 1$ and $\phi_\nu(x_k + \alpha_k d_k) < \phi_\nu(x_k)$.

vii. Set $x_{k+1} = x_k + \alpha_k d_k$, $k = k + 1$ and go to ii.
4.2 Optimization methods

4.2.1 Reduced gradient methods

The qp (4.3) can be resolved in the full space of free and independent variables, or in the reduced space of free variables by a suitable elimination of variables. Elimination of variables exploits that if \( n_x P - n_u M \gg n_u M \) and that \( n_u M \) is small, the reduced subproblem for the null-space step will be small (but dense). In the full space the sparsity of both the Hessian (which commonly requires analytic Hessians) and the Jacobian can be exploited to yield fast solutions (Rao, Wright, and Rawlings 1998). This section shows that a reduced gradient approach can be derived by following two different strategies. The first uses a sequential approach, see e.g. de Oliveira and Biegler (1995), while the second follows the simultaneous null-space approach (Nocedal and Wright 1999), (Biegler, Nocedal, and Schmid 1995). We only outline the central issues necessary to promote a qualitative comparison of the methods.

**Sequential approach (sQP)**

By iterating the model over the horizon \( P \), the transformation \( x^k = \Psi(x_0, u^k) \) allows the equivalent form

\[
\begin{align*}
\min_{u^k} & \quad f^k_p(u^k) \\
\text{s.t.} & \quad \Psi^k(x_0, u^k) \in \mathcal{X} \\
& \quad u^k \in \mathcal{U}
\end{align*}
\]

(4.4)

The transformation \( \Psi(\cdot) \) for linearized and discretized systems is essentially a projection onto the subspace \( \mathcal{U} \). The sequential approach solves the model at each iteration, i.e. the qp-subproblem is solved following a feasible path strategy. The KKT conditions for problem (4.1) are (temporarily assuming inactive bound constraints on \( x^k \) and \( u^k \) without loss of generality)

\[
\begin{align*}
\nabla_{x^k} f_k + \nabla_{x^k} c_k^T \lambda_k^E &= 0 \\
\nabla_{u^k} f_k + \nabla_{u^k} c_k^T \lambda_k^E &= 0 \\
c_k^E &= 0
\end{align*}
\]

Details on the partial derivatives are given in appendix C.4. We eliminate \( \lambda_k^E = -\left(\nabla_{x^k} c_k^E\right)^T \nabla_{x^k} f_k \), define \( S_k^T = -\nabla_{u^k} c_k^E^T \left(\nabla_{x^k} c_k^E\right)^{-T} \) and get the reformulated KKT conditions

\[
\begin{align*}
\nabla_{u^k} f_k + S_k^T \nabla_{x^k} f_k &= 0 \\
c_k^E &= 0
\end{align*}
\]
Note that the above result also can be derived by considering the total differential of \( c_E^k = 0 \), which is \( \frac{dk^k}{du} = \nabla_{x^k} c_E^k T \frac{dx^k}{du} + \nabla_{u^k} c_E^k T du^k = 0 \), and define \( S_k^T = \left( \frac{dx^k}{du} \right)_T = -\nabla_{u^k} c_E^k T \left( \nabla_{x^k} c_E^k \right)^{-T} \) (hence the notion of sensitivity\(^2\)). In the view of problem (4.4), consider the objective and model derivatives with respect to \( u^k \)

\[
\frac{dh}{du^k} = \nabla_{u^k} f_k + \left( \frac{du^k}{du^*} \right)_T \nabla_{x^k} f_k = \nabla_{u^k} f_k + S_k^T \nabla_{x^k} f_k
\]

\[
\frac{de^k}{du^k} = \nabla_{u^k} c_E^k + \nabla_{x^k} c_E^k S_k
\]

Note that the sensitivity matrix gives search directions \( d_k^u = S_k d_k^u \), hence \( \frac{de^k}{du^k} d_k^u = (\nabla c_E^k)^T d_k \). Also note that by defining \( Z_k^T = [S_k^T \ I] \) we have \( Z_k^T \nabla f_k^T = 0 \). Linearizing the reformulated KKT conditions with respect to \( u^k \) gives the Newton system

\[
\left[ Z_k^T \nabla^2 f_k^T + \nabla f_k \nabla Z_k^T \right] d_k^u = - \left[ \nabla_{u^k} f_k + S_k^T \nabla_{x^k} f_k \right]
\]

We observe that the following \( \mathcal{QP} \) in \( d_k^u \in \mathbb{R}^{n \times M} \) has the same KKT conditions (except for the term \( \nabla f_k \nabla Z_k^T \))

\[
\min_{d_k^u \in \mathbb{R}^{n \times M}} \left( \nabla_{u^k} f_k^T + S_k \nabla_{x^k} f_k^T \right) d_k^u + \frac{1}{2} \left( d_k^u \right)^T \left( S_k^T \nabla^2_{x^k} f_k S_k + \nabla^2_{u^k} f_k \right) d_k^u \quad \text{s.t.} \quad c_E^k^T + \frac{de^k}{du^*} d_k^u = 0
\]

(4.5)

The bound constraints in \( d_k^u \) are restated as

\[
\left[ S_k \quad -S_k \right] d_k^u \leq \left[ x_U^k - x_L^k \quad x^k - x_L^k \right]
\]

The algorithm evolves the model to get \( x^k = \Psi(x_0, u^k) \). Then the algorithm solves the \( \mathcal{QP} \) (4.5) for \( d_k^u \), giving \( u^{k+1} \) which again is used to evolve the model giving \( x^{k+1} \) and so on.

Neglecting the second order derivatives of the model, \( \nabla f_k \nabla S_k^T \), sacrifices the quadratic convergence of Newton’s method, but it gives a positive definite Hessian. This is also known as the Gauss-Newton method, which will deteriorate to linear convergence if the projected contributions of the model

\(^2\)This definition of \( S \) gives the same result as that of de Oliveira (1994), but is faster to compute in MATLAB which benefits from vectorization. Note that the inversion is not necessary to numerically solve for \( S \) from \( AS = B \).
are significant (Biegler 2000). Since the Hessian $H\mathcal{L}^*$ is positive definite, this means that we will have linear convergence (possibly to a saddle or maximum point of the original system) of a convex and small system due to the assumption on $v_M$. We also note that we will have quadratic convergence of (4.5) near the solution, if there are no active bounds at the solution. We observe from (4.4) that it is not meaningful to consider full-space sequential methods.

**Reduced Hessian approach (rSQP)**

In the null-space method a decomposition is applied to the KKT conditions to eliminate variables. Consider the SQP subproblem which at an iterate $k$ generates a search direction $d_k$ by solving

$$
\begin{align*}
\min_{d_k \in \mathbb{R}^{(n_x P + n_u) M}} \quad & g_k^T d_k + \frac{1}{2} d_k^T W_k (x_k, u_k) d_k \\
\text{s.t.} \quad & c^*_k(x, u; k) + A(x, u; k)^T d_k = 0 \\
& x^k \in X \\
& u^k \in U
\end{align*}
$$

(4.6)

Here $\nabla f_k = g_k$, $W_k$ (usually) is a positive definite approximation of $H\mathcal{L}_k$. Where $H\mathcal{L}_k$ is the Hessian of the Lagrangian function $\mathcal{L}(x^k, u^k, \lambda^k) = f_k(x^k, u^k) + \lambda^k^T c^*_k(x^k, u^k)$ evaluated at $(x^*, u^*, \lambda^*)$. $A(x, u; k)$ denotes the constraint Jacobian. The next iterate is computed as $(x_{k+1}, u_{k+1}) = (x_k, u_k) + \alpha_k (d_k^*, d_k^u)$ where $\alpha_k$ is the step length parameter chosen to reduce a suitable merit function. Denote $A(x, u; k) = A_k$ etc.

We partition $(x^k, u^k) \in \mathbb{R}^{(n_x P + n_u) M}$ into state and control variables through the basis given by a nonsingular matrix $[Y_k \ Z_k]$. This allows the representation of the search vector as $d_k = Y_k p_{Y,k} + Z_k p_{Z,k}$. Assume that $Z_k$ is a basis for $N(A^T_k)$, i.e. $A^T_k Z_k = 0$, and that $Y_k$ is a basis for $R(A^T_k)$. Hence, we decompose $d_k$ into a range and null-space component. The model constraint from problem (4.6) can now be rewritten as $c^*_k + A^T_k Y_k p_{Y,k} = 0$. Since $[Y_k \ Z_k]$ is nonsingular, assuming full column rank of $A_k$ leads to $p_{Y,k} = - (A^T_k Y_k)^{-1} c^*_k$ which gives us $d_k = -Y_k (A^T_k Y_k)^{-1} c^*_k + Z_k p_{Z,k}$. We arrive at the reduced size SQP subproblem (considering $p_{Y,k}$ as a constant)

$$
\begin{align*}
\min_{p_{Z,k} \in \mathbb{R}^{n_u M}} \quad & (Z_k^T g_k + Z_k^T W_k Y_k p_{Y,k})^T p_{Z,k} + \frac{1}{2} p_{Z,k}^T Z_k^T W_k Z_k p_{Z,k} \\
& x^k \in X \times \cdots \times X \\
& u^k \in U \times \cdots \times U
\end{align*}
$$

(4.7)

The choice of $Y_k$ and $Z_k$ is motivated by the partitioning into dependent and free variables. Biegler et al. (1995) argues that the partitioning $A^T_k =
\[
[C_k \ N_k] \text{ with }
Z_k = \begin{bmatrix}
-C_k^{-1}N_k \\
I
\end{bmatrix}
Y_k = \begin{bmatrix}
I \\
0
\end{bmatrix}
\tag{4.8}
\]

should be utilized, assuming a non-singular \(C_k\) and \(A_k^T Z_k = 0\). If we choose the natural partitioning \([C_k \ N_k]\) = \[
\begin{pmatrix}
\frac{\partial c_k}{\partial x^k} \\
\frac{\partial c_k}{\partial u^k}
\end{pmatrix}^T
\begin{pmatrix}
\frac{\partial c_k}{\partial x^k} \\
\frac{\partial c_k}{\partial u^k}
\end{pmatrix}^T
\] arising from linearization with respect to \((x^k, u^k)\), this leads to the following relations

\[
Z_k = \begin{bmatrix}
-C_k^{-1}N_k \\
I
\end{bmatrix} = \begin{bmatrix}
S_k \\
I
\end{bmatrix}
\]
\[
d_k^e = p_{Y,k} + S_k p_{Z,k}
\]
\[
d_k^u = p_{Z,k}
\]

Summarizing, the search direction in \texttt{rSQP} has an added range-space component \(p_{Y,k}\) which is not present in the \texttt{sSQP} method. Inserting \(p_{Y,k} = 0\) into (4.7) and comparing with (4.6), we observe that the search directions for the \texttt{sSQP} approach coincide with the \texttt{rSQP} approach for the choice

\[
W_k = \begin{bmatrix}
\nabla^2_{xx} f_k \\
\nabla^2_{uu} f_k
\end{bmatrix}
\]

and with \([C_k \ N_k]\) selected from the linearization. The step \(p_{Z,k}\) is in the null space of \(A_k\), i.e. it is tangential to the constraints, while \(p_{Y,k}\) is in the range space of \(A_k\). Then, informally \(p_{Z,k}\) aims at reducing the objective while \(p_{Y,k}\) searches for feasibility. Since the \texttt{sSQP} method is a feasible path method, \(p_{Y,k}\) is not needed.

In comparing the two approaches we observe that the sequential approach maintains feasibility of all iterates, while \texttt{rSQP} searches for feasibility and optimality simultaneously. In addition the sequential method solves the model at each iteration, while \texttt{rSQP} only solves the model once. We also observe that the sequential method does not utilize BFGS updates, while this must be utilized in \texttt{rSQP} since we do not assume available second order derivatives. Recall that we neglected the cross-term involving second order model derivatives in equation (4.5). We also note that the sequential approach only handles initial value problems (IVP), i.e. \(x_P \in \Omega_x\) cannot be guaranteed since it implements a shooting strategy in evolving the model over the horizon. The endpoint constraint changes the problem into a boundary value problem (BVP) which must be handled by simultaneous strategies. Therefore the sequential approach is limited to open-loop stable
and non-stiff systems. In fact, the stability of the algorithm requires an
infinite prediction horizon which is intractable unless the step length can be
increased to infinity, see de Oliveira (1994) and Chen and Allgöwer (1998a)
for details. We also observe that the reduction of the size of the \(QP\) to be
solved, introduces an additional cost of calculating \(S_k (sSQP)\) and \(Z_k (rSQP)\)
respectively.

Additional equality (or active inequality) constraints reduce the available
degrees of freedom, and consequently a manual decomposition of the Jacobian
\(A_k = [C_k N_k]\) as indicated in section 4.3 is not recommended. There is
a number of commercial routines available for both dense and sparse al-
gebra that can be applied. Decomposition strategies for sparse matrices are
implemented in the Harwell subroutine libraries MA28 and MA48 (Harwell
Laboratory 1995). We observe that in addition to assuming stability, we
must assume non-singularity of \(\nabla x^k e^k\) and \(C_k\). Note that these are sparse
lower triangular matrices of order \(n_x P\). Hence, solving for \(S_k (sSQP)\) and \(Z_k
(rSQP)\) is cheap i.e. of order \(O((n_x P)^p)\), with \(p = 2\) instead of \(p = 3\) due to
sparsity. Since the matrix is both sparse and lower triangular \(p \in [1, 2]\) could
be approached by a proper strategy. Recall that the efficiency of reduced
gradient algorithms relies on the assumption that \(n_x P - n_u M \gg n_u M\)
and that \(n_u M\) is small. Alternatives to computing the Jacobian by analytic
partial derivatives is by perturbation or by forward differences. This will
have a significant impact on the computational demands, see the results in
section 4.3.2.

4.3 Simulations

We implemented NMPC on two cases with three different optimization meth-
ods. The first is a basic full space SQP method following algorithm 4.1.
The second is the reduced Hessian method rFSQP, cf. algorithm 3.1, and
the third is the sequential method (sSQP). The first case is a CSTR while
the second case is grate sintering from chapter 2. The CSTR example was
thoroughly explored by application of various discretization methods and
finite difference approximations to the Jacobian. For the CSTR there are no
nonlinear inequality constraints, and rFSQP switches to nonlinear equality
constrained mode for this case, i.e. it is equivalent to a rSQP method for this
case.
4.3.1 Implementation issues

The basic SQP full-space method was implemented with the common $l_1$-penalty function. The rFSQP algorithm uses sparse linear algebra and, since rFSQP always remain feasible with respect to inequalities, uses an $l_1$-penalty function without penalization of inequality constraints. sSQP implemented an $l_1$-penalty function without penalization of equality constraints, since sSQP always remain feasible with respect to equalities. The different penalty functions are

\[
\phi_{basic}(x_k) = f(x_k) + \nu_k \|c_E(x_k)\|_1 + \nu_k \max \{c_T(x_k), 0\}
\]

\[
\phi_{rFSQP}(x_k) = f(x_k) + \nu_k \|c_E(x_k)\|_1
\]

\[
\phi_{sSQP}(x_k) = f(x_k) + \nu_k \max \{c_T(x), 0\}
\]

where $c_E(x_k)$ is nonlinear equality constraints, and $c_T(x_k)$ is nonlinear inequality constraints. The line search for all methods is backtracking line search (Dennis and Schmabel 1996).

The update rule for the penalty parameter is (Biegler, Nocedal, Schmid, and Ternet 2000):

\[
\nu_{k+1} = \max\left(1.001 + \|\lambda_{k+1}\|_\infty, (3\nu_k + \|\lambda_{k+1}\|_\infty)/4, \nu_0\right)
\]

where $\lambda_{k+1}$ is an estimate of the Lagrange multipliers.

The relaxed convergence criteria from Gill, Murray, and Wright (1981), section 8.2.3, was implemented with tolerance $10^{-5}$ for the basic SQP method and sSQP. In rFSQP the algorithm stops whenever a certain KKT measure is decreased below the tolerance $10^{-5}$. Hence, the rFSQP algorithm does not implement the relaxed termination criteria of Gill et al. (1981). The implementation of rFSQP is generally more carefully performed than the basic SQP and sSQP methods. Hence, the relaxed termination criteria used in basic SQP and sSQP partly compensates for a rudimentary implementation. However, as the discussion in section 4.2 indicates, the sSQP method may show linear convergence in certain circumstances, and relaxed termination criteria can therefore be of crucial importance in production codes as well. For the CSTR case the model was discretized with explicit and implicit Euler, Lobatto IIIC and ordinary Runge-Kutta 4. The Jacobian matrices with almost block-diagonal (ABD) structure for the selected discretization methods are given in appendix C. The CSTR case was implemented with both analytic Jacobian and finite difference approximations of the Jacobian. Finite differences were considered for both the full Jacobian (a dense matrix) and the elements along the block diagonal (a sparse matrix). In sSQP analytic and finite difference Jacobians were implemented as documented in
4.3 Simulations

appendix C.4. I.e. the sensitivity matrix $S$ was approximated directly by finite difference perturbations of the simulator. The CSTR case was investigated with different sampling rates and prediction and move horizons. For the sinter case only aSQP using MATLAB’s ode15s and rFSQP using Lobatto IIIC were investigated.

4.3.2 Case 1: CSTR

Case 1 is the following isothermal CSTR with 1st order reaction from Matsunara and Kato (1967) also investigated by de Oliveira (1994)

$$\frac{dx_1}{dt} = u_1 + u_2 - k_1 x_1$$

$$\frac{dx_2}{dt} = (C_{B_1} - x_2) \frac{u_2}{x_1} + (C_{B_2} - x_2) \frac{u_2}{x_1} - \frac{k_2 x_2}{1 + x_2}$$

(4.9)

with parameter values $k_1 = 0.2$, $k_2 = 1$, $C_{B_1} = 24.9$ and $C_{B_2} = 0.1$. For $(u_1, u_2) = (1, 1)$ the CSTR has three equilibrium points at $x_1 = 100$, $x_2 \in (0.633, 2.72, 7.07)$, with the middle equilibrium point being unstable, and the others stable. The system (4.9) was discretized with a time step $h$, prediction horizon $P$, move horizon $M$ and simulated for $N_{MPC}$ samples, i.e. the NMPC problem is repeatedly solved $N_{MPC}$ times. At time step 10 the process experiences a +50% step in $C_{B_1}$ which is seen by the NMPC algorithm through the feedback only. We choose $Q = 10 I_n$ and $R = I_{n_u}$ in equation (4.1) and penalize deviation from stationary values. I.e. the control objective is to keep the states and controls at their initial values $x = (100, 0.633)$ and $u = (1, 1)$.

We require that the physical bounds $(x_i, u_i) \geq 0$ are maintained over the horizons. The SQP-algorithms were initialized with the output from the previous call for each NMPC iteration. Note that integral action is not implemented. This is justified by the fact that we are mainly interested in comparing the optimization methods, and we expect that introducing integral action will not influence on this comparison. A representative simulation result is shown in figure (4.1). The process was simulated by MATLAB’s ode45 in all cases.

Note that with the given initial conditions and the given disturbance, this case is pathological with respect to inequality constraints, i.e. the active set is empty and unaltered throughout the horizon $P$. The control inputs in figure 4.1 are nearly constant after a short transient subsequent to the parameter disturbance. Observing this typical behavior of the NMPC methods, we searched for the optimal control among those at set point until the step appears and constant thereafter. This produced the contours of figure (4.2). The figure caption provides a more detailed description on how the contours
Figure 4.1: *NMPC of CSTR*. The figure shows typical results for NMPC of the CSTR case with $h = 1$. The various discretization methods produced nearly identical results. In the lower subfigure the solid curve is for $u_1$ and the dashed curve is for $u_2$. The step in $C_{B_1}$ enters at time step 10, and this drives the state $x_2$ away from the equilibrium. If the control inputs are kept at the equilibrium input $[1, 1]$, the system will settle at an equilibrium point at $x = (100, 15.94)$.

were generated. Observe the steep contours on the figure indicating that even minor deviations will influence on the result. Observe also that the contours were generated for the class of constant controls described above, and do not match the contours for the different NMPC implementations. The contours are elongated, i.e. the system is poorly conditioned.

The computations were implemented in MATLAB with the *qp*-routines available as *mex* files on a Compaq Deskpro EN / Pentium II / 450MHz / 128Mb RAM running Windows NT4.0. Computational results are shown in tables 4.1-4.3 The results in tables 4.1-4.3 are summarized in the following conclusions:

- **sSQP** is sensitive to the choice between implicit and explicit integration methods, while both basic **SQP** and $r(F)/SQP$ is insensitive to this.

- Finite difference approximations of the full Jacobian in basic **SQP** and $r(F)/SQP$ should be avoided.

- $r(F)/SQP$ is superior for large number of variables.
4.3 Simulations

Figure 4.2: Contours of NMPC of CSTR. Contours of constant control. The control \( u \) was fixed at the stationary value \( u = [1, 1] \) until the step in \( C_B \) entered. Then \( u \) was set to another constant value for remaining part of the horizon. The objective minimum 23.6 at \((u_1, u_2) = (0.67, 1.33)\) is marked by a \( \times \). Note that the optimum is located at the floor of a narrow valley with elongated contours. The condition number is \( 9 \cdot 10^{10} \).

In the list above the notation \( r(F)SQP \) emphasizes that in this case, \( rFSQP \) is equivalent to \( rSQP \). Note that a consequence of the first item is that simultaneous SQP methods can have fewer variables when implemented with implicit discretization methods. I.e., the step length \( h \) can be increased beyond the stability limit of explicit methods (but not beyond reasonable accuracy). Since the basic SQP and \( sSQP \) methods are approximately similar in implementation complexity, \( sSQP \) should be chosen when explicit discretization schemes suffice. In the face of more challenging processes reduced Hessian methods are superior provided that the assumption that there are few degrees of freedom continue to hold. This assumption commonly holds in NMPC. Note that none of the problems reported in tables 4.1-4.3 could be solved by the MATLAB NAG toolbox routine e04ucf. The CSTR example has also been solved by de Oliveira (1994), but there the focus is on viability of the \( sSQP \) method and no comparisons to other approaches are given.

As a preparation for section 4.3.4, some additional simulations were performed. The consequence of terminating \( sSQP \) early (after one SQP iteration) was investigated, since it is of interest to see whether this significantly im-
<table>
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<tr>
<th>Discretization method</th>
<th>Horizons ( h/P/M )</th>
<th># vars. tot/dep/free</th>
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Table 4.1: Nonlinear MPC on a CSTR. Basic SQP. The table shows results for the basic SQP method. \( h/P/M \) are the sampling time, prediction and move horizons. The \# vars. tot/dep/free are the total, dependent and free number of variables. Note that there are no active inequality constraints in this case. The Jacobian is either analytic or approximated by finite differences. In mode \( fd1 \) only elements along the block diagonal were approximated, while in mode \( fd2 \) the full (dense) Jacobian was approximated. Obj is the objective value measured by summing the actual process outputs and implemented control actions over the MPC horizon \( N_{MPC} \). CPU time is the time measured by MATLAB's \texttt{cputime} command from start to end of the main MPC loop.

pains the performance. On the CSTR case terminating after 1 SQP iteration gave nearly identical results as compared to figure 4.1 and table 4.1. For the CSTR case the sSQP algorithm always terminates after 3-4 iterations. The similarity between early termination and normal termination is explained by that the first step gets very close to the optimum, and the following steps only provide minor improvements to the first step. However, early termination is problem dependent and for the sintering case other results are achieved, see the discussion of figure 4.5 and 4.6 in section 4.3.4.
### 4.3 Simulations

<table>
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<tr>
<th>Discretization method</th>
<th>Horizons $h/P/M$</th>
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Table 4.2: *Nonlinear MPC on a CSTR: ssQP*. The table shows results for the ssQP method. The results for ode45 with $h = 2$ showed some ripple that were caused by the relaxed termination criteria. See table 4.1 for explanation of symbols.

#### 4.3.3 Large scale applications of rFSQP

The rFSQP algorithm was tested on (pathological) large problems by decreasing the sampling time $h$ to give very long prediction horizons in the CSTR case. The move horizon was limited to 20 in these simulations in order to limit the size of the constraint Jacobian for the qp\(^3\).

The rFSQP algorithm was tested on the CSTR case with 40000 dependent and 20 free variables. This was done by choosing a very small step length and adjusting the prediction and move horizons accordingly. The task manager image in figure 4.3 shows that the system is running close to its limits. In particular, the lack of physical memory is critical. Attempts to run rFSQP with 100000 variables failed with an "unhandled exception" message from Windows.

\(^3\)The NAG toolbox routine s04naf needs the Jacobian as a dense matrix.
<table>
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<th>Discretization method</th>
<th>Horizons $h/P/M$</th>
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Table 4.3: *Nonlinear MPC on a CSTR: rFSQP*. The table shows results for the rFSQP method. See table 4.1 for explanation of symbols.

The text below is a copy of the text output on screen during the first 90 iterations. The algorithm was interrupted after this, and the results are plotted in figure 4.4. The results show that the algorithm works well, but machine limitations limit application to large scale problems.

The rFSQP algorithm has an option that allows direct call of the subroutine MA28BD if a pivoting sequence from MA28AD is given. This reduces the computational burden in NMPC where the SQP algorithm is called repeatedly, since complete refactoring is not necessary at each call from the outer NMPC algorithm. From the printout below it is observed that each SQP iteration in the beginning takes about 45 seconds. This includes initialization, LU decomposition by MA28BD, calculation of the range and null space steps and a convergence test. However, disk swapping adds considerably to computational times and with more physical memory, the computational time will decrease.

It is important to note that inadequate memory handling in MATLAB causes memory leaks in the program, i.e. when MATLAB enters a subfunction it allocates memory to the internal variables. Upon exit, the variables are

URN:NBN:no-1287
deleted but memory does not seem to be completely deallocated. Hence, each time MATLAB calls a subfunction, it leaks memory up to the size of the local variables. To the best of the authors knowledge, the only solution to this problem is to make all variables global. In rFSQP all matrix variables are sparse and global, but vectors are not global. Note that if a subroutine allocates 10 vectors of 100000 variables at each call, MATLAB will leak up to

Figure 4.3: *Task manager crop image.* The image shows the task manager when running rFSQP on the CSTR case with 40000 dependent variables. As can be seen all physical memory is occupied, and the page file is almost fully occupied. The CPU load is very low due to excessive disk swapping.
2Mb (in double real) at each call.

Printout from screen:

*****************************************************************************
* NMPC/CSTR: RK4    *
* Frode Martinsen, 28/06/01    *
*****************************************************************************
RK4 w/rFSQP (ANALYTIC=1)
Total nos. of vars.: ntot=40020 (dependent=40000, free=20)
MPC: It:5/11999 (CTOT=3.3e+002s, CTnow=45s. Last iSQP=1)
MPC: It:10/11999 (CTOT=5.4e+002s, CTnow=41s. Last iSQP=1)
STEP =1
MPC: It:15/11999 (CTOT=2.6e+003s, CTnow=3.1e+002s. Last iSQP=4)
MPC: It:20/11999 (CTOT=4.3e+003s, CTnow=3.5e+002s. Last iSQP=4)
MPC: It:25/11999 (CTOT=8.9e+003s, CTnow=1.1e+003s. Last iSQP=4)
MPC: It:30/11999 (CTOT=1.4e+004s, CTnow=1.3e+003s. Last iSQP=4)
MPC: It:35/11999 (CTOT=1.6e+004s, CTnow=3.7e+002s. Last iSQP=4)
MPC: It:40/11999 (CTOT=1.8e+004s, CTnow=5.1e+002s. Last iSQP=4)
MPC: It:45/11999 (CTOT=2e+004s, CTnow=4e+002s. Last iSQP=4)
MPC: It:50/11999 (CTOT=2.2e+004s, CTnow=3.6e+002s. Last iSQP=4)
MPC: It:55/11999 (CTOT=2.4e+004s, CTnow=3.5e+002s. Last iSQP=4)
MPC: It:60/11999 (CTOT=2.6e+004s, CTnow=3.3e+002s. Last iSQP=4)
MPC: It:65/11999 (CTOT=2.8e+004s, CTnow=3.7e+002s. Last iSQP=4)
MPC: It:70/11999 (CTOT=2.9e+004s, CTnow=3.4e+002s. Last iSQP=4)
MPC: It:75/11999 (CTOT=3.1e+004s, CTnow=3.9e+002s. Last iSQP=4)
MPC: It:80/11999 (CTOT=3.3e+004s, CTnow=3.7e+002s. Last iSQP=4)
MPC: It:85/11999 (CTOT=3.5e+004s, CTnow=4.1e+002s. Last iSQP=4)
MPC: It:90/11999 (CTOT=3.7e+004s, CTnow=5.7e+002s. Last iSQP=4)

4.3.4 Case2: Grate sintering

The sintering process from chapter 2 is a batch process. Hence, stability of the nonlinear MPC algorithm with the objective (2.6) is not essential to the performance of the algorithm. The limited accuracy of the model, cf. section 2.7, indicates that analyzing nominal stability of the nonlinear MPC algorithm is of little value. Hence, checking whether the suggested objective (2.6) is a Lyapunov function is not considered. Due to the problem defined
Figure 4.4: \textbf{rFSQP on large scale CSTR.} The figure shows the results from rFSQP after interruption at NMPC iteration 90. Comparing with figure 4.1, the sampling period $h = 0.005$ used in this figure implies that 200 time steps here corresponds to 1 time step in figure 4.1. I.e. the 80 datapoints from the step enters in this figure corresponding to about a half time step in figure 4.1. Hence, the state and control values cannot be visually distinguished in the two figures, and the results are concluded to be good. Note that the step enters at time step 10 in both figures which is not the same physical time. Physical time is given by $h \cdot \text{timestep}$.

in equation (2.6), this is a large scale problem with a nonlinear inequality constraint and a large number of equality constraints.

The reduced model defined in section 2.5.2 was simulated with the implicit MATLAB solver \texttt{ode15s} in section 2.5. Attempts to simulate the model with explicit Runge-Kutta of 4th order (RK4) failed due to numerical instabilities (recall the condition number of $\sim 10^{14}$ for the constraint Jacobian $\frac{\partial f}{\partial x}$ at the initial point). In nonlinear MPC with rSQP and the model discretized by RK4, the algorithm spent about 90 seconds in forming the initial $[\frac{\partial f}{\partial x}, \frac{\partial f}{\partial u}]$ of size $P \cdot 5n_x \times (P \cdot 5n_x + M \cdot n_u) = 11600 \times 11640 \approx 270Mbyte$ (as a sparse matrix!) with $n_x = 29$ and $n_u = 1$. The horizons $P = 80$ and $M = 40$ were selected to give a prediction horizon of 40 minutes with a sampling rate $h = 30s$. Note that the reduced Hessian is of size $40 \times 40$, and approximating this by a dense BFGS matrix presents no limitations.

The algorithm spent about 130 seconds in LU-decomposition inside \texttt{MA28AD}.

\footnote{The PC used had only 128\text{MB} memory. Virtual memory on the disk was in use.}
The computed steps for the first SQP-iteration was in the order \( \|p_Y\| \sim 10^{28} \)
and \( \|p_Z\| \sim 10^{24} \) indicating a large error introduced by inadequate discretization. With the use of Lobatto IIIC, the sintering process could be simulated with a step length \( h = 1 \). With a 45 minute prediction horizon this leads to a problem with approximately \( 2 \times 78300 \) dependent variables\(^5\). A sparse Jacobian for this case requires about 3.2Mb using double real format.

Single shooting (ssQP) for the reduced sinter model did not converge. Lack of robustness of single shooting is well known, see (Barclay, Gill, and Rosen 1998) and (Ascher, Mattheij, and Russell 1995). The results presented for ssQP in figure 4.5 and 4.6 were obtained by limiting the number of SQP iterations to 5 and 1 respectively. The line search was aborted after 5 iterations in both cases. Note that aborting the line search was done in order to reduce the number of model evolutions to obtain \( \hat{x} \) (superscript notation defined above equation (4.1)). Aborting the line search will not guarantee that the step taken gives descent. The number of control breaks were limited to 3 by control action blocking. The sensitivity matrix then has three columns, each corresponding to one control break. Perturbing \texttt{ode15s} to get \( S \) is done by three evolutions, which took about 75 seconds. Note that \( S \) is a narrow and dense lower trapezoidal matrix. The computational times given in the figures are longer than the batch time, and the approach cannot be implemented in the industrial plant. The objective value in figure 4.5 (see text on top) is lower than the number given in figure 4.6.

### 4.4 Discussion

In this chapter we implemented different MPC strategies on two cases and investigated the computational load and quality. From tables 4.1-4.3 we observe that among the different NMPC methods, the ssQP method seems preferable in view of computational time. In NMPC computational time is limited, and feasibility of intermediate iterates is essential for stability (Mayne, Rawlings, Rao, and Scokaert 2000), (Scokaert, Mayne, and Rawlings 1999). SQP is an adaptive subproblem, i.e. its computational time is not deterministic. Consequently, in NMPC feasible path SQP methods are preferred since they allow termination prior to convergence (Mayne 1997). Such methods must solve the model constraints at each SQP iteration, which may be time consuming if the model is represented with an implicit discretization scheme. Hence, ssQP becomes computationally demanding if implicit dis-

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\(^5\)The 2\(s\) follows from the additional set of variables in Lobatto IIIC.
Figure 4.5: NMPC of reduced sinter model with SSQP, MAXIT=5. The figure shows the results applying SSQP to the reduced sinter model. The full sinter model was used as process simulator. The upper part shows the gas temperatures. The dashed line indicates the fusion temperature. The boldface curve is the measured ignition temperature, while the solid curves show the computed profiles at spatial discretization levels \( n = 2, 5, 10 \) where \( n = 10 \) is the bottom level. The second subfigure shows the solid temperature profiles at levels \( n = 1, 2, 5, 10 \) along with the measured temperature profile (boldface) at 15cm depth, cf. figure 2.11. The dashed line shows the fusion limit. The third subfigure shows the computed coke concentrations at levels \( n = 1, 2, 5, 10 \). The last subfigure shows the computed control input \( v \) (solid). The dashed-dotted line shows the control profile \( u_k \) computed for the last iteration of the NMPC algorithm, and is only included to show the effect of control action blocking, i.e. the time scale is not relevant for this profile.

cretization methods are applied, whereas rSSQP preforms equally well regardless of whether implicit or explicit discretization scheme is applied. Both methods require that the selected discretization scheme is appropriate, i.e. if the model cannot be simulated with a given method, it cannot be expected that the optimization algorithms perform well either.

Feasibility with respect to inequality constraints is easier to achieve. The FSQP method of Titis and co-workers (Lawrence and Titis 2000), (Lawrence and Titis 1996), and the rFSQP method from chapter 3 maintain feasibility with respect to inequality constraints, and asymptotic feasibility with respect to nonlinear equality constraints by combining these with an exact penalty function and an arc search. The feasible path SSQP method investigated
in section 4.2.1 does not seem to perform well in the presence of strong nonlinearities. This is contradictory to the needs for NMPC; problems with strong nonlinearities and trajectory tracking (Qin and Badgwell 2000).

The large scale example investigated in section 4.3.3 shows that application of rFSQP in the grate sintering case is not computationally feasible with the presently available computing equipment. Hence, this has not been solved. Grate sintering is a complex process with pronounced nonlinearities and where the time constants of the system differ by many decades in magnitude. Hence, application of real-time optimization methods like nonlinear model predictive control to the grate sintering process is challenging.

The thesis still contributes to the application of model based control to grate sintering. The thesis gives a framework for implementing nonlinear model based control of grate sintering by giving a control objective. Further, a nonlinear model along with an appropriate discretization scheme is presented. To complete the course of NMPC for grate sintering two directions may be investigated; providing a better discretization method or acquiring a better computer. Reimplementing rFSQP in C++ or FORTRAN may also be
4.5 Conclusion

The practical considerations discussed in this chapter explore the choices an engineer must take if he wants to implement NMPC at a given process. The interplay between discretization methods and optimization algorithms has been investigated informally.

First the engineer must select an appropriate discretization scheme. If he chooses an explicit discretization scheme, he can choose between sequential or simultaneous optimization methods. Sequential methods are easy to implement, while simultaneous methods are harder to implement. This applies in particular to reduced Hessian methods which may be quite sophisticated. If implicit discretization methods must be applied, the performance of zSQP deteriorates while rSQP does not degrade.
Chapter 5

Conclusion

5.1 Conclusions to the thesis

Grate sintering

A reduced order model of the grate sintering process was developed from models available in the literature. Both the full model and the reduced model were simulated with the MATLAB function ode15s, which is an implicit variable step length solver of varying order. Industrial experiments including special measurements were conducted, and the data was used for model adaption and assessing the control objective. The models were adapted by visual comparison to data collected from industrial experiments. Data analysis supports the proposed control objective. The reduced model is less computationally demanding, and reproduces the important process states satisfactorily.

A control objective for use in nonlinear MPC was suggested and assessed by data analysis based on industrial data.

In conclusion, the fusion model needs to be refined, the gas velocity must be included as a state and pressure must be used as control input before the model can be used in an industrial model based control setting. Improved numerical schemes must be investigated if the model is to be applied in real-time optimization. The reduced model provides an adequate basis on which to continue.

rFSQP

The optimization algorithm is described, and global and local convergence results are given. The algorithm was implemented in MATLAB and tested
on small scale problems. The algorithm is a reduced Hessian method and the algorithm is expected to be efficient for large scale problems with few degrees of freedom.

The algorithm worked well, and it is concluded that the present MATLAB implementation serves as a good alternative for small to medium scale problems with, say, up to 10000 variables. A number of possible algorithmic extensions to the algorithm may be implemented and tested on the existing platform. In particular, analytic Hessians and trust-region extensions should be investigated. A watch-dog algorithm should also be implemented.

NMPC

A qualitative comparison between sequential and simultaneous reduced gradient methods is given and illuminates the similarities and differences between these approaches. The comparison was supplemented with simulations on a simple nonlinear MPC case, where the interplay between choices among various optimization methods and discretization methods was investigated.

The rFSQP algorithm was tested on a simple large scale problem with promising results. However, the computing environment limits testing on very large scale problems with number of variables in the range from 100000 and upwards. Hence, the algorithm was not tested on the grate sintering case which has about 150000 variables when discretized with Lobatto IIIC.

The sequential method sSQP was tested on the sintering case with termination prior to convergence. The results are modestly encouraging, since the computational load is excessive. It is concluded that simultaneous optimization algorithms are well suited for problems where explicit discretization methods are inadequate.

The grate sintering case should be implemented with discretization schemes allowing fewer variables, or alternatively ran on a more powerful computer.

rFSQP should be reimplemented in C++ or FORTRAN to allow for large scale applications. Further testing on large scale applications, in particular problems with nonlinear inequalities, should be performed.
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Appendix A

Appendices to chapter 2

A.1 Sinter objective

The objective from equation (2.6) is restated

\[
\phi = \int_0^{t_{end}} \int_0^{t_{end}} w(z) \frac{1}{1 + e^{k_1(T_s - T_{fu})}} (T_s - T_{fu}) dt dz
\]

\[
\psi_j = \int_{t=0}^{t_{end}} \sigma(T_s)(T_s - T_{fu}) dt
\]

The double integral is approximated by a sum over the prediction horizon for each spatial element \( j \). Choosing \( P \cdot h = t_s \) where \( h \) is the sampling time and \( t_{end} \) is the sintering batch time. The integrals are approximated by summation:

\[
\phi = \sum_{j=1}^{n} w_j \sum_{k=1}^{P} \frac{1}{1 + e^{k_1(T_{s,k} - T_{fu})}} (T_{s,k} - T_{fu})
\]

\[
\psi_j = \sum_{k=1}^{P} f_k(T_s) = \sum_{k=1}^{P} \frac{1}{1 + e^{k_1(T_{s,k} - T_{fu})}} (T_{s,k} - T_{fu}) \text{ for } j = 1, \ldots, n
\]

where \( n \) is the spatial resolution and \( w_j \) are weights. The kernel \( f_k \) for a given \( j \) is considered.

\[
f_k = \frac{(T_{s,k} - T_{fu})}{1 + e^{k_1(T_{s,k} - T_{fu})}}
\]
The gradient is
\[ g_k = \frac{\partial f_k}{\partial T_{i,k}} = -\frac{k_1(T_{i,k} - T_{fu})e^{k_1(T_{i,k} - T_{fu})}}{(1 + e^{k_1(T_{i,k} - T_{fu})})^2} + \frac{1}{1 + e^{k_1(T_{i,k} - T_{fu})}} \]

The Hessian is
\[ H_k = \frac{\partial^2 f_k}{\partial T_{i,k}^2} = \frac{2k_1^2(T_{i,k} - T_{fu})e^{k_1(T_{i,k} - T_{fu})}}{(1 + e^{k_1(T_{i,k} - T_{fu})})^3} - \frac{2k_1e^{k_1(T_{i,k} - T_{fu})}}{(1 + e^{k_1(T_{i,k} - T_{fu})})^2} - \frac{k_1^2(T_{i,k} - T_{fu})e^{k_1(T_{i,k} - T_{fu})}}{(1 + e^{k_1(T_{i,k} - T_{fu})})^2} \]

The variable vector for the reduced sinter model with \( n \) spatial stages is
\[ x = [x_1^T, x_2^T, \ldots, x_n^T, u_0^T, \ldots, u_M^T]^T \]

where the subscript is the time index \( k \) and the superscript is the spatial index \( j \). The gradient of \( \psi_{xj} \) is formed as \( \nabla_x \psi_j = [0, \ldots, 0, g_{1,j}, \ldots, 0]^T \) which gives \( \nabla_x \psi_j = [0, \ldots, 0, g_{1,j}, \ldots, 0, g_{2,j}, \ldots, 0, g_{P,j}, \ldots, 0]^T \). The objective gradient is
\[ \nabla_x \phi = \sum_{j=1}^{n} w_j \nabla_x \psi_j = [0, \ldots, 0, w_1 g_{1,j}, w_2 g_{2,j}, \ldots, w_n g_{n,j}, 0, \ldots, 0, w_1 g_{1,j}, w_2 g_{2,j}, \ldots, w_n g_{n,j}, 0, \ldots, 0, \ldots, 0, w_1 g_{1,j}, w_2 g_{2,j}, \ldots, w_n g_{n,j}, 0, \ldots, 0]^T \]

finally
\[ \nabla \phi = [\nabla_x \phi^T, \nabla_u \phi^T]^T = [\nabla_x \phi^T, 0, \ldots, 0]^T \]

The objective Hessian is formed as a block diagonal matrix with \( \nabla^2 \phi_j = w_j H_{k,j}, k = 1, \ldots, P \) along the block diagonal. Observe that there are no couplings across spatial discretization boundaries or time indexes.

### A.2 Pitot measurements

The pitot measurements are shown in figure A.1. These measurements give an estimate of the gas velocity in the pipe following the cyclones, see figure 2.8. The gas velocity in the sintering pans is upward limited by the gas velocity shown in the figure. Through consideration of the pressure drops across the two pans connected in parallel an estimate of the gasflow through the pan can be achieved. This relies on identification of cracks, channelling effects and pipe leaks. The gas volumetric flow can be calculated from the pitot measurements. This allows further adaption of the gasflow predicted by the model. This is left as future work.
A.2 Pitot measurements

Figure A.1: *Experiment 1: Pitot measurements.* The figure shows measurements placed after the cyclones shown in figure 2.8 during all three batches included in experiment 1. Subfigure 1 shows the pitot pressure measured by a dP-cell connected to a pitot sensor. Subfigure 2 shows the gas temperature measured at the same spot. The third subfigure shows the absolute pressure which is calculated by $p_{atm} - p_{2,bsd}$ where $p_{2,bsd}$ is the solid curve in figure 2.11, subfigure 2. Subfigure 4 shows gas density calculated from the ideal gas law by assuming dry air and using $p_{abs}$ from subfigure 3. Subfigure 5 shows the calculated gas velocity using the relation $v = \sqrt{\frac{2 \cdot 0.8 \cdot p_{atm}}{\rho_g}}$. 
Appendix B

Appendix to chapter 3

B.1 Proof of lemma 3.3

The lemma is restated for ease of reading:

**Lemma B.1** Suppose assumptions 3.1-3.6 hold. Suppose $x_k \in X_I$ is not a KKT point for the NLP, $B_k$ is symmetric positive definite and $\eta_k > 0$. Then

1) $D\phi_k(x_k, d_k) < 0$, and

2) $\langle \nabla c_i^T(x_k), d_k \rangle < 0$, for all $i \in J_k^c$

3) $\phi_k(x_j) - \phi_k(x_{j+1}) \geq \gamma \nu \left[ \left\| Z_j^T g_j \right\|^2 + \left\| c_j \right\|_1 \right]$ for the good iterates $j$ and constant $\nu_j$ in (3.11).

**Proof:** The descent property follows by an appropriate choice of the penalty parameter $\nu$ in (3.11). The directional derivative is

$$D\phi_k(x_k, d_k) = \langle g_k, d_k \rangle - \nu_k \left\| c_k \right\|_1 = \langle g_k, Y_k y_k \rangle + \langle Z_k^T g_k, p_{Z,k} \rangle - \nu_k \left\| c_k \right\|_1$$

From (3.15) and (3.18) $\langle g_k, Y_k y_k \rangle = \langle \lambda_k, c_k \rangle$. Recalling $\langle \lambda_k, c_k \rangle \leq \lambda_k \left\| c_k \right\|_1$ and by choosing $\nu_k \geq \| \lambda_k \|_\infty + 2\rho$ for a constant $\rho > 0$, we get

$$D\phi_k(x_k, d_k) \leq \langle Z_k^T g_k, p_{Z,k} \rangle - 2\rho \left\| c_k \right\|_1$$

We have $B_k p_{Z,k} = -\langle \zeta_k w_k + Z_k^T g_k \rangle$ from (3.17). Considering $B_k s_k = \alpha_k B_k p_{Z,k}$ and equation (3.38) as in Biegler et al. (1995), section 3.4,

$$\cos \theta_k^{BFGS} = \frac{\langle s_k^T B_k s_k \rangle}{\| s_k \| \| B_k s_k \|} = \frac{\langle Z_k^T g_k + \zeta_k w_k, p_{Z,k} \rangle}{\| Z_k^T g_k + \zeta_k w_k \| \| p_{Z,k} \|}$$
is well-defined. We have that
\[
D\phi_k(x_k, d_k) \leq -\| Z_k^T g_k + \zeta_k w_k \| \| p_{Z,k} \| \cos \theta_k^{BF} - \zeta_k \langle w_k, p_{Z,k} \rangle - 2\rho \| c_k \|_1
\]
holds for all \( k \). This is equation (68) in Biegler et al. (1995), and the derivation for the good iterates indexed by \( j \) follows
\[
\frac{\| s_k \|}{B_k s_k} = \frac{\| p_{Z,k} \|}{\| Z_k^T g_k + \zeta_k w_k \|}
\]
and the assumption \( \beta_3 > 1 \) is valid since \( \beta_3 \) is an upper bound. We get
\[
D\phi_k(x_k, d_k) \leq -\frac{\beta_1}{\beta_3} \| Z_j^T g_j \|^2 + \left[ 2\zeta_j \cos \theta_j^{BF} \| g_j^T Z_j w_j \| - \zeta_j w_j^T p_{Z,j} \right] - 2\rho \| c_j \|_1
\]
Choosing
\[
2\zeta_j \cos \theta_j^{BF} \| g_j^T Z_j w_j \| - \zeta_j w_j^T p_{Z,j} \leq \rho \| c_j \|_1
\]
gives for all good iterates
\[
D\phi_k(x_k, d_k) \leq -\frac{\beta_1}{\beta_3} \| Z_j^T g_j \|^2 - \rho \| c_j \|_1 \tag{B.3}
\]
which is zero only at KKT points according to (3.44). As in Biegler et al. (1995) we get the update rule (for all iterates)
\[
\zeta_k \left[ 2 \cos \theta_k^{BF} \| g_k^T Z_k w_k \| + w_k^T B_k^{-1} Z_k^T g_k + \zeta_k w_k^T B_k^{-1} w_k \right] \leq \rho \| c_k \|_1 \tag{B.4}
\]
This inequality is clearly consistent for a sufficiently small and positive \( \zeta_k \), hence \( 0 < \zeta_k \leq 1 \) is feasible and gives descent. For the non-good iterates the angle \( \theta_k^{BF} \) is \( \pi/2 \) so
\[
-\zeta_k w_k^T p_{Z,k} \leq \rho \| c_k \|_1 \tag{B.4}
\]
holds, giving
\[
D\phi_k(x_k, d_k) \leq -\| Z_k^T g_k + \zeta_k w_k \| \| p_{Z,k} \| \cos \theta_k^{BF} - \rho \| c_k \|_1
\]
which is nonpositive, and zero only at KKT points since \( c_k = 0 \) implies \( w_k = 0 \). The first claim is proved.

To prove item ii), strict feasibility, from lemma 3.2 i) we have \( \gamma_{k-1} < 0 \) otherwise by lemma 3.2 ii) and equation (3.51), the algorithm would have
stopped in step (vii). Then, since $Z_k^T \nabla e_{I,k} = 0$, $i \in J_k^c$ we have by (3.15) and the associated definition of $c_k$

$$\langle \nabla e_{I,L}^i(x_k), d_k \rangle = \langle Y_k^T \nabla e_{I,L}^i(x_k), p_{I,k} \rangle = r_k \gamma_{k-1} < 0$$

for $i \in J_k^c$.

To establish the third claim we follow the derivation of lemma 4.1 of Biegler et al. (1995). From (B.3) we have

$$D\phi_k(x_k, d_k) \leq - b_2 \left( \| Z_j^T g_j \|^2 + \| c_j \|_1 \right)$$

where $b_2 = \{ \beta_1 / \beta_3, \rho \}$. Continuing as in Biegler et al. (1995) we establish

$$\| d_j \|^2 \leq 3 \gamma_0^2 \left\| \frac{p_{Z,j}}{\gamma_0} \right\|^2 + 3 \gamma_0^2 \| c_j \|^2$$

where $\| c_j \|^2 \leq \sup_{x_j \in X_j} \| c(x_j) \| \| c_j \|_1$, since $\| \cdot \|_1 \leq \| \cdot \|_1$. From (B.2), the assumption $\| w_k \| \leq \kappa_c \| c_k \|^{1/2}, \| \cdot \|_1 \leq \| \cdot \|_1$, $\zeta_j \leq 1$ and $a^2 + 2ab + b^2 \leq 3a^2 + 3b^2$ for $a, b \geq 0$ we have

$$\| p_{Z,j} \|^2 \leq \frac{3}{\beta_2^2} \left( \| Z_j^T g_j \|^2 + \| p_{Z,j} \|^2 + \| c_j \|_1 \right)$$

giving

$$\| d_j \|^2 \leq - \frac{9 \beta_0^2}{\beta_2^2} \| p_{Z,j} \|^2 + \left( \frac{9 \beta_0^2}{\beta_2^2} \kappa_c^2 + 3 \gamma_0^2 \sup_{x_j \in X_j} \| c(x_j) \| \right) \| c_j \|_1$$

$$\leq b_3 \left( \| Z_j^T g_j \|^2 + \| c_j \|_1 \right)$$

where

$$b_3 = \max \left\{ \frac{9 \beta_0^2}{\beta_2^2}, \frac{9 \beta_0^2}{\beta_2^2} \kappa_c^2 + 3 \gamma_0^2 \sup_{x_j \in X_j} \| c(x_j) \| \right\}$$

The non-zero lower bound on $\alpha > \frac{1 - \theta \kappa_0 \beta_1}{\beta_2 \beta_3}$ holds and the Armijo condition then holds for $\alpha_j = \tau \alpha$. Then $-D\phi_k(x_j, d_j) \geq b_2 \left( \| Z_j^T g_j \|^2 + \| c_j \|_1 \right)$ in equation (3.40) gives

$$\phi_k(x_j) - \phi_k(x_{j+1}) \geq \gamma \nu \left( \| Z_j^T g_j \|^2 + \| c_j \|_1 \right)$$
where

$$\gamma_j = \theta_j^{BFGS} b_2 \min \left\{ 1, \frac{(1 - \theta_j^{BFGS}) \tau b_2}{b_1 b_3} \right\}$$

where \( \min \) is only needed to handle an \( \alpha_j = 1 \). \( \square \)
Appendix C

Appendices to chapter 4

The almost block diagonal (ABD) form used in nonlinear MPC in chapter 4 is derived in detail below. The ABD form depends on the discretization method. General ABD forms are given for explicit Euler, Runge-Kutta of 4th order (RK4) and for Lobatto IIIc. The ABD forms are given for a general nonlinear model $\dot{x} = f(x, u)$ with prediction horizon $N$ and move horizon $M$. Only the model constraint over the horizon is considered, but additional constraints can be fitted into the same scheme. Note that for distributed systems the Jacobian $\nabla_{x,u} f(x, u)$ has a sparse structure that should be exploited. This is not considered in the following, since it is problem dependent.

C.1 Explicit Euler

Explicit Euler gives the discretization scheme

$$x_{k+1} = x_k + hf(x_k, u_k)$$

where $h$ is the time-step. Introduce

$$g(x_k, u_k) = -(x_{k+1} - x_k) + hf(x_k, u_k), \quad k = 0, \ldots, N - 1$$

Define the variable vector

$$\bar{x} = [x_1^T \cdots x_N^T u_0^T \cdots u_M^T]^T$$

Newton’s method for solving this nonlinear equation is given by

$$J(\bar{x})p_k = -g(\bar{x}), \quad k = 0, \ldots, N - 1 \quad (C.1)$$
where \( J(\vec{x}) = \nabla_{\vec{x}} g(\vec{x}) \) with the vector function

\[
g(\vec{x}) = \begin{bmatrix}
-x_1 + f(x_0, u_0) \\
-x_2 + f(x_1, u_1) \\
\vdots \\
-x_N + f(x_{N-1}, u_{M})
\end{bmatrix} = \begin{bmatrix}
g_1(x_1, u_0) \\
g_2(x_2, x_1, u_0) \\
\vdots \\
g_N(x_N, x_{N-1}, u_{M})
\end{bmatrix}
\]

(C.2)

The Jacobian is defined by

\[
J(\vec{x}) = \nabla_{\vec{x}} g(\vec{x}) = \begin{bmatrix}
\nabla x g_1(\vec{x}) \\
\nabla x g_2(\vec{x}) \\
\vdots \\
\nabla x g_N(\vec{x})
\end{bmatrix} = \\
\begin{bmatrix}
\nabla x_1 g_1 & \nabla x_2 g_1 & \ldots & \nabla x_N g_1 & \nabla u_0 g_1 & \ldots & \nabla u_M g_1 \\
\nabla x_1 g_2 & \nabla x_2 g_2 & \ldots & \nabla x_N g_2 & \nabla u_0 g_2 & \ldots & \nabla u_M g_2 \\
\vdots & \ddots & \ddots \\
\nabla x_1 g_N & \nabla x_2 g_N & \ldots & \nabla x_N g_N & \nabla u_0 g_N & \ldots & \nabla u_M g_N
\end{bmatrix}
\]

which by defining

\[
\nabla x f_k = A_k \\
\nabla u f_k = B_k
\]

gives

\[
J(\vec{x}) = \\
\begin{bmatrix}
-I & \ & \ & \ & hB_0 \\
(I + hA_1) & -I & \ & \ & hB_1 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
(I + hA_M) & -I & \ & \ & hB_M \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
(I + hA_{N-1}) & -I & \ & \ & hB_M
\end{bmatrix}
\]

(C.3)

The nonlinear system (C.1) is now defined by substituting in (C.2) and (C.3). The Jacobian is sparse, a property that can be utilized by sparse optimization algorithms.
C.2 Runge-Kutta 4

RK4 for the system $\dot{x} = f(x, u)$ is defined by the discretization scheme

\[ \begin{align*}
x_{k+1} &= x_k + \frac{h}{6}(y_1 + 2y_2 + 2y_3 + y_4) \\
y_1 &= h f(x_k, u_k) \\
y_2 &= h f(x_k + \frac{h}{6}, u_k) \\
y_3 &= h f(x_k + \frac{h}{2}, u_k) \\
y_4 &= h f(x_k + \frac{h}{2}, u_k) \\
y_4 &= h f(x_k + y_3, u_k)
\end{align*} \]

Observe that the property $u_k = u_k + \frac{h}{3} = u_k + \frac{h}{2} = u_k + y_3$ has been utilized. Define the variable vector

\[ \bar{x} = \begin{bmatrix} y_{11} & y_{12} & y_{13} & y_{14} & x_1 & y_2 & \cdots & y_{24} & x_2 & y_{24} & x_4 & \cdots & x_N & u_0 & \cdots & u_M \end{bmatrix} \]

and the vector function

\[ g(\bar{x}) = \begin{bmatrix} -y_{11} + h f(x_0, u_0) \\
-y_{12} + h f(x_0 + \frac{h}{6}, u_0) \\
-y_{13} + h f(x_0 + \frac{h}{2}, u_0) \\
-y_{14} + h f(x_0 + y_3, u_0) \\
-x_1 + \frac{h}{6}(y_{11} + 2y_{12} + 2y_{13} + y_{14}) \\
-x_2 + h f(x_1, u_1) \\
-x_2 + h f(x_1 + \frac{h}{2}, u_1) \\
-x_2 + h f(x_1 + y_{23}, u_1) \\
-x_3 + \frac{h}{6}(y_{21} + 2y_{22} + 2y_{23} + y_{24}) \\
\vdots \\
-x_N + \frac{h}{6}(y_{N1} + 2y_{N2} + 2y_{N3} + y_{N4}) \\
\end{bmatrix} = \begin{bmatrix} g_1(y_{11}, u_0) \\
g_2(y_{12}, u_0) \\
g_3(y_{13}, u_0) \\
g_4(y_{14}, u_0) \\
g_5(y_{11}, y_{12}, y_{13}, y_{14}, x_1) \\
g_6(x_1, y_2, u_1) \\
g_7(y_{21}, y_{22}, y_{23}, u_1) \\
g_8(y_{21}, y_{23}, y_{24}, u_1) \\
g_9(y_{21}, y_{22}, y_{23}, y_{24}, x_2) \\
\vdots \\
\end{bmatrix} = \begin{bmatrix} g_1 \\
g_2 \\
ge_3 \\
ge_4 \\
ge_5 \\
ge_6 \\
ge_7 \\
ge_8 \\
ge_9 \end{bmatrix} \]

where the last vector emphasizes that the initial pattern is repeated over the horizon $N$. The Jacobian matrix is defined by

\[ J(\bar{x}) = J(y, x, u) = \begin{bmatrix} \nabla_{\bar{x}}g_1(\bar{x}) \\
\nabla_{\bar{x}}g_2(\bar{x}) \\
\vdots \\
\nabla_{\bar{x}}g_N(\bar{x}) \end{bmatrix} = \begin{bmatrix} \nabla y_{11}g_{11} & \cdots & \nabla y_{14}g_{11} & \nabla x_1g_{11} & \cdots & \nabla y_{N4}g_{11} & \nabla x_Ng_{11} & \nabla u_0g_{11} & \cdots & \nabla u_Mg_{11} \\
\nabla y_{11}g_{15} & \cdots & \nabla y_{14}g_{15} & \nabla x_1g_{15} & \cdots & \nabla y_{N4}g_{15} & \nabla x_Ng_{15} & \nabla u_0g_{15} & \cdots & \nabla u_Mg_{15} \\
\nabla y_{11}g_{21} & \cdots & \nabla y_{14}g_{21} & \nabla x_1g_{21} & \cdots & \nabla y_{N4}g_{21} & \nabla x_Ng_{21} & \nabla u_0g_{21} & \cdots & \nabla u_Mg_{21} \\
\nabla y_{11}g_{N5} & \cdots & \nabla y_{14}g_{N5} & \nabla x_1g_{N5} & \cdots & \nabla y_{N4}g_{N5} & \nabla x_Ng_{N5} & \nabla u_0g_{N5} & \cdots & \nabla u_Mg_{N5} \end{bmatrix} \]
By defining

\[ \nabla_x f|_{x_k, u_k} = A_k^0 \quad \nabla_u f|_k = B_k^0 \]
\[ \nabla_x f|_{x_k + \frac{1}{2} \Delta t, u_k} = A_k^1 \quad \nabla_u f|_{x_k + \frac{1}{2} \Delta t, u_k} = B_k^1 \]
\[ \nabla_x f|_{x_k + \frac{1}{2} \Delta t, u_k} = A_k^2 \quad \nabla_u f|_{x_k + \frac{1}{2} \Delta t, u_k} = B_k^2 \]
\[ \nabla_x f|_{x_k + \Delta t, u_k} = A_k^3 \quad \nabla_u f|_{x_k + \Delta t, u_k} = B_k^3 \]

the Jacobian for RK4 becomes
Comparing the variable vectors for explicit Euler and RK4 reveals that the number of variables is considerably larger in RK4. Assuming $x_k \in \mathbb{R}^{n_x}$ and $u_k \in \mathbb{R}^{n_u}$ the number of variables in explicit Euler is $\theta_{euler} = n_x N + n_u M$. In RK4 the dimension of $y_i$ equals the dimension of $x$ giving $\theta_{RK4} = 5n_x N + n_u M$. Observe that the degrees of freedom $n_u M$ is unaltered by the choice of discretization schemes. Assuming $n_u M \ll n_x N$ shows that RK4 has approximately 5 times the number of variables as compared to explicit Euler. Hence, the increased order of accuracy of RK4 comes at the expense of a larger optimization problem. Note that the calculations above are somewhat counteracted by the enlarged stability region of RK4 allowing longer step-lengths.

Considering the sintering case from section 2.3 with the state vector $x = [T_g, T_s, X_C]$ of dimension $n_x = (n_z - 1) + 2n_z = 29$ if the spatial dimension is $n_z = 10$. Choosing a batch time of 40 minutes and a sampling interval of 30 seconds gives a prediction horizon of $N = 80$. The control action has dimension $n_u = 1$ and the move horizon is chosen as $M = 40$. This gives

$$\begin{align*}
\theta_{euler} &= n_x N + n_u M = 29 \cdot 80 + 1 \cdot 40 = 2360 \\
\theta_{RK4} &= 5n_x N + n_u M = 5 \cdot 29 \cdot 80 + 1 \cdot 40 = 11640
\end{align*}$$

Note that due to the stiffness of the system choosing the sampling interval as 30 seconds leaves both explicit Euler and RK4 numerically unstable.

**C.3 Lobatto IIIC**

Lobatto IIIC is an A-stable implicit Runge-Kutta method with second order accuracy. The Butcher table is

$$
c | A \\
\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
1 & \frac{1}{3} & -\frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\
\end{array}
$$

Since the last row of $A$ equals $b^T$ Lobatto IIIC is a FSAL method. The discretization scheme for a time-invariant system can be written as

$$
\begin{bmatrix}
\frac{1}{h}(X_1 + X_2 - 2x_{k-1}) - f(X_1, U) \\
\frac{1}{h}(-X_1 + X_2) - f(X_2, U)
\end{bmatrix} = 0
$$

and setting $x_k = X_2$. Choosing the variable vector

$$\tilde{x} = \begin{bmatrix} X_{1,1} & X_{1,2} & X_{2,1} & X_{2,2} & \cdots & X_{N,1} & X_{N,2} & U_1 & \cdots & U_M \end{bmatrix}$$
where the first index is the time index over the prediction/move horizons gives the following right-hand side:

\[
g(\tilde{x}) = \begin{bmatrix}
\frac{1}{h}(X_{1,1} + X_{1,2} - 2x_0) - f(X_{1,1}, U_1) \\
\frac{1}{h}(-X_{1,1} + X_{1,2}) - f(X_{1,2}, U_1) \\
\frac{1}{h}(X_{2,1} + X_{2,2} - 2X_{1,2}) - f(X_{2,1}, U_2) \\
\frac{1}{h}(-X_{2,1} + X_{2,2}) - f(X_{2,2}, U_2) \\
\vdots \\
\frac{1}{h}(X_{N,1} + X_{N,2} - 2X_{N-1,2}) - f(X_{N,1}, U_M) \\
\frac{1}{h}(-X_{N,1} + X_{N,2}) - f(X_{N,2}, U_M)
\end{bmatrix}
= 0
\]

Observe that \(x_{k-1}\) has been replaced by \(X_{k-1,2}\) throughout the horizon. By defining

\[
\nabla_X f|_{X_{k,1}, U_k} = A^1_k \\
\nabla_X f|_{X_{k,2}, U_k} = A^2_k \\
\nabla_U f|_{X_{k,1}, U_k} = B^1_k \\
\nabla_U f|_{X_{k,2}, U_k} = B^2_k
\]

the constraint Jacobian becomes:
\[ J(\bar{x}) = \begin{bmatrix}
\frac{4}{\pi} + A_1^1 & \frac{4}{\pi} \\
-\frac{4}{\pi} & \frac{4}{\pi} + A_1^2 \\
-\frac{2L}{\pi} & \frac{4}{\pi} + A_2^1 & \frac{4}{\pi} \\
-\frac{4}{\pi} & \frac{4}{\pi} + A_2^2 & \frac{4}{\pi} & \frac{4}{\pi} + A_3^1 \\
-\frac{2L}{\pi} & \frac{4}{\pi} + A_3^2 & \frac{4}{\pi} & \frac{4}{\pi} + A_4^1 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
-\frac{2L}{\pi} & \frac{4}{\pi} + A_{M-1}^1 & \frac{4}{\pi} & \frac{4}{\pi} + A_{M-2}^2 & \frac{4}{\pi} + A_M^1 \\
-\frac{4}{\pi} & \frac{4}{\pi} + A_{M-2}^2 & \frac{4}{\pi} & \frac{4}{\pi} + A_{M-1}^2 & \frac{4}{\pi} + A_M^2 \\
\end{bmatrix} \]
For the grate sintering case with prediction data etc. as discussed for RK4, but with a sampling time of $h = 1s$, a dense Jacobian will require about 12.2Gb in double real, while a sparse Jacobian will require about 1.6Mb of memory.

### C.4 sSQP

The sensitivity matrix $S$ for the sequential method (de Oliveira 1994), pp.19-20, is considered in the following. Given the system

\[
\begin{align*}
\dot{x} &= f(x, u) \\
y &= c(x)
\end{align*}
\]

Define

\[
\begin{align*}
\nabla_x f_k &= A_k \\
\nabla_u f_k &= B_k \\
\nabla_x c_k &= C_k
\end{align*}
\]

We have

\[
\begin{align*}
\frac{\partial y_{k+1}}{\partial u_k} &= \frac{\partial y_{k+1}}{\partial x_{k+1}} \cdot \frac{\partial x_{k+1}}{\partial u_k} = C_{k+1} B_k \\
\frac{\partial y_{k+2}}{\partial u_k} &= \frac{\partial y_{k+2}}{\partial x_{k+2}} \cdot \frac{\partial x_{k+2}}{\partial u_k} \cdot \frac{\partial x_{k+1}}{\partial u_k} = C_{k+2} A_{k+1} B_k \\
\frac{\partial y_{k+2}}{\partial u_{k+1}} &= \frac{\partial y_{k+2}}{\partial x_{k+2}} \cdot \frac{\partial x_{k+2}}{\partial u_{k+1}} \cdot \frac{\partial x_{k+1}}{\partial u_k} = C_{k+2} B_{k+1}
\end{align*}
\]

which gives the general case

\[
S_{ij} = \begin{cases} 
0 & \text{if } i > j \\
C_{k+i} B_{k+j-1} & \text{if } i = j \\
C_{k+i} \left( \prod_{m=1}^{i-j} A_{k+i-m} \right) B_{k+j-1} & \text{otherwise}
\end{cases}
\]
The sensitivity matrix for a prediction horizon $P$ and move horizon $M$ becomes (with $k = 0$ and $C_i = I$ for all $i$)

$$
S = \begin{bmatrix}
B_0 \\
A_1 B_0 \\
A_2 A_1 B_0 \\
\vdots \\
A_M B_0 \\
\prod_{m=1}^{M} A_m B_0 \\
\prod_{m=1}^{M+1} A_m B_0 \\
A_{M+1} B_M + B_{M+1} \\
\vdots \\
A_{N-1} B_{M-1} \\
\prod_{m=1}^{N-1} A_m B_0 \\
\prod_{m=M+1}^{N-1} A_m B_M + \cdots + A_{N-1} B_{N-1} + B_N
\end{bmatrix}
$$

where

$$\tilde{B} = \prod_{m=M+1}^{N-1} A_m B_M + \prod_{m=M+2}^{N-1} A_m B_{M+1} + \cdots + A_{N-1} B_{N-1} + B_N$$

Considering the lower leftmost element of $S$ it is observed that this element corresponds to the observability matrix of the linearized system. Complete observability then suffices to guarantee full rank of $S$ since all other elements are truncated versions of the lower left element. Full rank of $S$ implies observability of all (unstable) modes, and the system may be stabilized by a suitable strategy. Note that pinning down unstable modes by an end-point constraint $x_{N}^u = 0$ is susceptible to numerical roundoff errors (Rawlings 2000). The stability proof of the sequential method is only valid for open loop stable systems (de Oliveira and Biegler 1995).

If the discretization scheme is known beforehand (i.e. if solvers like MATLAB’s ode15s are not used), an analytic Jacobian can be implemented without the need for extensive for-loops as would be the case if the elements of $S$ were to be constructed explicitly. Note that by perturbation of inputs to the simulator, the Jacobian constructed by finite differences in the simulator outputs gives the sensitivity matrix directly. I.e. perturbing each control $u_i$ over the horizon $M$ gives the variations in each output $y_{i,j}$ for $i = 1, \ldots, n_y$ and $j = 1, \ldots, N$. This results in $n_u M$ calls to the simulator. If the process can be stably discretized with explicit Euler or RK4 considerable savings can be achieved. Note that the grate sintering case from chapter 2 cannot be stably discretized with explicit methods, while such methods work well with
the CSTR-example. We consider explicit Euler only in the following, but observe that the approach fits equally well with all (explicit and implicit) discretization schemes.

For explicit Euler the right hand side function is given by equation (C.2) and the Jacobian is given by equation (C.3). Partition the Jacobian from equation (C.3) such that the parts for the states and the controls are separated in matrices $A$ and $B$ as below:

$$
A = \begin{bmatrix}
-I & -I \\
(I+hA_1) & -I \\
\vdots & \ddots & \ddots \\
(I+hA_M) & -I \\
(I+hA_{M-1}) & -I
\end{bmatrix}
$$

and

$$
B = \begin{bmatrix}
hB_0 \\
hB_1 \\
\vdots \\
hB_M
\end{bmatrix}
$$

The sensitivity matrix from chapter 4 is given by $S = -\left(\nabla_{x^k} h^k\right)^{-1} \nabla_{u^k} h^k = -A^{-1}B$ with $A$ and $B$ given above in the explicit Euler case. Since

$$
A^{-1} = \begin{bmatrix}
-I & -I \\
-\tilde{A}_1 & -I \\
-\tilde{A}_2 \tilde{A}_1 & -\tilde{A}_2 & -I \\
\vdots & \ddots & \ddots \\
-\prod_{m=1}^{N-1} \tilde{A}_m & \cdots & -\tilde{A}_{N-1} & -I
\end{bmatrix}
$$

where $\tilde{A}_j = (I + hA_j)$, the sensitivity formed by $S = -A^{-1}B$ is given by equation (C.4). Observe that partitioning of the Jacobian into appropriate submatrices $A$ and $B$ continue to hold for the other discretization methods as well. Hence, analytic sensitivity matrices can easily be formed for RK4 and Lobatto IIIIC as well.

This gives two alternative methods for forming the sensitivity matrix. If analytic derivatives are know the last approach should be chosen. If
the discretization scheme is given (and not hidden inside the solver as in \texttt{ode15s} or \texttt{HYSYS}) the latter approach may be chosen (with matrices $A$ and $B$ adapted to the discretization scheme), even if analytic derivatives are not known. This is of particular interest with implicit discretization methods where the model can be hard to solve, since a simple evolution does not suffice. This is seen by the fact that perturbing the ”derivative” function $f(x)$ in $\dot{x} = f(x,u)$ in $x$ and $u$ to get $A_k$ and $B_k$ and composing $A$ and $B$ from these may be cheaper than simulating the system to get $S$ directly. If the discretization scheme is hidden inside the simulator numerical perturbation to get $S$ directly is the only option.

For large scale systems it is essential that the matrix $A$ is formed directly as a sparse matrix. In the grate sintering case with approximately 10000 variables the storage of a full $A$ would require $10000^2 \times 2 = 200 \, M\!b$ in double precision, and about $2 \cdot 10000 \times 2 = 40 \, M\!b$ (depending on the non-zero structure of the $A_k$’s) in sparse form. The sensitivity matrix $S$ (and $B$) has much smaller dimension if $n_u M$ is small. In the grate sintering case $S$ has dimension $10000 \cdot 1$ since there is only one control. The dimension of $S$ is the same as the dimension of $B$. 
Appendix D

Reprint of the CCA-paper

This is a reprint of the paper Martinsen, Johansen, and Foss (1999). The issues in this paper was not pursued further during the progress of the doctoral work. The paper suggests a generic multi-model for hyperbolic PDE's. The main drawback is that the switching between zone-boundaries causes problems when the system is being integrated by conventional solvers like MATLAB's ode15s. The results in the paper were obtained by significant de-tuning of the model parameters to allow integration by explicit schemes. The approach is thus viable for PDE's that can be integrated by explicit solvers, but extensions to stiff and unstable systems are left as future work.
A control relevant dynamic model of grate sintering

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Abstract

In this paper a control relevant nonlinear dynamic model of grate sintering is presented. The model is designed for control purposes for use in future model predictive control (MPC) strategies. A multi-model approach is utilized where the model is presented as a convex combination of locally affine models. The model performance is compared to global models listed in the literature by simulations and by comparison to industrial plant data.

1 Introduction

The metallurgical process of sintering prepares the (iron) ore to form suitable feed for the blast furnace. Granulated ore and coke are mixed, moistened with water and micro-pelletized to form the charge. The charge is loaded onto a grate and leveled to form a bed which is ignited by a gas-fueled ignition hood. A heat wave and coke combustion zone travels down through the bed under the influence of a suction pressure. Hot gas from the combustion zone passes through moist charge deeper in the bed where water evaporates. The process can be divided in five subsequent zones: heat exchange, fusion, combustion, drying and over-moist charge. This is illustrated in figure 2 a). The main purpose of sintering is to convert weakly-bounded granules into a partially fused porous sinter cake suitable for feeding to the blast furnace. Sintering is a complex process involving flow of gas through a packed bed, heat and mass transfer between gas and solids, heterogeneous chemical reactions and melting of solids.

Several models of the sintering process are presented in the literature [1], [2], [3], [4], [5], [6], [7], [8]. These models are presented as nonlinear PDE's, and mainly focus on reproducing important process quantities. There are few reported results on model based control of the sintering process. Kwon et al. [9] uses a linear MPC scheme with an identified input/output model to control the burn-through point of traveling grate sintering. The reported real-time experiments and simulations demonstrates that the chosen MPC algorithm performs well. In the present work, the problem of controlling production rate and quality is directly addressed by identifying a model from designed experiments. As argued below there is an economic criteria restricted by constraints involved, and investigating MPC as a means to control grate sintering is motivated. We seek to exploit the underlying structure of the sintering process to develop a structured model which later on can be utilized to develop a robust control strategy for the sintering process. In the present approach the global nonlinear PDE model is approximated by a convex combination of locally linear or affine models. The local (zone) models are interconnected by both boundary values and propagation of zone positions as sintering proceeds. The interconnection of the zones are handled by the multi-modeling techniques of Johansen and Foss [10]. This method gives good interpolation of zones and is chosen since exact zone boundaries are uncertain and overlap.

Early attempts to model the sintering process divided the process into zones [1]. This approach was later abandoned [2]. The present approach re-investigates this approach, but the motivation for this differs from earlier works. The model in this paper aims at a control relevant model, not a detailed first principles model. In a control relevant model reproducing the internal states is not as important as reproducing the outputs. This becomes important in a state space oriented MPC strategy due to the need for either measuring or estimating the next internal state value $x_{k+1}$. If $x_{k+1}$ cannot be measured and estimation is hard, it is likely that the MPC algorithm performs poorly. In such a case an input/output oriented MPC strategy might perform better, despite the model being less accurate in reproducing the internal states.

The present paper will emphasize the development of the control relevant model, and the control algorithm itself is to be investigated in a later paper.
2 Model

A model can be derived either from physical knowledge, identified from data or as a combination of these. A control relevant model is tailored to the selected control strategy, i.e. the control strategy influence on what information the model should produce. For the sintering process the overall goal is to produce sinter at prescribed quality and rate at the lowest possible cost. Manipulated inputs are coke, water, ignition energy and air flow, while the feed is regarded as a disturbance. The process dependent outputs are quality in terms of mechanical strength and reducibility [11], and production rate. The amplitude and shape of the heat wave determines the quality: Increased coke content increases the maximum sintering temperature, $T_{s,\text{max}}$ [8], but to achieve high reducibility $T_{s,\text{max}}$ should not be too high [12]. In addition proper ignition is necessary to establish the initial conditions for sintering [2]. The process variable influencing on production rate is mainly the permeability of the bed which in turn is influenced mainly by water content. There is an optimal water content yielding the highest bed permeability, i.e. there is an optimum in both coke [12] and water content [13] which can be formulated in a MPC criterion. Bounds on $T_{s,\text{max}}$ and minimum ignition energy are formulated as constraints in the MPC formulation. Due to the large (hot) recycle and time delays present the process is considered difficult to control, with quality and production rates being hard to predict [5].

The recycle stream is an important process variable serving as an on-line measure of mechanical sinter quality: Poor mechanical quality will give increased recycle rate, which in turn reduces the production rate. Reducibility can be quantified from the temperature profile in the fusion zone [12]. Since modeling the sinter quality is difficult, it is identified from experimental data not modeled explicitly at this stage. The stationary equations of the Voice permeability $P$ in the laminar and turbulent flow regimes are respectively:

$$R_l = v \left( \frac{D_p}{2} \right)^{1.0} = \frac{1}{15 \, \eta_p} \cdot \left( \frac{v}{\eta_p} \right)^{0.5} \cdot \frac{d_p}{L}$$

$$R_t = v \left( \frac{D_p}{2} \right)^{0.5} = \sqrt{1 - \frac{1}{15 \, \eta_p}} \cdot \left( \frac{v}{\eta_p} \right)^{0.5} \cdot \frac{d_p}{L}^{0.5}$$

The productivity relation thus becomes:

$$G = \frac{v}{G_s} = \frac{P}{G_s} \cdot \left( \frac{\Delta p}{L} \right)^n$$  \hspace{1cm} (1)

where $n = 0.5$ for turbulent flow and $n = 1$ for laminar flow. The mass air flow $G$ serves as an on-line measure of production rate. Note that when significant melting occurs $d_p$ becomes a conceptual parameter.

The discussion above on in- and outputs is represented graphically in figure 1.

A mechanistic model based on models reported in literature is presented in section 2.1, and a state-space multi-model is suggested in section 2.2. The models considered in this paper does not incorporate radial distributions, and the industrial process considered is batch-wise sintering of manganese ore in Greenawalt pans.

2.1 Mechanistic model

The general PDE model is stated in appendix A. Parameter uncertainties are present in the global models, since essential parameters typically are determined from empirical formulas valid only under idealized conditions. In industrial sintering processes the formation of cracks and channels leads to areas where air passes through without interacting with the mass in the sinter bed. In particular, the mass, $h_m$, and heat, $h_c$, transfer coefficients are calculated from the Nusselt and Sherwood numbers. These number are again calculated from the empirical relations [14]:

$$Nu = \frac{h \cdot d_p}{k} = \frac{1}{\pi} \left( 2 + 1.1 \, Pr^{1/3} \, Re^{0.6} \right)$$  \hspace{1cm} (2)

$$Sh = \frac{h \cdot d_p}{D_{OC}} = \frac{1}{\pi} \left( 2 + 1.1 \, Sc^{1/3} \, Re^{0.6} \right)$$  \hspace{1cm} (3)

valid for an idealized bed with homogeneous packing. In an industrial bed the gas flowing through channels and large cracks are not interacting with the solid, and the values estimated from the empirical relations for an idealized bed will deviate from the actual values. Various heuristics are utilized to overcome this in the literature, i.e. altering the constants of the empirical relations [2], [3], [7], and introducing a scaling factor [5], [6].

The kinetic parameters of coke combustion, fusion and solidification of solids and condensation are also not known in detail. The kinetic model of coke combustion is discussed in [1] assuming the reaction $C + O_2 \rightarrow CO_2$. The kinetics of fusion of solids is described by empirical schemes based on slag diagrams [6] or linear schemes based on process experience [5]. The kinetics of condensation of water is derived from laboratory tests [15] or...
by heuristics and experience [2]. In addition the heat capacity of the solid and the void fraction will change in a complicated way as sintering proceeds. The average particle diameter, \( d_p \), will not have a physical interpretation once melting in the fusion zone has occurred. Still all cited models utilize some equivalent particle diameter when melting has occurred.

Assuming infinite fast gas dynamics a mechanistic energy balance yields the pressure drop as the isothermal relation:

\[
\frac{\partial p}{\partial z} = 15\rho \mu v (1 - \varepsilon)^2 \frac{d^2 \varepsilon^3}{d^2 \varepsilon^3} + 1.75 \rho v^2 (1 - \varepsilon) \frac{d \varepsilon^3}{d \varepsilon^3}
\]

(4)

The pressure profile \( \frac{\partial p}{\partial z} \) is highly nonlinear in \( \varepsilon \) and \( d_p \), and estimating them by use of the Ergun relation will lead to uncertain values. Consequently the models available in literature uses heuristic estimates of the profiles \( \frac{\partial d}{\partial z} \) and \( \frac{\partial \varepsilon}{\partial z} \). All these phenomena gives rise to a model with many uncertain parameters, which must be accounted for when applying model based control to the sintering process.

2.2 State-space multi-model

The bed is divided in a fixed number \( n_x \) of vertical layers named elements \( \Delta z \). Each element is allocated a model type \( M_{z,i} \), \( i \in \{1, \ldots, 5\} \). These zone models are models of the natural zone partitioning depicted in figure 2a). The allocation is based on process knowledge, i.e. as the state of the element as a function of either \( T_s \), \( \rho \), and \( x_C \), \( x_{H_2O}(t) \). Once the model in an element has changed from \( M_{z,i} \) to \( M_{z,i-1} \), it can never change back to \( M_{z,i} \).

As an example the transition from \( M_{z,A} \) to \( M_{z,B} \) is controlled by the ignition temperature of coke \( T_{C,ign} \approx 900-1050^\circ C \), i.e. in an element \( \Delta z \) with solid temperature in this range, both \( M_{z,A} \) and \( M_{z,B} \) is calculated, and the resulting states become a weighted sum of the two models. Similar heuristics controls the transition between other zone models. The void fraction profile \( \frac{\partial \varepsilon}{\partial z} \) is estimated by combining the weighting functions, the measured pressure and the Ergun relation in equation (4). A graphical illustration of the modeling concept and weighting functions is presented in figure 2b). Note that a transition spans more than one element in general. In addition the same technique can be applied independent of the model type, linear vs. nonlinear etc., allocated to the individual elements. However, if the structure of the zone models differs explicit handling of initial conditions must be done to prevent inconsistencies. In the present model the model structure inside each zone is identical (linear or affine), and such initialization problems does not occur.

Viewed as a discretization of a system of PDE’s, the described multi-modeling technique is related to the finite element method (FEM)\(^1\). Extensions to FEM is that in the present approach interpolation is done in the state-space as well as in time and the spatial domain.

3 Simulations

Simulations of the global and multi-model approaches are compared to measurements taken on an industrial plant. The plant data and simulations are shown in figure 3.

The temperature dependent aggregated parameters of the mechanistic model were manually tuned against the plant data. Similarly, the parameters associated with each of the five multi-models were tuned against the

\(^1\)FEM is applied in [6].
The mechanistic model was simulated by applying Newton iterations to an implicit finite difference scheme giving unconditional stability. The stability of the multi-model simulation scheme has not been analyzed. The linear weighting functions can be replaced by smooth functions, and the elements $\Delta z$ of the multi-model can be decoupled from the spatial discretization resolution of the implicit difference scheme. The relation between FEM and the proposed state-space multi-model algorithm should be pursued further. A multi-model uncertainty class should be defined and identified. The control algorithm itself is to be investigated in a later paper.

The simulations showed that the performance of the simpler model gave satisfactory results as compared to the mechanistic model. However, an improved mechanistic model can give better simulation performance. The proposed multi-model algorithm reveals an interesting relation between multi-modeling techniques and finite-element methods which suggests a direction for future research. This also suggests that stability issues of the proposed multi-model algorithm can be analyzed with methods previously applied to FEM. Finally, multi-models have so far been extensively investigated for data driven models, while the present case is motivated by acknowledging that models published in the literature have important parameter uncertainties.

### 4 Discussion

Noting that simplified kinetics of fusion and water evaporation/condensation have been utilized, some improvements of the mechanistic model are expected upon introducing the results of Patisson et al. [6], [15]. The model does not incorporate radial spatial inhomogeneities, which are known to appear regularly in industrial applications in form of channels, cracks and inhomogeneous filling and mixing. Such inhomogeneities causes radial temperature and concentration gradients, in addition to the axial gradients modeled herein. Future work on mechanistic modeling should incorporate radial gradients, possibly with additional simplifying assumptions.

Manual tuning of parameters in a non-linear, coupled distributed system is non-optimal, and a suitable identification scheme should be implemented. Manual tuning of the parameters of the (affine) multi-model is again non-optimal, and work is in progress to implement augmented Kalman filtering in each operating regime. The observability of the (distributed) system is yet to be investigated. Tuning has only been performed for one set-point $x_{e_i}$, $x_{w_i}$ and is not expected to be robust to set-point variations. The affine multi-model uncertainty problem can be adressed by the method of Slupphaug and Foss [16].

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### A Mechanistic model

The following states are included in the model $x = [T_1, T_2, x_{e}, x_{w}, x_{O_2}, x_{N_2}, x_{CO_2}, x_{H_2O}]$; i.e. temperature of solids and gas, coke concentration in solid, liquid water content\(^2\) and gas composition including water vapor. Void fraction and particle size are estimated from

\(^2\)Liquid and solids are lumped in one phase.
measured values, the pressure profile and (4).
\[ \frac{\partial T}{\partial t} + k_1 (T_s - T_g) = g(T_s) \]
\[ \frac{\partial T_s}{\partial t} + v \frac{\partial T_s}{\partial z} + k_2 (T_s - T_g) = 0 \]
\[ \frac{\partial q}{\partial t} = -M_C R_e(T_s) \]
\[ \frac{\partial x}{\partial t} = -M_C v^4 T_s \]
\[ \frac{\partial p}{\partial t} + v \frac{\partial p}{\partial z} = r_j \]

where \( k_1, k_2 \) and \( k_3 \) are aggregated temperature dependent parameters and
\[ g(T_s) = [k_3 R_e(T_s) \Delta H_r - k_3 R_f(T_s) \Delta H_f - k_3 r_{H,0} \Delta H_b(T_s)] \]
\[ r_1(T_s) = -R_e(T_s) \]
\[ r_2(T_s) = 0 \]
\[ r_3(T_s) = R_e(T_s) \]
\[ r_4(T_s) = r_{H,0}(v) \]

Relations for \( R_e(T_s) \) are given by [1], \( R_f(T_s) \Delta H_f \) and \( r_{H,0} \) by [7]. Kinetic parameters is only considered for coke combustion, fusion and drying in the model. Shrinkage and slump is not included. The heat of coke combustion is released to the solid phase, see discussion in [5]. Limestone is not utilised in the industrial plant, and is not included in the model.

### B Notation

**Parameters:**
- \( \varepsilon \) - void fraction
- \( d_p \) - average particle diameter
- \( h_m \) - mass transfer coefficient
- \( h_c \) - heat transfer coefficient
- \( k \) - thermal conductivity of gas
- \( v \) - gas velocity
- \( \mu \) - viscosity
- \( \rho \) - density
- \( D_{ON} \) - axial gas dispersion coefficient (\( O_2-N_2 \))
- \( G \) - mass flow rate of gas
- \( G_s \) - gas volume per sinter mass
- \( L \) - height of bed
- \( p \) - pressure
- \( \kappa_g \) - adiabatic constant
- \( \Delta H \) - heat of reaction
- \( c_p \) - specific heat capacity

**Dimensionsless numbers:**
- \( Re \) - Reynolds number: \( Re = \frac{\varepsilon_d d_g}{\mu} \)
- \( Sh \) - Sherwood number: \( Sh = \frac{h_o d_g}{D_{ON}} \)
- \( Sc \) - Schmid number: \( Sc = \frac{\mu}{\rho D_{ON}} \)
- \( Nu \) - Nusselt number: \( Nu = \frac{h_o d_g}{k} \)
- \( Pr \) - Prandtl number: \( Pr = \frac{\varepsilon d_g}{k} \)

### References


