Ramprasad Yelchuru

Quantitative methods for controlled variables selection

Doctoral thesis
for the degree of philosophiae doctor

Trondheim, May 2012

Norwegian University of Science and Technology
Natural Sciences and Technology
Department of Chemical Engineering

NTNU

Norwegian University of Science and Technology

Doctoral thesis
for the degree of philosophiae doctor

Natural Sciences and Technology
Department of Chemical Engineering

ISBN ISBN 978-82-471-3627-0 (printed version)
ISBN ISBN 978-82-471-3628-7 (electronic version)
ISSN 1503-8181

Doctoral theses at NTNU, 2012:168

Printed by Skipnes Kommunikasjon AS

Summary

Optimal operation is important to improve productivity to be more competitive, and therefore, increase profitability. Optimal operation can be viewed to constitute the control layer (supervisory layer plus regulatory layer) and optimization layer in the hierarchical decomposition of plantwide control. The task of control layer is to keep controlled variables at given set points and the task of optimization layer is to provide optimal set points. For simple implementation, we want to update the set points less frequently while obtaining an acceptable loss in the presence of disturbances. This can be achieved by appropriate controlled variables selection and keeping them at constant set points. This approach is termed as "self-optimizing control" as this approach automatically lead the operation close to optimal operation. Physically, in self-optimizing control, the selected controlled variables can be seen as the set of variables whose optimal values are insensitive to disturbances and controlling these (at constant set point) would reduce the need for frequent set point updates. The selected controlled variables obtained in "self-optimizing control" link the optimization layer and the control layer.

Self-optimizing control provides a mathematical framework and we use this framework to select the controlled variables $\mathbf{c}$ as linear combinations of measurements $\mathbf{y}$, $\mathbf{c} = \mathbf{H}\mathbf{y}$, with the aim to minimize the steady state loss from optimal operation. In "self-optimizing control", we keep the controlled variables $\mathbf{c}$ at constant set points using feedback, and this feedback introduces implementation errors. The focus of this thesis is to devise systematic and good methods to arrive at controlled variables by finding optimal $\mathbf{H}$ that minimize the steady state loss of optimality in the presence of both disturbances and implementation errors.

There are three main contributions in this thesis. The first contribution is to provide (i) a convex formulation to find the optimal combination matrix $\mathbf{H}$ for a given measurement set, and (ii) a Mixed-Integer Quadratic

Programming (MIQP) methodology to select optimal measurement subsets that result in minimal steady state loss in the presence of disturbances. The methods provided in this thesis are exact for quadratic problems with linear measurement relations. The MIQP methods can handle additional structural constraints compared to the Branch and Bound (BAB) methods reported in literature for these problems. The MIQP methods are evaluated on a toy example, an evaporator example, a binary distillation column example with 41 stages and a Kaibel column example with 71 stages.

Second contribution is to develop convex approximation methods that incorporate structural constraints to improve the dynamic controllability properties, such as fast response, control loop localization and to reduce time delays between the manipulated variables ($\mathbf{u}$) and the controlled variables ($\mathbf{c}$). For these cases, $\mathbf{H}$ is structured, for example, decentralized $\mathbf{H}$ or triangular $\mathbf{H}$. The decentralized $\mathbf{H}$ is to obtain $\mathbf{c}$ as combination of measurements of a individual process unit. These structured $\mathbf{H}$ cases in self-optimizing control are non-convex. Hence, we propose a few new ideas and convex approximation methods to obtain good upper bounds for these structured $\mathbf{H}$ problems. The proposed methods are evaluated on random cases, an evaporator case study and a binary distillation column case study with 41 stages.

Third contribution is to extend the self-optimizing control ideas to find optimal controlled variables in the regulatory layer. The regulatory layer is designed to facilitate stable operation, to regulate and to keep the operation in the linear operating range. The regulatory layer performance is quantified using the state drift criterion. Quantitative method for the regulatory layer selection with one, two or more closed loops is proposed to minimize the drift in states. The proposed quantitative methods are evaluated on a distillation column with 41 stages and a Kaibel column with 71 stages case studies.

To summarize, in self-optimizing control, for selecting the controlled variables $\mathbf{c}$ as linear combinations of measurements $\mathbf{y}$, $\mathbf{c} = \mathbf{H}\mathbf{y}$, (a) we developed MIQP methods that belong to a convex sub class to find globally optimal $\mathbf{H}$ and optimal measurement subsets; (b) we developed convex approximation methods to find good upper bounds to find optimal decentralized/triangular $\mathbf{H}$ and optimal measurement subsets; (c) we extended the self-optimizing control concepts to find $\mathbf{c}$ in the regulatory layer and proposed a quantitative method that minimizes the state drift to arrive at optimal regulatory layer with $1, 2$ or more closed loops.

In conclusion, we developed quantitative methods for controlled variables selection in both supervisory layer and regulatory control layer. We demonstrated the developed methods on a few representative case studies.

Acknowledgements

I thank Prof. Sigurd Skogestad for providing me the opportunity to work under his supervision. I express my deep gratitude to him for the constant support, encouragement, motivation and guidance. During these four years, I was amazed at his passion for research, enthusiasm and the attitude of always welcoming discussions. I am indebted to him for increasing my appetite to research and for enabling me to arrive at personal benchmarks to become a productive researcher.

I would like to thank Prof. Bjarne Foss and Prof. Terje Hertzberg for educating me in the areas of optimal control and design of experiment techniques. I would also like to thank other professors in PROcess Systems engineering in Trondheim (PROST) for the interaction throughout these years. I am indebted to Norwegian University of Science and Technology, Trondheim and Process Systems Group for providing me the scintillating environment for my doctoral research. The funding from Research Council of Norway through GASMAKS program is grealy acknowledged.

I cherish moments of enlightening discussions with my previous and present colleagues at the Process Control group , Henrik Manum, Mehdi Panahi, Andreas Linhart, Johannes Jäschke, Håkon Dahl-Olsen, Magnus Glosli Jacobsen, Deeptanshu Dwivedi, Maryam Ghadrdan, Esmaeil Jahanshahi and Ivan Dones and I admire them for their wisdom, humility and attitude. I was fortunate to share office with Andreas Linhart, Mehdi Panahi and Naresh Doni Jayavelu during my graduate studies.

Equally cherishable are the moments I spent with my Telugu friends Venkat, Ravindra, Madhu, Giri, Chandra, Dheeraj, Kishore, Naresh, Prabandh, Srikanth, Phani, Gireesh, Sree Ganesh, Praveen and lunch mates Martin, Michal, Nagaraj, Ralf, Pierre, Vinod, Katherina, Elena, Chiara, Simone and Camilla during my stay in Trondheim. My wonderful friends other

than those mentioned above, to list whose names would be endless, have been a great source of solace in times of need besides the enjoyment they had given me in their company. I am thankful to my friends in making me feel at home in Trondheim.

Thanks to my parents and my wife Swapna, for bestowing their support, love, affection and for the trust on me. I am always indebted to my siblings and cousins for their encouragement, support, affectionate love and friendship.

Ramprasad Yelchuru

Trondheim, May, 2012

Table of Contents

List of Figures

List of Tables

Chapter 1

Introduction

Optimal operation of plants under various disturbances is crucial for the profitability of the integrated process plants. The research objective of this thesis is to provide systematic methods to automatically propagate the business objectives of a process plant to the selection of controlled variables. In this chapter, motivation and scope of the thesis are discussed in the broad area of plantwide control. An overview of the thesis, author's contributions and a list of publications emerged from this thesis are given.

1.1 Motivation and scope

Efficient process operation is important to improve the operating margins, to be more competitive, and therefore profitability. Efficient operation often requires higher process automation. In most cases, process outputs (controlled variables) are assumed to be known during automation or controller design. The higher automation in process systems with the assumed controlled variables may make it difficult to stay agile in the dynamic market conditions and to translate the business objectives for optimal operation. The business objectives can be energy efficiency, environmental impact or sustainability of process plant. The cost function could be anyting, e.g. environmental impact. The scope of the thesis is to find the controlled variables that allow automatic propagation of the business objectives to process operation and a control policy that is simple, easy to implement in practice. The simple control policies are derived explicitly based on the overall business objectives such as minimizing the costs or maximizing the profits and allow for automatic propagation of the business objectives.

Skogestad has formulated a self optimizing control method (Skogestad, 2000) to find controlled variables (CV) by explicitly accounting for the eco-

nomic objectives. By controlling these CV at constant set points, the operation is kept close to the economic steady state optimum in the presence of disturbances and implementation errors. As the appropriate selection of CV and controlling them (at constant set point) automatically lead the operation close to optimal operation, this method is termed as "self-optimizing control". The ideas of "self-optimizing control" dates back to (Morari et al., 1980), who stated that "we want to find a function $\mathbf{c}$ of the process variables which when held constant, leads automatically to the optimal adjustments of the manipulated variables, and with it, the optimal operating condition". Mathematically, we can write it as $\mathbf{c} = \mathbf{f}(\mathbf{y})$, where $\mathbf{c}$ are controlled variables, $\mathbf{f}$ is a function of measurements $\mathbf{y}$. In this thesis, we want to find $\mathbf{c}$ as linear combination of measurements, that is, $\mathbf{c} = \mathbf{H}\mathbf{y}$ and $\mathbf{H}$ is measurement combination matrix. In summary, the self-optimizing control framework may be used to select combination matrix $\mathbf{H}$, and there by controlled variables $\mathbf{c}$, that minimize the deviation of process operation from the optimum on steady state basis.

1.2 Thesis overview

In Chapter 2, we briefly describe the previous results on self-optimizing control and the contribution of the thesis. We also describe other alternative approaches to optimizing control briefly.

Chapter 3, we present the convex formulations for optimal controlled variable combinations and optimal measurement selection using Mixed Integer Quadratic Programming (MIQP) method. We evaluated the developed methods on a toy problem, an evaporator case study, a binary distillation column case study with 41 stages and a Kaibel column with 71 stages. The simplicity of formulating MIQP is demonstrated on a toy problem. The advantages of MIQP methods in handling some practically relevant structural constraints over the existing methods are demonstrated on an evaporator case study and a Kaibel column.

Chapter 4, the controlled variable ($\mathbf{c} = \mathbf{H}\mathbf{y}$) selection problems with a particular structure in $\mathbf{H}$ (i.e. a few elements in $\mathbf{H}$ are zero) are non-convex in self-optimizing control. Hence, we present an MIQP based convex approximation method to find an upper bound to find particular structured $\mathbf{H}$ and controlled variables $\mathbf{c} = \mathbf{H}\mathbf{y}$. The particular structure in $\mathbf{H}$ is of immense practical significance to improve the dynamical controllability (i.e. fast response, control loop localization). An example of particular structured $\mathbf{H}$

is decentralized **H** or block diagonal **H**, where each controlled variable is a combination of measurements of a process unit. The MIQP based convex approximation methods are evaluated on an evaporator case study and a binary distillation column case study with 41 stages. The presented convex approximation methods are observed to provide good upper bounds, which are of significant practical importance.

Chapter 5, the ideas of self-optimizing control are extended to find optimal controlled variables ($\mathbf{c} = \mathbf{Hy}$) that minimize state drift in the regulatory layer based on steady state analysis. The regulatory layer that minimizes the state drift with $1, 2$ or more closed loops for process plants is studied. Based on the acceptable state drift threshold the minimum number of closed loops (minimum regulatory layer) is obtained. The developed methods are evaluated on a binary distillation column case study with 41 stages and a Kaibel column case study with 71 stages to arrive at regulatory layer with 1, 2 or more closed loops.

Chapter 6 presents the ease and practicality of controlling the measurement combinations in dynamic simulations. The dynamic performance in terms of rejecting the disturbances is evaluated for a distillation column with 41 stages.

Chapter 7 sums up and concludes the thesis. Finally, we discuss the directions for future work.

1.3 Thesis contributions

There are three main contributions in this thesis to select controlled variables for a process plant in self-optimizing control framework.

(1) Convex formulations for optimal controlled variable combinations and optimal measurement selection using Mixed Integer Quadratic Programming (MIQP)(Chapter 3).

(2) An MIQP based convex approximation to obtain an upper bound in finding controlled variables, $\mathbf{c} = \mathbf{Hy}$, where **H** has a particular structure (Chapter 4).

(3) Extending the self-optimizing control to find optimal controlled variables that minimize state drift in the regulatory layer based on steady

state analysis and to find regulatory layer with $1, 2$ or more closed loops (Chapter 5).

1.4 Publications

Chapter 3

Yelchuru, R., Skogestad, S., Manum, H., 2010. MIQP formulation for controlled variable selection in self optimizing control. In: DYCOPS, July 7-9, Brussels. pp. 61–66.

Yelchuru, R., Skogestad, S., 2010. MIQP formulation for optimal controlled variable selection in self optimizing control. In: PSE Asia, July 25-28, Singapore. pp. 206–215.

Yelchuru, R., Skogestad, S., Dwivedi, D., 2011. Optimal measurement selection for controlled variables for Kaibel distillation column, AIChE National Meeting, October 16-21, Minneapolis. Presentation 652e.

Yelchuru, R., Skogestad, S., 2012. Convex formulations for optimal selection of controlled variables and measurements using Mixed Integer Quadratic Programming. Manuscript accepted for publication in Journal of Process Control.

Chapter 4

Yelchuru, R., Skogestad, S., 2010. Optimal controlled variable selection for individual process units in self optimizing control with MIQP formulations, In: Nordic Process Control Workshop, August 19 - 21, Lund, Sweden, Poster presentation.

Yelchuru, R., Skogestad, S., 2011. Optimal controlled variable selection for individual process units in self optimizing control with MIQP formulation. In: American Control Conference, June 29 - July 01, San Francisco, USA. pp. 342–347.

Yelchuru, R., Skogestad, S., 2011. Optimal controlled variable selection with structural constraints using MIQP formulations. In: IFAC World Congress, August 28 - September 2, Milano, Italy. pp. 4977–4982.

Chapter 5

Yelchuru, R., Skogestad, S., 2012. Regulatory layer selection through partial control. In: Nordic Process Control Workshop, Jan 25 - 27, Techni-

cal University of Denmark, Kgs Lyngby, Denmark.

Yelchuru, R., Skogestad, S., 2012. Quantitative methods for optimal regulatory layer selection. Accepted for ADCHEM 2012, Singapore.

Yelchuru, R., Skogestad, S., 2012. Quantitative methods for Regulatory control layer selection. Manuscript submitted for publication in Journal of Process Control.

Co-authored publications

Skogestad, S., Yelchuru, R. Jäschke , J., 2011. Optimal use of measurements for control, optimization and estimation using the loss method: Summary of existing results and some new, Book chapter in: M. Huba, S. Skogestad, M. Fikar, M. Hovd, T.A. Johansen, B. Rohal'-Ilkiv (Editors): Selected topics on constrained and nonlinear control, Workbook, ISBN:978-80-968627-3-3.

Panahi, M., Skogestad, S., Yelchuru, R., 2010, Steady State Simulation for Optimal Design and Operation of a GTL Process", Advances in Gas Processing (Volume 2). Proceedings of the 2nd Annual Gas Processing Symposium, pp. 275-284, Elsevier, ISBN-978-0-444-53588-7.

Bibliography

Morari, M., Stephanopoulos, G., Arkun, Y., 1980. Studies in the synthesis of control structures for chemical processes. Part I: formulation of the problem. process decomposition and the classification of the control task. analysis of the optimizing control structures. AIChE Journal 26 (2), 220–232.

Skogestad, S., 2000. Plantwide control: The search for the self-optimizing control structure. Journal of Process Control 10, 487–507.

Chapter 2

Brief overview of control structure design and methods

Optimal operation of the process plants is vital for improved productivity and profitability in the presence of disturbances. The objective of control structure selection is to automatically propagate the business objectives to process operation. In this chapter, we present a method to find controlled variables explicitly based on business objectives in self-optimizing control framework. We focus on the self-optimizing control based methods in this thesis. The self-optimizing control framework, the previously established methods for self-optimizing control framework and the thesis contributions are presented briefly. A short overview of other methods for optimal operation are presented.

2.1 Control structure design

The control structure design plays a vital role in operating the process plant optimally. Control structure design deals with the selection of controlled variables (CV/outputs) and manipulated variables (MV/inputs), and the pairings or interconnections between these variables. The control structure design is vital issue that needs to be addressed by control engineers in process plants. The control community was criticized for the dearth of theory to address control structure design (Foss, 1973). Morari & co-workers (Morari et al., 1980; Morari and Stephanopoulos, 1980a,b) have introduced interesting theories on hierarchical control, multilevel optimization and on

control structure design.

2.2 Plantwide control

Plantwide control deals with the control philosophy of the overall plant and on the structural decisions. Structural decisions include selection of controlled variables and set points, $\mathbf{c}$ and $\mathbf{c}_s$, selection of measured variables $\mathbf{y}$, selection of manipulated variables $\mathbf{u}$, selection of control configurations (the structure interconnecting measurements and manipulated variables), selection of type of controller (the control law) (Skogestad, 2000). The selection of control structure based on economics is stressed by Narraway and co-workers for the effect of disturbances (Narraway et al., 1991; Narraway and Perkins, 1993).

The scope of this thesis is limited to the selection of controlled variables and measurements for optimal operation. The plantwide control system for an overall plant is organized in a hierarchical structure (Figure 2.1), based on the time scale separation between the layers.

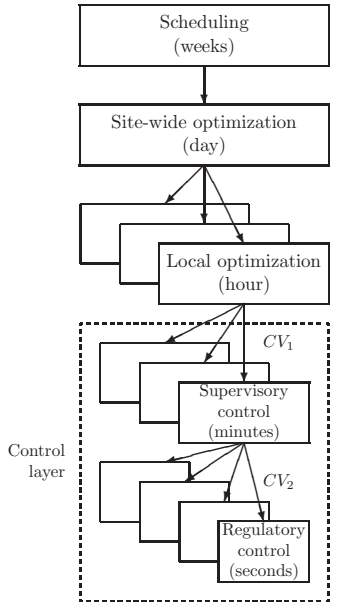

Figure 2.1: Control system hierarchy for plantwide control in chemical plants (Findeisen et al., 1980; Skogestad and Postlethwaite, 1996)

The typical time scale separation of various layers (Figure 2.1) in plantwide control (Findeisen et al., 1980) are *Scheduling* (weeks), *Site-wide optimiza-*

tion (days), *Local optimization* (hours), *Control layer* (minutes and seconds) (Skogestad and Postlethwaite, 1996). The business objectives, like economic profitability or cost (J) of plant operation are achieved by cascading the objectives down from scheduling to the control layer. The interaction between the layers is through the set points from upper layer to bottom layer. The interaction between the optimization layer and control layer is through the set points that are updated only once in an hour, whereas the control layer operates continuously.

A review of plantwide control is presented and control structure design is viewed as a subtask of plantwide control procedure (Larsson and Skogestad, 2000). The selection of controlled variables is important in control structure design to operate the process plant optimally. The local optimization layer can be either real time optimization (RTO) (Forbes and Marlin, 1996) or optimizing controller (Engell, 2007) or NCO tracking (Srinivasan et al., 2003; Kadam et al., 2007) or extremum seeking methods (Srinivasan et al., 2003; Ariyur and Krstic, 2003; Guay and Zhang, 2003). The interaction of controlled variables selection and the local optimization layer is depicted in Figure 2.2. When a disturbance ($\mathbf{d}$) affects the process, the controller $\mathbf{K}$

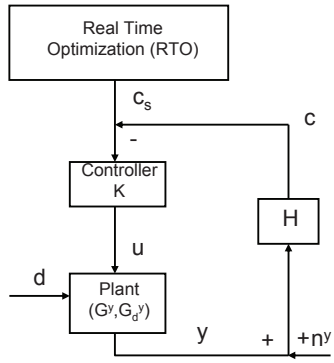

Figure 2.2: Feedback implementation of optimal operation with separate layers for optimization and control (Kassidas et al., 2000) (Engell, 2007). The controller K could be any controller including MPC. Self-optimizing control framework deals with selection of the controlled variables $\mathbf{c} = \mathbf{H}\mathbf{y}$

tries to keep the controlled variables $\mathbf{c}$ at their set points $\mathbf{c}_s$. The disturbances affecting the process are estimated by the optimizer from the process measurements. Then the optimizer provides new optimal set points $\mathbf{c}_s$ for the control layer based on a model of the plant and are implemented in the

control layer using local feedback loop.

In this setup, there are two classes of systems, *Constrained systems*, *Fully or partially unconstrained systems*. At the optimal point, all degrees of freedom are used for satisfying constraints in constrained systems and one or more the degrees of freedom are unconstrained in fully or partially unconstrained systems. For the constrained systems, active constraint control is used for controlling the optimally active constraints (Maarleveld and Rijnsdorp, 1970). Whenever the active constraints are not measurable, indirect measurements are used to infer the actual value of the constraint. An adaptive active constraint policy (Arkun and Stephanopoulos, 1980) can be used, when the optimally active constraints sets vary in the presence of disturbances. In presence of unconstrained degrees of freedom at optimal point, it is not clear on how to utilize these unconstrained degrees of freedom to meet the economic objectives. The focus of this thesis is to devise methods to find $\mathbf{c}$ that minimize the steady state loss in the economic objectives for these unconstrained degrees of freedom.

2.3 Real-time optimization

The integration of Real-Time Optimization (RTO) with the control layer can be viewed as Figure 2.2 with optimization layer being RTO. RTO uses the steady state process model online. The steady state process model parameters are partitioned as varying parameters and fixed parameters and the process measurements are used to estimate the varying parameters of the process model online. The model with the newly estimated parameters is used for optimization. Then the optimization gives the optimal set points $\mathbf{c}_s$ to the control layer (Forbes and Marlin, 1996; Marlin and Hrymak, 1997). The usage of approximate process models is studied to facilitate faster convergence in optimization (Loeblein and Perkins, 1998). RTO operates at a slower time scale as it involves parameter estimation and optimization and is costly. The uncertainties in entities of RTO in the presence of disturbances are addressed (Zhang et al., 2001, 2002; Zhang, 2010). Dynamic versions of the RTO-framework are also presented (Kadam et al., 2003). But a very limited work is reported on the interaction of the RTO and control layer (the controlled variables)(Marlin and Hrymak, 1997; Adetola and Guay, 2010).

2.4 Self-optimizing control

Economically optimal operating point

The steady state optimization problem defining the plant's economic operating point is formulated as

$$\begin{aligned} \min_{\mathbf{u}_s} \quad & J(\mathbf{x}, \mathbf{u}_s, \mathbf{d}) \\ \text{st.} \quad & \mathbf{g}_1(\mathbf{x}, \mathbf{u}_s, \mathbf{d}) = 0 \\ & \mathbf{g}_2(\mathbf{x}, \mathbf{u}_s, \mathbf{d}) \leq 0 \end{aligned} \tag{2.1}$$

Where J is a scalar cost function to be maximized (i.e. profit, yield, selectivity) or minimized (i.e. production cost, by-products), $\mathbf{x} \in \mathbb{R}^{n_x}$, $\mathbf{u}_s \in \mathbb{R}^{n_{u_s}}$ and $\mathbf{d} \in \mathbb{R}^{n_d}$ are states, steady state degrees of freedom and disturbances, respectively. Steady state degrees of freedom ($\mathbf{u}_s$) are different from available DOF ($\mathbf{u}_T$), as few available DOF are associated with variables such as levels do not have any effect on steady state operation. Hence the steady state DOF must be chosen suitably. The equality constraint $\mathbf{g}_1$ represents the steady state process model expressing the relationship between $\mathbf{x}$ and independent variables $(\mathbf{u}_s, \mathbf{d})$. The inequality constraints $\mathbf{g}_2$ represents the limits that must be satisfied during operation such as safety limits, saturation limits of actuators, equipment capacity limits and environmental aspects. The steady state model equation $\mathbf{g}_1$ is solved to express $\mathbf{x} = \mathbf{f}(\mathbf{u}_s, \mathbf{d})$ and the active constraints of optimization problem in (2.1) are implemented to result in the optimization problem in reduced space as

$$\min_{\mathbf{u}} \quad J(\mathbf{u}, \mathbf{d}) \tag{2.2}$$

Where $\mathbf{u}$ are the unconstrained degrees of freedom. In order to keep the operation at optimum, the optimization problem (2.2) should be solved for $\mathbf{u} = \mathbf{u}_{\text{opt}}(\mathbf{d})$ for any disturbance $\mathbf{d}$ and the resulting optimal cost is $J_{\text{opt}}(\mathbf{u}_{\text{opt}}(\mathbf{d}), \mathbf{d})$. The cost function J as a function of input $\mathbf{u}$ and disturbance $\mathbf{d}$ is shown in Figure 2.3. The optimal inputs for disturbances $\mathbf{d}^*$ (solid), and $\mathbf{d}$ (dotted) are $\mathbf{u}_{\text{opt}}(\mathbf{d}^*)$ and $\mathbf{u}_{\text{opt}}(\mathbf{d})$, respectively. In other words the input $\mathbf{u}$ should be updated according to the disturbance affecting the system to keep the operation optimal. The loss by keeping the input $\mathbf{u}$ constant at $\mathbf{u} = \mathbf{u}_{\text{opt}}(\mathbf{d}^*)$ when there is a disturbance $\mathbf{d}$ is also illustrated in Figure 2.3. Hence, for any disturbance $\mathbf{d}$, if we update the input to any $\mathbf{u}$ then we will incur loss from optimal operation as shown in Figure 2.3. The associated loss can be quantified as (Skogestad and Postlethwaite, 1996)

$$L = J(\mathbf{u}, \mathbf{d}) - J_{\text{opt}}(\mathbf{u}_{\text{opt}}(\mathbf{d}), \mathbf{d}) \tag{2.3}$$

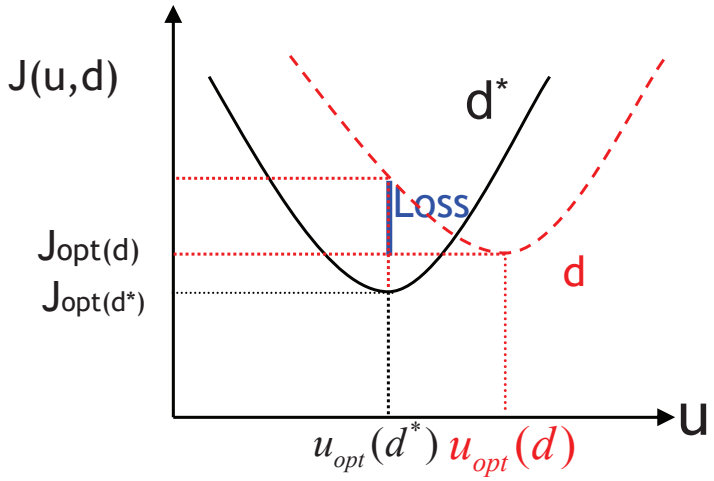

Figure 2.3: Cost function as a function of disturbances $\mathbf{d}^*$ and $\mathbf{d}$ and inputs $\mathbf{u}$; Illustration of loss by keeping input $\mathbf{u}$ constant at $\mathbf{u} = \mathbf{u}_{\text{opt}}(\mathbf{d}^*)$ when there is a disturbance $\mathbf{d}$

.

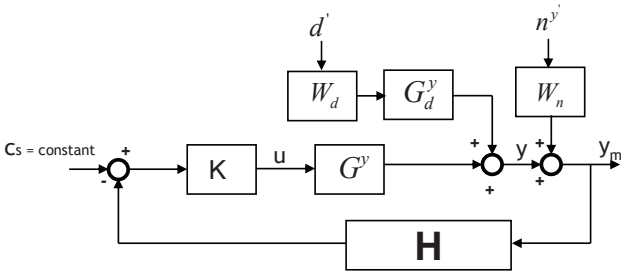

Figure 2.4: Feedback diagram

.

In self optimizing control framework, input $\mathbf{u}$ is manipulated to keep $\mathbf{H}\mathbf{y}_m$ at constant set point $\mathbf{c}_s$ using a feedback diagram as in Figure 2.4 and the associated loss is defined as

$$L_c = J(\underbrace{\mathbf{u}}_{to\ keep\ \mathbf{H}\mathbf{y}_m\ at\ \mathbf{c}_s}, \mathbf{d}) - J_{\text{opt}}(\mathbf{u}_{\text{opt}}(\mathbf{d}), \mathbf{d}) \tag{2.4}$$

Note that the feedback in the self-optimizing control framework introduces implementation errors and the loss (2.4) is a function of both disturbances and implementation errors (i.e. $L_c = \text{f}(\mathbf{d}, \mathbf{n}^c)$, where $\mathbf{n}^c = \mathbf{H}\mathbf{n}^y$). In this self-optimizing control framework, the emphasis is on the controlled variables, $\mathbf{c} = \mathbf{H}\mathbf{y}$, selection as individual/combination of measurements and to keep them at constant set points by adjusting the unconstrained degrees of freedom in a feedback fashion.

2.5 Previously proposed methods for selection of self-optimizing controlled variables

2.5.1 Brute force optimization method

Brute force optimization methods are used in self-optimizing control framework to select CV earlier, where the loss for various alternatives of selected measurements as CV are calculated directly and are compared. In these brute force methods, disturbances $\mathbf{d}$ and implementation errors $\mathbf{n}^c$ are treated as random variables and the $L_{c,wc}, L_{c,av}$ are obtained by considering various realizations of $\mathbf{d} \in \mathscr{D}$ and $\mathbf{n}^c \in \mathscr{E}$ for each alternative. $\mathscr{D}, \mathscr{E}$ denote the allowable sets of $\mathbf{d}$ and $\mathbf{n}^c$. Note that for each realization, two optimization problems (i.e. equation (2.1) and equation (2.1) with additional constraint as selected CV at constant set point) are solved. These steps are repeated for all the possible alternatives and the one with the smallest worst-case loss and the average loss are selected as the optimal candidate CV.

$$L_{c,wc}(\mathbf{d}, \mathbf{n}^c) = max_{\mathbf{d}\in\mathscr{D}, \mathbf{n}^c\in\mathscr{E}} \quad L_c(\mathbf{d}, \mathbf{n}^c) \tag{2.5}$$

$$L_{c,av}(\mathbf{d}, \mathbf{n}^c) = \mathbb{E}\left[L_c(\mathbf{d}, \mathbf{n}^c)\right] \quad \forall \mathbf{d} \in \mathscr{D},\ \forall \mathbf{n}^c \in \mathscr{E} \tag{2.6}$$

where $\mathbb{E}[.]$ is expectation operator. Note that the active constraints can change in the brute force approach.

2.5.2 Other methods

Mahajanam et al. (2001) proposed a short-cut method for CV selection to remove the poor choices and to generate prospective alternatives without solving the non-convex optimization problems (i.e. equation (2.1) with additional constraint as selected CVs at constant set points). The short-cut method uses scaling on CV to have similar effect on the steady state process economics. This short-cut method is scaling dependent and cannot consider linear combinations of disturbances in the allowed disturbance space. Cao (2003) proposed to use analytical gradient of the optimization problem (equation (2.1)) as controlled variables. Although gradient as controlled variable and controlling it at a constant set point zero guarantees optimal operation, it suffers a few drawbacks for practical usage. The drawbacks are the complexity to obtain analytical gradient and the requirement of information on states, unmeasured disturbances.

2.5.3 Local methods

As the brute force evaluation for all the possible measurement alternatives as controlled variables is intractable, local methods are developed to pre screen and identify the promising CV. Local methods are developed based on the local analysis of loss and linearized steady state model at an operating point (see section 2.4), with an assumption that the plant economics are governed by the plant pseudo/steady state behavior.

A key idea in the self-optimizing framework of Skogestad and co-workers (Skogestad and Postlethwaite, 1996) is to minimize the loss ($L = J - J_{\text{opt}}(\mathbf{d})$) rather than directly minimizing the cost J. In the subsequent discussions, we term this local method with loss minimization as the minimum loss method.

Problem formulation

Classification of variables

- $\mathbf{u}$ - unconstrained steady state degrees of freedom (inputs) for optimization (it does not actually matter what they are as long as they form an independent set).
- $\mathbf{d}$ - disturbances, including process parameter changes.
- $\mathbf{y}$ - all available measurements. The manipulated variables (MV, often the same as the inputs $\mathbf{u}$) are generally included in the measurement set $\mathbf{y}$. This will allow, for example, for simple control policies where

the inputs are kept constant. Of course, the set $\mathbf{y}$ can also include measured disturbances ($\mathbf{d}_m$, a subset of $\mathbf{d}$).

- $\mathbf{n}^y$ - measurement noise (error) for $\mathbf{y}$, $\mathbf{y_m} = \mathbf{y} + \mathbf{n}^y$.
- $\mathbf{c} \in \mathbb{R}^{n_c}$ where $n_c = n_u$ - selected controlled variables $\mathbf{c} = \mathbf{H}\mathbf{y}$.

Cost function

We consider an unconstrained optimization problem, where the objective is to adjust the input $\mathbf{u}$ to minimize a quadratic cost function at steady-state

$$J(\mathbf{u},\mathbf{d}) = J(\mathbf{u}^*,\mathbf{d}^*) + \begin{bmatrix}\mathbf{J}_u^* & \mathbf{J}_d^*\end{bmatrix}\begin{bmatrix}\Delta\mathbf{u}\\ \Delta\mathbf{d}\end{bmatrix} + \frac{1}{2}\begin{bmatrix}\Delta\mathbf{u}\\ \Delta\mathbf{d}\end{bmatrix}^T\begin{bmatrix}\mathbf{J}_{uu}^* & \mathbf{J}_{ud}^*\\ \mathbf{J}_{ud}^{*T} & \mathbf{J}_{dd}^*\end{bmatrix}\begin{bmatrix}\Delta\mathbf{u}\\ \Delta\mathbf{d}\end{bmatrix} \quad (2.7)$$

Here $\Delta\mathbf{u} = \mathbf{u} - \mathbf{u}^*$ and $\Delta\mathbf{d} = \mathbf{d} - \mathbf{d}^*$ represent deviations from the nominal optimal point $(\mathbf{u}^*, \mathbf{d}^*)$. $\mathbf{J}_u^*$ and $\mathbf{J}_d^*$ are first derivatives of J with respect to $\mathbf{u}$ and $\mathbf{d}$, $\mathbf{J}_{uu}^*$, $\mathbf{J}_{ud}^*$ and $\mathbf{J}_{dd}^*$ are second derivatives of J with respect to $\mathbf{u}$, $\mathbf{u}$ and $\mathbf{d}$, and $\mathbf{d}$, respectively at $(\mathbf{u}^*, \mathbf{d}^*)$. The nominal point is assumed to be optimal, which implies that $\mathbf{J}_u^* = 0$. To further simplify notation, we assume that the variables have been shifted so that the nominal optimal point is zero $(\mathbf{u}^*, \mathbf{d}^*) = (0, 0)$ and also $\mathbf{y}^* = 0$, then we have $\mathbf{u} = \Delta\mathbf{u}$, $\mathbf{d} = \Delta\mathbf{d}$ and $\mathbf{y} = \Delta\mathbf{y}$. From the derivation below, we find that the values of $\mathbf{J}_d^*$ and $\mathbf{J}_{dd}^*$ are not needed for finding the optimal $\mathbf{H}$, because they do not affect the optimal input $\mathbf{u}$.

Measurement model

A linear steady-state model is assumed for the effect of $\mathbf{u}$ and $\mathbf{d}$ on the measurements $\mathbf{y}$

$$\mathbf{y} = \mathbf{G}^y\mathbf{u} + \mathbf{G}_d^y\mathbf{d} = \tilde{\mathbf{G}}^y\begin{bmatrix}\mathbf{u}\\ \mathbf{d}\end{bmatrix} \quad (2.8)$$

In Figure 3.1, $\mathbf{G}^y$ and $\mathbf{G}_d^y$ are transfer functions, but in this thesis only steady-state gains in (2.8) are used for selecting $\mathbf{H}$.

Further assumptions

- Any active constraints are controlled and $\mathbf{u}$ spans the remaining unconstrained subspace.

- We want to find as many controlled variables $\mathbf{c}$ as there are degrees of freedom, that is, $n_c = \dim(\mathbf{c}) = \dim(\mathbf{u}) = n_u$. Then $\mathbf{HG}^y$ is a square $n_u \times n_u$ matrix.
- We need at least as many independent measurements $\mathbf{y}$ as there are degrees of freedom $\mathbf{u}$ ($\text{rank}(\mathbf{G}^y) = n_u$) to get offset free control of all CV ($\mathbf{c}$). This requires $n_y \geq n_u = n_c$.
- We write $\mathbf{d} = \mathbf{W}_d \, \mathbf{d}'$ where $\mathbf{W}_d$ is a diagonal matrix giving the expected magnitude of each disturbance and $\mathbf{d}'$ is of unit magnitude (see below for further definition of "unit magnitude").
- Similarly, $\mathbf{n}^y = \mathbf{W}_{n^y} \, \mathbf{n}^{y'}$ where $\mathbf{W}_{n^y}$ is a diagonal matrix with the magnitude of the noise for each measurement, and the vector $\mathbf{n}^{y'}$ is of unit magnitude (see below).

Problem

Keeping the inputs $\mathbf{u}$ constant at $\mathbf{u}_{\text{opt}}(\mathbf{d}^*)$ for a new disturbance $\mathbf{d}$ will give a loss as illustrated in Figure 2.3. Instead in this thesis, the $\mathbf{u}$ is adjusted in a feedback fashion (see Figures 2.2 and 2.4) to keep the measured controlled variables $\mathbf{c}$ at a constant set point $\mathbf{c}_s = 0$. Mathematically, we have

$$\mathbf{c}_m = \mathbf{H} \underbrace{(\mathbf{y} + \mathbf{n}^y)}_{\mathbf{y}_m} = \mathbf{c}_s = 0 \tag{2.9}$$

The problem can now be stated as: Find the optimal matrix $\mathbf{H}$ such that "magnitude" of the loss

$$L = J(\mathbf{u}, \mathbf{d}) - J_{\text{opt}}(\mathbf{d}) \tag{2.10}$$

is minimized for the expected $\mathbf{d}$ and $\mathbf{n}^y$, when $\mathbf{u}$ is adjusted such that $\mathbf{c}_m = 0$ in (2.9) is satisfied.

The "magnitude" of the loss and the "unit magnitude" of the expected $\mathbf{d}'$ and $\mathbf{n}^{y'}$ still needs to be defined. Two possibilities are considered.

- Worst-case loss, L_{wc}, when the combined normalization vectors for disturbances and measurement noise have 2-norm less than 1,

$$\left\| \begin{bmatrix} \mathbf{d}' \\ \mathbf{n}^{y'} \end{bmatrix} \right\|_2 \leq 1 \tag{2.11}$$

- Average or expected loss, $L_{avg} = \mathbb{E}(L)$, for a normal distributed set $\begin{bmatrix} \mathbf{d}' \\ \mathbf{n}^{y'} \end{bmatrix} \in \mathcal{N}(0, 1)$. $\mathbb{E}(.)$ is expectation operator.

It is sometimes argued that the worst-case loss is not likely to occur, but this is not really true in this case since we use the combined 2-norm for disturbances and noise in (2.11). This means that the "unlikely" combination with all $\mathbf{d}'$s and $\mathbf{n}^{y'}$s being 1 at the same time will not occur. This is discussed in more detail in the Appendix of Halvorsen et al. (2003).

2.5.4 Solution to minimum loss problem

The objective is to derive the solution to the above problem. This solution has previously been called the "exact local method" (Halvorsen et al., 2003).

Expression for $\mathbf{u}_{\text{opt}}(\mathbf{d})$

We find the optimal input $\mathbf{u}$ for a given disturbance $\mathbf{d}$ (Halvorsen et al., 2003). Expanding the gradient $\mathbf{J}_u$ around the nominal optimal point $(\mathbf{u}^*, \mathbf{d}^*) = (0, 0)$ gives

$$\mathbf{J}_u(\mathbf{u}, \mathbf{d}) = \underbrace{\mathbf{J}_u^*(\mathbf{u}^*, \mathbf{d}^*)}_{=0} + \mathbf{J}_{uu}^* \mathbf{u} + \mathbf{J}_{ud}^* \mathbf{d} \tag{2.12}$$

where $\mathbf{J}_u(\mathbf{u}^*, \mathbf{d}^*) = 0$ because the nominal point is assumed to be optimal. We assume that we change the input to remain optimal, i.e. we have $\mathbf{u} = \mathbf{u}_{\text{opt}}(\mathbf{d})$ and $\mathbf{J}_u(\mathbf{u}, \mathbf{d}) = 0$, and we get

$$\mathbf{u}_{\text{opt}} = -\mathbf{J}_{uu}^{*^{-1}} \mathbf{J}_{ud}^* \mathbf{d} \tag{2.13}$$

Note that we are considering a quadratic problem (2.7), where the Hessian matrices are assumed constant, i.e. $\mathbf{J}_{uu} = \mathbf{J}_{uu}^*$ and $\mathbf{J}_{ud} = \mathbf{J}_{ud}^*$.

Expression for the loss L in terms of $\mathbf{u} - \mathbf{u}_{\text{opt}}(\mathbf{d})$

Consider a given disturbance $\mathbf{d}$ and a non-optimal input $\mathbf{u}$. A second order Taylor's expansion of the cost J around the "moving" optimum point, $\mathbf{u}_{\text{opt}}(\mathbf{d})$, gives

$$\begin{aligned} J(\mathbf{u}, \mathbf{d}) = \underbrace{J(\mathbf{u}_{\text{opt}}(\mathbf{d}), \mathbf{d})}_{J_{\text{opt}}(\mathbf{d})} + \underbrace{\mathbf{J}_{u,opt}}_{=0}(\mathbf{u} - \mathbf{u}_{\text{opt}}(\mathbf{d})) \\ + \frac{1}{2}(\mathbf{u} - \mathbf{u}_{\text{opt}}(\mathbf{d}))^T \mathbf{J}_{uu,opt}(\mathbf{u} - \mathbf{u}_{\text{opt}}(\mathbf{d})) \end{aligned} \tag{2.14}$$

Note that for a truly quadratic problem, this is an exact expression and $\mathbf{J}_{uu,opt} = \mathbf{J}_{uu}^* = \mathbf{J}_{uu}$. Because we are expanding around an optimal point $J_{u,opt} = 0$ and we get the following expression for the loss

$$L(\mathbf{u}, \mathbf{d}) = J(\mathbf{u}, \mathbf{d}) - J_{\text{opt}}(\mathbf{d}) = \frac{1}{2}\mathbf{z}^T\mathbf{z} = \frac{1}{2}\|\mathbf{z}\|_2^2 \tag{2.15}$$

where we have introduced

$$\mathbf{z} \triangleq \mathbf{J}_{uu}^{1/2}(\mathbf{u} - \mathbf{u}_{\text{opt}}(\mathbf{d})) \tag{2.16}$$

This simple expression for the loss is a key result that allows us to end up with a convex optimization problem.

Optimal sensitivities

Note from (2.13) that we can write $\mathbf{u}_{\text{opt}} = \mathbf{F}^u\mathbf{d}$ where $\mathbf{F}^u = -\mathbf{J}_{uu}^{-1}\mathbf{J}_{ud}$. More generally, we can write

$$\mathbf{y}_{\text{opt}} = \mathbf{F}\mathbf{d} \tag{2.17}$$

where $\mathbf{F}$ is the optimal sensitivity of the outputs (measurements) with respect to the disturbances. Here, $\mathbf{F}$ can be obtained using (2.8) and (2.13),

$$\mathbf{y}_{\text{opt}} = \mathbf{G}^y\mathbf{u}_{\text{opt}} + \mathbf{G}_d^y\mathbf{d} = (-\mathbf{G}^y\mathbf{J}_{uu}^{-1}\mathbf{J}_{ud} + \mathbf{G}_d^y)\mathbf{d}$$

that is,

$$\mathbf{F} = (-\mathbf{G}^y\mathbf{J}_{uu}^{-1}\mathbf{J}_{ud} + \mathbf{G}_d^y) \tag{2.18}$$

However, (2.18) is not generally a robust way to obtain $\mathbf{F}$, for example $\mathbf{J}_{uu}, \mathbf{J}_{ud}$ can be difficult to obtain numerically, and taking the difference in (2.18) can also be unreliable numerically. Thus, for practical use it is usually better to obtain $\mathbf{F}$ directly from its definition, $\mathbf{F} = \frac{d\mathbf{y}_{\text{opt}}}{d\mathbf{d}}$. This typically involves numerical re-optimization for each disturbance.

The loss L as a function of disturbances and noise

We here just present the derivation of the main result (Halvorsen et al., 2003; Alstad et al., 2009). We start from the loss expression in (2.15), $L = \frac{1}{2}\|\mathbf{z}\|_2^2$ where $\mathbf{z} = \mathbf{J}_{uu}^{1/2}(\mathbf{u} - \mathbf{u}_{\text{opt}})$. We want to write $\mathbf{z}$ as a function of $\mathbf{d}$ and $\mathbf{n}^y$, given that the input $\mathbf{u}$ should be adjusted to satisfy (2.9). We start by writing $\mathbf{u} - \mathbf{u}_{\text{opt}}$ as a function of $\mathbf{c} - \mathbf{c}_{\text{opt}}$. We have $\mathbf{c} = \mathbf{H}\mathbf{y}$, so

$$\begin{aligned}\mathbf{c} &= \mathbf{H}\mathbf{y} = \mathbf{H}\mathbf{G}^y\mathbf{u} + \mathbf{H}\mathbf{G}_d^y\mathbf{d}\\ \mathbf{c}_{\text{opt}} &= \mathbf{H}\mathbf{y}_{\text{opt}} = \mathbf{H}\mathbf{G}^y\mathbf{u}_{\text{opt}} + \mathbf{H}\mathbf{G}_d^y\mathbf{d}\end{aligned}$$

Thus, $\mathbf{c} - \mathbf{c}_{\text{opt}} = \mathbf{H}\mathbf{G}^y(\mathbf{u} - \mathbf{u}_{\text{opt}})$, or

$$(\mathbf{u} - \mathbf{u}_{\text{opt}}) = (\mathbf{H}\mathbf{G}^y)^{-1}(\mathbf{c} - \mathbf{c}_{\text{opt}}) \tag{2.19a}$$

where $\mathbf{H}\mathbf{G}^y$ is the square gain matrix from the inputs $\mathbf{u}$ to the selected controlled variables $\mathbf{c}$.

The next step is to express $(\mathbf{c} - \mathbf{c}_{\text{opt}})$ as a function of $\mathbf{d}$ and $\mathbf{n}^y$. From (2.17) we have that

$$\mathbf{c}_{\text{opt}} = \mathbf{HFd} \tag{2.19b}$$

From (2.9) we have that $\mathbf{H}(\mathbf{y} + \mathbf{n}^y) = \mathbf{c}_s$ (constant), or

$$\mathbf{c} = \mathbf{Hy} = -\mathbf{Hn}^y + \mathbf{c}_s \tag{2.19c}$$

Here, $\mathbf{c}_s = 0$, since we assume the nominal point is optimal. Since the signs for $\mathbf{n}^y$ and $\mathbf{d}$ do not matter for the expressions we derive below (from (2.11) we can have both positive and negative changes), we can write

$$\begin{aligned} \mathbf{u} - \mathbf{u}_{\text{opt}} &= (\mathbf{HG}^y)^{-1}\mathbf{H}(\mathbf{Fd} + \mathbf{n}^y) \\ &= (\mathbf{HG}^y)^{-1}\mathbf{H}(\mathbf{FW}_d\mathbf{d}' + \mathbf{W}_{n^y}\mathbf{n}^{y'}) \\ &= (\mathbf{HG}^y)^{-1}\mathbf{HY}\begin{bmatrix} \mathbf{d}' \\ \mathbf{n}^{y'} \end{bmatrix} \end{aligned} \tag{2.19d}$$

where we have introduced

$$\mathbf{Y} = [\mathbf{FW}_d \quad \mathbf{W}_{n^y}] \tag{2.20}$$

Note that $\mathbf{W}_d$ and $\mathbf{W}_{n^y}$ are usually diagonal matrices, representing the magnitude of the disturbances and measurement noises, respectively.

In summary, we have derived that for the given normalized disturbances $\mathbf{d}'$ and for the given normalized measurement noises $\mathbf{n}^{y'}$ the loss is given by (Halvorsen et al., 2003)

$$L = \frac{1}{2}\mathbf{z}^T\mathbf{z} \tag{2.21}$$

where

$$\mathbf{z} = \mathbf{J}_{uu}^{1/2}(\mathbf{u} - \mathbf{u}_{\text{opt}}) = \underbrace{\mathbf{J}_{uu}^{1/2}(\mathbf{HG}^y)^{-1}\mathbf{HY}}_{\mathbf{M}(\mathbf{H})}\begin{bmatrix} \mathbf{d}' \\ \mathbf{n}^{y'} \end{bmatrix} \tag{2.22}$$

Worst-case and average loss for a given H (analysis using loss method)

The above expressions give the loss for a given $\mathbf{d}'$ and $\mathbf{n}^{y'}$, but the goal is the find the "magnitude" of the loss L for the expected set for example as given in (2.11). Here "magnitude" can be defined in different ways, and for a given $\mathbf{H}$ the worst-case loss (Halvorsen et al., 2003) and average loss (Kariwala et al., 2008) are given by

$$L_{wc} = \frac{1}{2}\bar{\sigma}(\mathbf{M})^2 \tag{2.23}$$

$$L_{avg} = \mathbb{E}(L) = \frac{1}{2}\|\mathbf{M}\|_F^2 \tag{2.24}$$

where

$$\mathbf{M}(\mathbf{H}) = \mathbf{J}_{uu}^{1/2}(\mathbf{H}\mathbf{G}^y)^{-1}\mathbf{H}\mathbf{Y} \tag{2.25}$$

Here $\bar{\sigma}(\mathbf{M})$ denotes the maximum singular value (induced 2-norm) of the matrix $\mathbf{M}(\mathbf{H})$, and $\|\mathbf{M}\|_F = \sqrt{\sum_{i,j}\mathbf{M}_{ij}^2}$ denotes the Frobenius norm of the matrix $\mathbf{M}$. Use of the norm of $\mathbf{M}$ to analyze the loss is known as the "exact local method" (Halvorsen et al., 2003). Note that these loss expressions are for a given matrix $\mathbf{H}$.

The controlled variable selection problem using self-optimizing control framework based on local analysis is to select the matrix $\mathbf{H}$ and associated controlled variables, $\mathbf{c} = \mathbf{H}\mathbf{y}$, that results in the minimum worst-case loss (2.23) and/or average loss (2.24). The CV selection problem by selecting $\mathbf{H}$ based on local methods (2.23) was originally believed to be non-convex (Halvorsen et al., 2003). Hence, previously few qualitative requirements, minimum singular value rule (Halvorsen et al., 2003), minimum loss method (Halvorsen et al., 2003) and null space method (Alstad and Skogestad, 2007) are proposed to find the controlled variables that minimize the deviation from optimal operation.

2.5.5 Qualitative requirements for self-optimizing CV

Skogestad (2000) presents several qualitative requirements for a good self-optimizing controlled variable $\mathbf{c}$:

Requirement 1: Its *optimal* value should be insensitive to disturbances, i.e. $\mathbf{c}_{\text{opt}}(\mathbf{d})$ small.

Requirement 2: It should be easy to measure and control accurately (its implementation error should be small).

Requirement 3: Its value should be sensitive to changes in the manipulated input ($\mathbf{u}$), that is, the gain from $\mathbf{u}$ to $\mathbf{c}$ should be large.

Requirement 4: For cases with two or more controlled variables, the selected controlled variables should not be closely correlated.

The first requirement deals with sensitivity to disturbances, while requirements 2-4 deal with the implementation errors. All these requirements need to be fulfilled in order to guarantee a good self-optimizing controlled variable. Note that requirement 1 says that the $\mathbf{c}_{\text{opt}}$ should be insensitive to disturbances and not $\mathbf{c}$.

2.5.6 Minimum singular value rule

The minimum singular value rule is to select the controlled variables based on a scaled steady-state gain from the inputs to the candidate outputs (Skogestad and Postlethwaite, 1996; Halvorsen et al., 2003; Alstad, 2005). From (2.21) and (2.25) we have that

$$L = \frac{1}{2}\|\mathbf{z}\|_2^2 \tag{2.26}$$

where

$$\mathbf{z} = \mathbf{J}_{uu}^{1/2}(\mathbf{u} - \mathbf{u}_{\text{opt}}) = \mathbf{J}_{uu}^{1/2}\mathbf{G}^{-1}(\mathbf{c} - \mathbf{c}_{\text{opt}}) = \mathbf{J}_{uu}^{1/2}\mathbf{G}^{-1}\mathbf{e}_c \tag{2.27}$$

The $\mathbf{J}_{uu}^{1/2}$ matrix exists as $\mathbf{J}_{uu}$ is positive definite (Horn and Johnson, 1991), $\mathbf{e}_c = \mathbf{c} - \mathbf{c}_{\text{opt}}$ and $\|\mathbf{z}\|_2$ denotes the 2-norm of the vector. The variables are scaled as follows:

- Scale each candidate controlled variable c_i such that the optimal variation for the considered disturbances and implementation errors bounds is unity. Then the combined scaled error norm for each candidate controlled variables is $\|e'_{c,i}\|_2 = \|c'_i - {c_{i,\text{opt}}}'\|_2 \leq 1$.
- Scale each u_i such that a unit change in each input has the same effect on the cost function (J).

Now let $\mathbf{G}'$ be the scaled steady-state gain and from eq. (2.26) we have that the worst-case loss is

$$\begin{aligned} L_{wc} = \max_{\|\mathbf{e}'_c\|_2 \leq 1} L &= \max_{\|\mathbf{e}'_c\|_2 \leq 1} \frac{1}{2}\|\mathbf{z}\|_2^2 \\ &= \frac{1}{2}(\bar{\sigma}(\mathbf{J}_{uu}^{1/2}\mathbf{G}'^{-1}))^2 = \frac{1}{2}(\bar{\sigma}(\alpha^{1/2}\mathbf{G}'^{-1}))^2 = \frac{\alpha}{2}\frac{1}{\underline{\sigma}((\mathbf{G}')^2} \end{aligned} \tag{2.28}$$

where the constant $\alpha = \bar{\sigma}(\mathbf{J}_{uu})$ is independent of the choice of the controlled variable and $\underline{\sigma}(\mathbf{G}')$ denotes the minimum singular value of $\mathbf{G}'$. The maximum singular value $\bar{\sigma}$ is the induced 2-norm of a matrix. As we scaled the $\mathbf{u}$ to have same effect on cost function, $\mathbf{J}_{uu}$ is unitary. The last equality holds as the maximum singular value of $\mathbf{G}'^{-1}$ is the minimum singular value of $\mathbf{G}'$ (i.e. $\bar{\sigma}(\mathbf{G}'^{-1}) = \frac{1}{\underline{\sigma}(\mathbf{G}')}$). Hence to minimize the worst-case loss (2.28), we should select controlled variables that result in the largest minimum singular value for the scaled steady state gain.

This method requires appropriate scaling of the inputs and outputs. Selecting an exact scaling is difficult as we cannot study each and every possible combination of disturbances and implementation errors bounded by $\left\| \begin{bmatrix} \mathbf{d} \\ \mathbf{n}^y \end{bmatrix} \right\|_2 \leq 1$. For a more detailed discussion of the minimum singular value and illustrating examples, see Halvorsen et al. (2003). The singular value method has been applied to many case studies, see e.g. Skogestad (2000) and the references therein.

2.5.7 Minimum loss method

The optimal $\mathbf{H}$ can be found by minimizing either the worst-case loss (2.23) or the average loss (2.24). Fortunately, Kariwala et al. (2008) prove that the $\mathbf{H}$ that minimizes the average loss in equation (2.24) is super optimal, in the sense that the same $\mathbf{H}$ minimizes the worst-case loss in (2.23). Hence, only minimization of the Frobenius norm in (2.24) is considered in this thesis. The square does not effect the optimal solution and can be omitted. In summary, the problem is to find the combination matrix $\mathbf{H}$ that minimizes the Frobenius norm of $\mathbf{M}$:

Theorem 1 Minimum loss method (Alstad et al., 2009) *To minimize the average and worst-case loss for expected combined disturbances and noise, ($\|[\mathbf{d}', \mathbf{n}^{y'}]^T\|_2 \leqslant 1$), find the H that solves the problem*

$$\min_{\mathbf{H}} \left\| \mathbf{J}_{uu}^{1/2} (\mathbf{H}\mathbf{G}^y)^{-1} \mathbf{H}\mathbf{Y} \right\|_F \tag{2.29}$$

where $\mathbf{Y} = [\mathbf{F}\mathbf{W}_d \quad \mathbf{W}_{\mathbf{n}^y}]$.

The objective in (2.29) is to find the non-square $n_u \times n_y$ matrix $\mathbf{H}$ (note that $n_u = n_c$).

2.5.8 Null space method

The null space method of selecting $\mathbf{H}$ such that $\mathbf{H}\mathbf{F} = 0$ (Alstad and Skogestad, 2007) follows if we neglect measurement noise such that $\mathbf{Y} = [\mathbf{F}\mathbf{W}_d \quad \underline{\underline{0}}]$, where $\underline{\underline{0}}$ is zero matrix of $n_y \times n_y$ size, and assume that we have enough measurements to make $\mathbf{H}\mathbf{F} = 0$. In the presence of measurements, $n_y \geq n_d + n_u$, it is always possible to find a non trivial $\mathbf{H}$ in the left-null space of $\mathbf{F}$ to result in zero loss.

This method is useful, when controlled variables are selected as combination of measurements $n_y \geq n_u + n_d$ and to get perfect disturbance rejection.

Selection of optimal measurements does not play any role in this method as every measurement set with greater than $n_u + n_d$ measurements give perfect disturbance rejection.

2.6 Thesis contribution in self-optimizing control framework

The major focus of this thesis to find an optimal **H** that minimizes the loss (2.24) from optimal operation in the presence of disturbances. The optimal **H** selection for a given measurement set is shown as a constrained QP (Alstad et al., 2009). Using the method (Alstad et al., 2009) gives an optimal **H** for a chosen measurement set, but still finding an optimal measurement subset is an important problem.

2.6.1 Measurement subset selection with full H

Measurement subset selection with full **H** for optimal CV is an important problem. To solve this problem, customized branch and bound methods are developed (Kariwala and Cao, 2009, 2010a). In this thesis, alternatively, we formulated a standard Mixed Integer Quadratic Programming approach to find the optimal measurement subsets. The developed MIQP based method is discussed in detail in Chapter 3. The developed MIQP based method allows for additional structural constraints compared to the bidirectional branch and bound methods (Kariwala and Cao, 2009, 2010a). MIQP method takes longer time than the bidirectional branch and bound methods, but are acceptable as the measurement subset selection is done offline. Including more number of measurements for CV combination averages out the measurement noise contribution in the loss.

2.6.2 Measurement subset selection with structured H

Combining the measurements from different sections in a process with full **H** may result in poor controllability and dynamic properties. To overcome these, it may be desirable to have structured **H**. Structured **H** imposes limitation, that is, we may require some elements in **H** to be zero. For example, for dynamic reasons we may want to combine measurements from given process section, and we require a (decentralized) block diagonal (BD)

(2.30) or triangular (T) $\mathbf{H}$ (2.31).

$$\mathbf{H}_{BD} = \begin{bmatrix} \mathbf{H}_1 & 0 & \cdots & 0 \\ 0 & \mathbf{H}_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{H}_{n_{iu}} \end{bmatrix} \tag{2.30}$$

$$\mathbf{H}_{T} = \begin{bmatrix} \mathbf{H}_{11} & \mathbf{H}_{12} & \cdots & \mathbf{H}_{1n_{iu}} \\ 0 & \mathbf{H}_{22} & \cdots & \cdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{H}_{n_{iu}n_{iu}} \end{bmatrix} \tag{2.31}$$

The optimization problem here is to minimize (2.24) with a structure in $\mathbf{H}$. This is a non-convex optimization problem and an iterative method is proposed (Heldt, 2010). In this thesis, we propose various convex approximation methods to find structured $\mathbf{H}$ that provides a sub optimal solution and serve as good upper bounds. We further extend the convex approximation methods to find optimal measurement subset with a structure in $\mathbf{H}$ using MIQP framework. These methods are discussed in detail with two representative case studies in Chapter 4.

2.7 Other related concepts

A short overview of other methods for ensuring optimal process operation are given. As uncertainties are unavoidable in process systems, the effects of uncertainty for optimal operation are also presented. We provide only a brief overview of the methods and for comprehensive details, we refer the reader to the references provided at the end of this chapter.

2.7.1 Experimental methods

Experimental methods require carefully designed experiments to measure or infer the objective function to operate the plant optimally (Box, 1957). The experiments are designed to facilitate the estimation of the gradient information. Based on the estimated gradient information, a new set of experiments are designed until the estimated gradient converges to zero (i.e. to the optimum). Requirement of frequent experiments in the presence of disturbances make experimental methods impractical for continuous process plants for optimal operation. In addition, performing the carefully designed experiments are often resource intensive and introduces additional disturbance to process operation.

2.7.2 Necessary conditions of optimality tracking

In Necessary conditions of optimality (NCO) tracking, the inputs are updated directly to maintain the analytical gradient of the Lagrangian function associated with the optimal process operation at zero (Srinivasan et al., 2003; Kadam et al., 2007). For steady state optimization, iterative input updates are used to converge to optimal steady state operating point (François et al., 2005; Gros et al., 2009). Slow speed of convergence caused by inaccurate gradient information usually makes these difficult to use in practice.

2.7.3 Extremum seeking control

Extremum seeking control is an experimental method. The process is driven towards optimum by imposing an excitation signal to the process. Hence in these methods both the identification of process states and obtaining optimal inputs are combined (Ariyur and Krstic, 2003). This method is based on the direct measurement of objective function or based on the dependency of states and disturbances to objective function. Adaptive extremum seeking controller is proposed to minimize an objective function as penalty on both the performance error and control action (El-Farra and Christofides, 2001). The drawbacks of extremum seeking methods are the convexity of the disturbance space to guarantee the convergence of estimation, the assumption of state feedback and slow speed of convergence.

2.7.4 Optimizing controllers based on economics

In contrast to minimizing the tracking error as in classical control theory, an optimization problem is solved online by using the process economics as the objective function in optimizing controllers (Kassidas et al., 2000; Engell, 2007). These are useful but slow speed of convergence make these difficult to use in practice.

2.7.5 Model predictive control

Model predictive control (MPC) has gained importance in control community (Garcia et al., 1989; Mayne et al., 2000). Numerous versions of linear/nonlinear MPC and their industrial installations are reported (Qin, 2003; Maciejowski, 2002; Rawlings and Mayne, 2009). MPC works based on a moving horizon philosophy, a sequence of control actions is chosen according to a prediction of future trajectory of the system and applied to the plant until new measurement is available. Then a new input sequence is determined at the next sampling time. The advantages of MPC are the ability

to handle input, output constraints and interactions. The MPC controllers can be formulated to track set points or to drive the controlled variables to a desired range. Robust MPC implementation can be found in Camacho and Bordons (1998).

Nonlinear MPC (NMPC) uses a nonlinear process model to predict the future trajectory of the system. NMPC is applied for chemicals, polymers and air and gas processing plants (Qin, 2003).

Linear MPC solve a quadratic optimization problem and nonlinear MPC solve a nonlinear optimization problem online. The computation requirement can inhibit the usage of these controllers in practice. To overcome the online optimization solving in MPC, explicit MPC is proposed, where the inputs are calculated using an explicit state feedback controller developed offline (Pistikopoulos et al., 2000; Grancharova et al., 2004). The idea in explicit MPC is to divide the state space into regions and to form an explicit state feedback control law for each region. But these methods fail as the number of regions grow with the process dimensions.

2.7.6 Regulatory control layer

The plantwide control system for the overall plant is in most cases organized in a hierarchical structure (Figure 2.1), based on time scale separation between the layers. The main objective of the upper slower "supervisory" layer is to keep the "economic" or primary controlled variables CV_1 close to their economic optimal set points. On the other hand, the objectives of the lower faster "regulatory" layer is to facilitate stable operation, to regulate and to keep the operation in the linear operating range (Skogestad and Postlethwaite, 2005) without the need to reconfigure the loops in the regulatory layer. Ideally, we would like to have a tool that based on a process model, automatically selects structure of the regulatory control layer, including the controlled variables (CV_2) and pairing with manipulated variables (valves).

The regulatory control layer has received the attention of various researchers, for example, Buckley (1964), Lee and Weekman (1976), Arkun and Stephanopoulos (1980), Shinnar (1981), Narraway and Perkins (1993), Hovd and Skogestad (1993), Narraway and Perkins (1994), Luyben (1996), Luyben et al. (1998), Wang and McAvoy (2001), Kookos and Perkins (2002), Konda et al. (2005), de Araújo et al. (2007), Kariwala and Cao (2010b). These are either based on heuristic, procedural or mathematical methods. A few mathematical approaches formulate mixed integer non linear programming (MINLP) problems (Narraway and Perkins, 1993, 1994; Kookos and Perkins, 2002) to find suitable controlled variables CV_2 and their pairings with MV. These are combinatorial in nature and are very time consuming

and generally global optimality cannot be guaranteed.

Thesis contribution: Controlled variables selection for regulatory control layer

In this thesis, we quantify the regulatory layer performance with state drift criterion and propose quantitative methods to identify regulatory layer controlled variables CV_2. The quantitative methods are described and evaluated for representative case studies in detail in Chapter 5.

2.8 Conclusions

The control hierarchy of plantwide control problems is described. The context of control structure design problem for the process plant is described. The self-optimizing framework is used to develop a controlled variable selection method, which explicitly account for the business objectives is described. The previous work on self-optimizing control, namely maximum gain rule, exact local method, null space method are described. The contribution of the thesis in self optimizing control framework is briefly described. Various other methods for optimal operation are briefly mentioned.

Bibliography

Adetola, V., Guay, M., 2010. Integration of real-time optimization and model predictive control. Journal of Process Control 20 (2), 125 – 133.

Alstad, V., 2005. Studies on selection of controlled variables. Ph.D. thesis, Norwegian University of Science and Technology, Department of Chemical Engineering.

Alstad, V., Skogestad, S., 2007. Null space method for selecting optimal measurement combinations as controlled variables. Ind. Eng. Chem. Res. 46, 846–853.

Alstad, V., Skogestad, S., Hori, E., 2009. Optimal measurement combinations as controlled variables. Journal of Process Control 19 (1), 138–148.

Ariyur, K. B., Krstic, M., 2003. Real-Time Optimization by Extremum-Seeking Control. Wiley-Interscience.

Arkun, Y., Stephanopoulos, G., 1980. Studies in the synthesis of control structures for chemical processes: Part IV. design of steady-state optimizing control structures for chemical process units. AIChE Journal 26 (6), 975–991.

Box, G. E. P., 1957. Evolutionary operation: A method for increasing industrial productivity. Journal of the Royal Statistical Society. Series C (Applied Statistics) 6 (2), 81–101.

Buckley, P. S., 1964. Techniques of process control. John Wiley & Sons, New York, USA.

Camacho, E., Bordons, C., 1998. Model Predictive Control. Springer.

Cao, Y., 2003. Self-optimizing control structure selection via differentiation. Proceedings of the European Control Conference, 445–453.

de Araújo, A. C., Govatsmark, M., Skogestad, S., 2007. Application of plantwide control to the hda process. I - steady-state optimization and self-optimizing control. Control Engineering Practice 15 (10), 1222 – 1237.

El-Farra, N., Christofides, P., 2001. Integrating robustness, optimality and constraints in control of nonlinear processes. Chem. Eng. Sci. 56, 1841–1868.

Engell, S., 2007. Feedback control for optimal process operation. Journal of Process Control 17 (3), 203 – 219, special Issue ADCHEM 2006 Symposium.

Findeisen, W., Nailey, F., Brdys, M., Malinowski, K., Tatjewski, P., Wozniak, A., 1980. Control and Coordination in Hierachical Systems. John Wiley & Sons.

Forbes, J. F., Marlin, T. E., 1996. Design cost: A systematic approach to technology selection for model-based real-time optimization systems. Computers & Chemical Engineering 20 (6-7), 717 – 734, fifth International Symposium on Process Systems Engineering.

Foss, A., 1973. Critique of chemical process control theory. AIChE Journal 19, 209–214.

François, G., Srinivasan, B., Bonvin, D., 2005. Use of measurements for enforcing the necessary conditions of optimality in the presence of constraints and uncertainty. Journal of Process Control 15 (6), 701 – 712.

Garcia, C. E., Prett, D. M., Morari, M., May 1989. Model predictive control: theory and practice a survey. Automatica 25, 335–348.

Grancharova, A., Johansen, T., Kocijan, J., 2004. Explicit model predictive control of gas-liquid separation plant via orthogonal search tree partitioning. Comput. Chem. Eng. 28, 2481–2491.

Gros, S., Srinivasan, B., Bonvin, D., 2009. Optimizing control based on output feedback. Computers and Chemical Engineering 33 (1), 191 – 198.

Guay, M., Zhang, T., 2003. Adaptive extremum seeking control of nonlinear dynamic systems with parametric uncertainties. Automatica 39 (7), 1283 – 1293.

Halvorsen, I. J., Skogestad, S., Morud, J. C., Alstad, V., 2003. Optimal selection of controlled variables. Ind. Eng. Chem. Res. 42.

Heldt, S., 2010. Dealing with structural constraints in self-optimizing control engineering. Journal of Process Control 20 (9), 1049 – 1058.

Horn, R. A., Johnson, C. R., 1991. Topics in matrix analysis. Cambridge.

Hovd, M., Skogestad, S., 1993. Procedure for regulatory control structure selection with application to the FCC process. AIChE Journal 39 (12), 1938–1953.

Kadam, J., Marquardt, W., Schlegel, M., Backx, T., Bosgra, O., Brouwer, P.-J., Dünnebier, G., Hessem, D., Wolf, A. T. S., 2003. Towards integrated dynamic real-time optimization and control of industrial processes. FOCAPO 2003. 4th Int. Conf. of Computer-Aided Process Operations, Proceedings of the Conference held at Coral Springs, Florida, January 12-15, 2003, 593–596.

Kadam, J. V., Marquardt, W., Srinivasan, B., Bonvin, D., 2007. Optimal grade transition in industrial polymerization processes via NCO tracking. AIChE Journal 53 (3), 627–639.

Kariwala, V., Cao, Y., 2009. Bidirectional branch and bound for controlled vaiable selection. Part II: Exact local method for self-optimizing control. Computers and Chemical Engineering 33, 1402–1414.

Kariwala, V., Cao, Y., 2010a. Bidirectional branch and bound for controlled vaiable selection. Part III: Local average loss minimization. IEEE Transactions on Industrial Informatics 6, 54–61.

Kariwala, V., Cao, Y., 2010b. Branch and bound method for multiobjective pairing selection. Automatica 46 (5), 932 – 936.

Kariwala, V., Cao, Y., Janardhanan, S., 2008. Local self-optimizing control with average loss minimization. Ind. Eng. Chem. Res. 47, 1150–1158.

Kassidas, A., Patry, J., Marlin, T., 2000. Integrating process and controller models for the design of self-optimizing control. Computers & Chemical Engineering 24 (12), 2589 – 2602.

Konda, N. V. S. N. M., Rangaiah, G. P., Krishnaswamy, P. R., 2005. Plantwide control of industrial processes: An integrated framework of simulation and heuristics. Industrial & Engineering Chemistry Research 44 (22), 8300–8313.

Kookos, I. K., Perkins, J. D., 2002. Regulatory control structure selection of linear systems. Computers & Chemical Engineering 26 (6), 875 – 887.

Larsson, T., Skogestad, S., 2000. Plantwide control - A review and a new design procedure. Modeling, Identification and Control 21 (4), 209–240.

Lee, W., Weekman, V. W., 1976. Advanced control practice in the chemical process industry: A view from industry. AIChE Journal 22 (1), 27–38.

Loeblein, C., Perkins, J., 1998. Economic analysis of different structures of on-line process optimization systems. Comput. Chem. Eng. 22 (9), 1257–1269.

Luyben, W. L., 1996. Simple regulatory control of the eastman process. Industrial & Engineering Chemistry Research 35 (10), 3280–3289.

Luyben, W. L., Luyben, M. L., Tyreus, B. D., 1998. Plantwide process control. McGraw-Hill, USA.

Maarleveld, A., Rijnsdorp, J., 1970. Constraint control on distillation columns. Automatica 6 (1), 51 – 58.

Maciejowski, J. M., 2002. Predictive Control with Constraints. Prentice Hall.

Mahajanam, R., Zheng, A., Douglas, J., 2001. A shortcut method for controlled variable selection and its application to the butane alkylation process. Ind. Eng. Chem. Res. 40 (14), 3208–3216.

Marlin, T., Hrymak, A., 1997. Real-time operations optimization of continuous processes. In: Proceedings of CPC V, AIChE Symposium Series vol. 93. pp. 156–164.

Mayne, D. Q., Rawlings, J. B., Rao, C. V., Scokaert, P. O. M., Jun. 2000. Constrained model predictive control: Stability and optimality. Automatica 36 (6), 789–814.

Morari, M., Stephanopoulos, G., 1980a. Studies in the synthesis of control structures for chemical processes: Part II: Structural aspects and the synthesis of alternative feasible control schemes. AIChE Journal 26 (2), 232–246.

Morari, M., Stephanopoulos, G., 1980b. Studies in the synthesis of control structures for chemical processes: Part III: Optimal selection of secondary measurements within the framework of state estimation in the presence of persistent unknown disturbances. AIChE Journal 26 (2), 247–260.

Morari, M., Stephanopoulos, G., Arkun, Y., 1980. Studies in the synthesis of control structures for chemical processes. Part I: formulation of the problem. process decomposition and the classification of the control task. analysis of the optimizing control structures. AIChE Journal 26 (2), 220–232.

Narraway, L., Perkins, J., 1994. Selection of process control structure based on economics. Computers & Chemical Engineering 18, Supplement 1 (0), S511 – S515.

Narraway, L., Perkins, J., Barton, G., 1991. Interaction between process design and process control: economic analysis of process dynamics. Journal of Process Control 1 (5), 243 – 250.

Narraway, L. T., Perkins, J. D., 1993. Selection of process control structure based on linear dynamic economics. Industrial & Engineering Chemistry Research 32 (11), 2681–2692.

Pistikopoulos, E., Dua, V., Bozinis, N., Bemporad, A., Morari, M., 2000. On-line optimization via off-line parametric optimization tools. Comput. Chem. Eng. 24, 175–185.

Qin, S. J. Badgwell, T. A., 2003. A survey of industrial model predictive control technology. Control Engineering Pactice 11.

Rawlings, J., Mayne, D., 2009. Model Predictive Control Theory and Design. Nob Hill Pub.

Shinnar, R., 1981. Chemical reactor modelling for purposes of controller design. Chemical Engineering Communications 9 (1-6), 73–99.

Skogestad, S., 2000. Plantwide control: The search for the self-optimizing control structure. Journal of Process Control 10, 487–507.

Skogestad, S., Postlethwaite, I., 1996. Multivariable Feedback Control, 1. Edition. Wiley.

Skogestad, S., Postlethwaite, I., 2005. Multivariable Feedback Control, 2. Edition. Wiley.

Srinivasan, B., Bonvin, D., Visser, E., Palanki, S., 2003. Dynamic optimization of batch processes: II. Role of measurements in handling uncertainty. Computers & Chemical Engineering 27 (1), 27 – 44.

Wang, P., McAvoy, T., 2001. Synthesis of plantwide control systems using a dynamic model and optimization. Industrial & Engineering Chemistry Research 40 (24), 5732–5742.

Zhang, Y., 2010. Robust dynamic real-time optimization under parametric uncertainty for plant-wide processes. 8th World Congress on Intelligent Control and Automation (WCICA), 4078 –4083.

Zhang, Y., Monder, D., Forbes, J., 2002. Real-time optimization under parametric uncertainty: A probability constrained approach. J. Proc. Control 12 (3), 373–389.

Zhang, Y., Nader, D., Forbes, J., 2001. Results analysis for trust constrained real-lime optimization. Journal of Process Control 11, 329–341.

Chapter 3

Convex formulations for optimal selection of controlled variables and measurements using Mixed Integer Quadratic Programming

Based on an accepted paper in
Journal of Process Control

The appropriate selection of controlled variables is important for operating a process optimally in the presence of disturbances. Self-optimizing control provides a mathematical framework for selecting the controlled variables as combinations of measurements, $\mathbf{c} = \mathbf{Hy}$, with the aim to minimize the steady state loss from optimal operation. In this paper, we present (i) a convex formulation to find the optimal combination matrix $\mathbf{H}$ for a given measurement set, and (ii) a Mixed-Integer Quadratic Programming (MIQP) methodology to select optimal measurement subsets that result in minimal loss. The methods presented in this paper are exact for quadratic problems with linear measurement relations. The MIQP methods can handle additional structural constraints compared to the branch and bound (BAB) methods reported in literature. The MIQP methods are evaluated on a toy test problem, an evaporator example, a binary distillation column example with 41 stages and a Kaibel column with 71 stages.

3.1 Introduction

Control structure selection deals with the selection of controlled variables (CVs/outputs) and manipulated variables (MVs/inputs), and the pairings or interconnections of these variables (Foss, 1973; Skogestad, 2000). A comprehensive review of input/output selection methods was provided by van de Wal and de Jager (2001). These input/output selection methods use desirable control system properties, (state, structural, input-output) controllability, achievable performance as criteria to arrive at CVs that are easy to control. However, these CV selection criteria fail to take into account more overall objectives, like economic profitability or cost (J). The selection of control structure based on economics is stressed by Narraway and co-workers (Narraway et al., 1991; Narraway and Perkins, 1993) for the effect of disturbances, but they do not formulate rules or procedures to select controlled variables.

In this paper, we consider the link between (economic) optimization and control as illustrated in Figure 3.1. Self-optimizing control (SOC) (Skogestad, 2000) aims at achieving acceptable operation by maintaining selected CVs ($\mathbf{c}$ in Figure 3.1) at constant or slowly varying set points. The idea dates back to (Morari et al., 1980), who stated that "we want to find a function $\mathbf{c}$ of the process variables which when held constant, leads automatically to the optimal adjustments of the manipulated variables, and with it, the optimal operating condition". Self-optimizing control makes use of the degrees of freedom in $\mathbf{c} = \mathbf{Hy}$, which link the optimization and control layers. There are three elements in the self-optimizing control approach. They are off-line static optimization to compute $\mathbf{H}$ to find controlled variables $\mathbf{c} = \mathbf{Hy}$, on-line slow time-scale static RTO to compute $\mathbf{c}_s$ and fast time-scale feedback control that adjusts $\mathbf{u}$. In this paper, we present the off-line static optimization approach to select $\mathbf{H}$, based on steady-state economics, but because the variables $\mathbf{c}$ are controlled in the feedback layer, one gets much faster updates in the inputs $\mathbf{u}$ than with the online slow time-scale RTO that computes $\mathbf{c}_s$. The dynamic performance of control structures obtained from self-optimizing control for various processes are reported (de Araújo et al., 2007; Vasudevan et al., 2009; Panahi and Skogestad, 2011). The idea of self-optimizing control is to put as much optimization as possible into the control layer. That is, when there is a disturbance, we want the system "go in the right direction" on the fast time scale, and not have to wait for optimization layer (RTO) to take the optimal action, which may take a long time, since RTO needs to estimate the disturbances (e.g., using data reconciliation) before taking action.

For example, consider the process of cake baking. The (original) physical degree of freedom is the oven heat input ($\mathbf{u} = Q$). However, baking the "optimal" cake is difficult when using the heat input directly for optimization (with the human as the RTO), and would require frequent changes in Q. However, we have available other measurements, including the oven temperature T. Consider the two candidate "measurements"

$$\mathbf{y} = [Q \quad T]^T$$

Clearly, the best variable to keep constant is T, so we choose $\mathbf{c} = \mathbf{H}\mathbf{y} = h_{11}Q + h_{12}T = T$ as the controlled variable, that is, we choose $\mathbf{H} = [0 \quad 1]$. With a temperature controller (thermostat), we (the human RTO) may use the temperature set point ($\mathbf{c}_s$) as the optimization variable. Clearly, the introduction of the self-optimizing variable $\mathbf{c} = T$, simplifies the real-time optimization effort and requires less frequent changes than when using Q.

Instead of the two layer structure in Figure 3.1, one could combine the layers and use real time optimization more directly by using a dynamic or steady state process model online to obtain an optimal input $\mathbf{u}_{\text{opt}}(\mathbf{d})$ for a disturbance $\mathbf{d}$. However, such a centralized solution would be costly in terms of modeling, implementation and maintenance (Forbes and Marlin, 1996) and would normally operate at a slower time scale than the feedback layer in Figure 3.1. A related alternative is optimizing controllers where the MVs ($\mathbf{u}$) are updated directly to maintain the gradient of the Lagrangian function associated with the optimal process operation at zero (Srinivasan et al., 2003). Based on how the gradient is obtained, these methods are categorized as Necessary conditions of optimality (NCO) tracking (Srinivasan et al., 2003; Kadam et al., 2007) or extremum seeking approaches (Ariyur and Krstic, 2003; Guay and Zhang, 2003). The former approaches use analytical gradients, whereas the latter use operational data to estimate gradients. Although these optimizing controllers may be useful, slow speed of convergence caused by inaccurate gradient information usually makes these difficult to use in practice.

Importantly, self-optimizing control which deals with the selection of $\mathbf{H}$ should not be viewed as an alternative to these other methods, including real time optimization or model predictive control (MPC), but rather as a complement, as illustrated in Figure 3.1. By appropriate selection of the variables $\mathbf{c} = \mathbf{H}\mathbf{y}$, we may reduce or eliminate the need for reoptimizing $\mathbf{c}_s$ independently of the approach we use for online optimization.

To quantify "acceptable operation" we introduce a scalar cost function J which should be minimized for optimal operation. In this paper, we assume that the (economic) cost mainly depends on the (quasi) steady-state

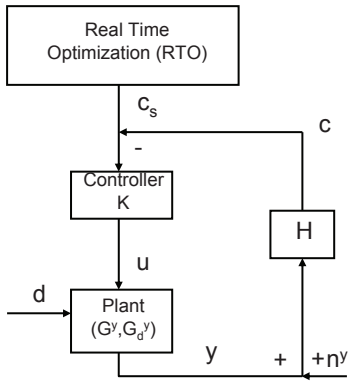

Figure 3.1: Feedback implementation of optimal operation with separate layers for optimization and control (Kassidas et al., 2000) (Engell, 2007). The controller K could be any controller including MPC. Self-optimizing control deals with selection of the controlled variables $\mathbf{c} = \mathbf{H}\mathbf{y}$

.

behavior, which is a good assumption for most continuous plants in the process industry. When selecting $\mathbf{c} = \mathbf{H}\mathbf{y}$, the cost function J is further assumed to be quadratic and the steady-state process model is assumed linear. Almost all steady-state unconstrained optimal operation problems can be approximated this way, usually by linearizing at the nominally optimal point. The scope of this paper is to provide systematic and good methods to select controlled variables (CVs, $\mathbf{c} \in \mathbb{R}^{n_c}$) associated with the unconstrained steady state degrees of freedom ($\mathbf{u} \in \mathbb{R}^{n_u}$) that minimize the loss, $L(\mathbf{u}, \mathbf{d}) = J(\mathbf{u}, \mathbf{d}) - J_{\text{opt}}(\mathbf{d})$, from economically optimal operation. The number of selected CVs is equal to the number of steady state degrees of freedom ($n_c = n_u$).

More specifically, the objective is to find a linear measurement combination,

$$\mathbf{c} = \mathbf{H}\mathbf{y} \tag{3.1}$$

such that control of these indirectly leads to acceptable operation with a small loss $L(\mathbf{u}, \mathbf{d}) = J(\mathbf{u}, \mathbf{d}) - J_{\text{opt}}(\mathbf{d})$, in spite of unknown disturbances, $\mathbf{d}$, and measurement noise (error), $\mathbf{n}^y$. If the original optimization problem is constrained, then we assume that all optimally active constraints are kept constant (controlled) and we consider the lower-dimensional unconstrained subspace. Depending on the disturbance range considered, there may be several constrained regions, and the procedure of finding $\mathbf{H}$ needs to be

repeated in each constrained region.

In this paper, we consider three problems related to finding optimal controlled variables, $\mathbf{c} = \mathbf{H}\mathbf{y}$,

Problem 3.1 Full $\mathbf{H}$, where the CVs are combinations of all measurements $\mathbf{y}$.

Problem 3.2 Measurements selection problems, where some columns in $\mathbf{H}$ are zero.

Case 3.2.1 Given subset of measurements.

Case 3.2.2 Optimal subset of measurements.

Case 3.2.3 Best individual measurements for decentralized control.

Compared to previous work (Kariwala and Cao, 2010), some additional restrictions are allowed for:

Case 3.2.4 Restriction on number of measurements from specified sections of the process.

Case 3.2.5 Addition of extra measurements to a given set.

Problem 3.3 Structured $\mathbf{H}$, where specified elements in $\mathbf{H}$ are zero; for example a block diagonal $\mathbf{H}$.

The problem of finding CVs as optimal measurement combinations (Problem 3.1) in the presence of disturbances and measurement noise was originally believed to be non convex and thus difficult to solve numerically (Halvorsen et al., 2003), but later it has been shown that this problem may be reformulated as a quadratic optimization problem with linear constraints (Alstad et al., 2009). The same problem was solved using generalized singular value decomposition method (Kariwala, 2007; Heldt, 2010). However, the problems of selecting individual measurements or linear combinations of a subset of measurements as controlled variables (Problems 3.2 and 3.3) are more difficult because of their combinatorial nature.

To solve Problem 3.2, effective partial bidirectional branch and bound (PB^3) methods have been developed (Kariwala and Cao, 2009) that exploit the monotonicity properties. However, these methods are cannot be used directly in the presence of the restrictions in Cases 3.2.4 and 3.2.5 as the monotonicity is not guaranteed. In this paper, we propose a different method to solve Problem 3.2 by reformulating the minimum loss method problem as a Mixed-Integer Quadratic Programming (MIQP) problem. The

MIQP formulations are simple and intuitive. The proposed MIQP formulations solve a convex quadratic optimization problem at each node in the search tree. These form a subclass of MIQP that are convex and hence these methods give globally optimal **H** that results in measurement combinations as CVs. The additional restrictions Cases 3.2.4 and 3.2.5 can easily be handled with the MIQP based methods, whereas the branch and bound methods (Kariwala and Cao, 2009) would require further customization. Problem 3.3 is non-convex and cannot be solved by the methods presented in this paper and will be the topic of future work.

This paper is organized as follows: A self-contained summary of the minimum loss method formulation for SOC is presented in Section 3.2. The transformation of non-convex SOC problem to convex QP problem is discussed in Section 3.3 (Problem 3.1). The MIQP formulation for CV selection in SOC is presented in Section 3.4 (Problem 3.2). The evaluation of developed methods is performed on a toy problem, on an evaporator example, on a binary distillation column example with 41 stages and on a 4-product Kaibel column with 71 stages and are discussed in Section 3.5. A discussion on Problem 3.3 is presented in Section 3.6. The conclusions from this work are discussed in Section 3.7.

3.2 Minimum loss method

The key idea in the self-optimizing framework of Skogestad and co-workers (Skogestad and Postlethwaite, 1996) is to minimize the loss ($L = J - J_{\text{opt}}(\mathbf{d})$) from optimal operation when there are disturbances.

To find the minimum cost for a given disturbance $J_{\text{opt}}(\mathbf{d})$, we first find an expression for $\mathbf{u}_{\text{opt}}(\mathbf{d})$. We then evaluate the steady-state loss from this policy when $\mathbf{u}$ is adjusted in a feedback fashion such that $\mathbf{c} = \mathbf{H}\mathbf{y}$ is kept constant.

3.2.1 Problem formulation

Classification of variables

- $\mathbf{u} \in \mathbb{R}^{n_u}$ - unconstrained steady state degrees of freedom (inputs) for optimization (it does not actually matter what they are as long as they form an independent set).
- $\mathbf{d} \in \mathbb{R}^{n_d}$ - disturbances, including parameter changes.
- $\mathbf{y} \in \mathbb{R}^{n_y}$ - all available measurements. The manipulated variables (MVs, often the same as the inputs $\mathbf{u}$) are generally included in the

measurement set $\mathbf{y}$. This will allow, for example, for simple control policies where the inputs are kept constant. Of course, the set $\mathbf{y}$ can also include measured disturbances ($\mathbf{d}_m$, a subset of $\mathbf{d}$).

- $\mathbf{n}^y$ - measurement noise (error) for $\mathbf{y}$, $\mathbf{y_m} = \mathbf{y} + \mathbf{n}^y$.
- $\mathbf{c} \in \mathbb{R}^{n_c}$ where $n_c = n_u$ - selected controlled variables $\mathbf{c} = \mathbf{H}\mathbf{y}$.

Cost function

We consider an unconstrained optimization problem, where the objective is to adjust the input $\mathbf{u}$ to minimize a quadratic cost function for a steady-state process

$$J(\mathbf{u},\mathbf{d}) = J(\mathbf{u}^*,\mathbf{d}^*) + \begin{bmatrix}\mathbf{J}_u^* & \mathbf{J}_d^*\end{bmatrix}\begin{bmatrix}\Delta\mathbf{u}\\ \Delta\mathbf{d}\end{bmatrix} + \frac{1}{2}\begin{bmatrix}\Delta\mathbf{u}\\ \Delta\mathbf{d}\end{bmatrix}^T\begin{bmatrix}\mathbf{J}_{uu}^* & \mathbf{J}_{ud}^*\\ \mathbf{J}_{ud}^{*T} & \mathbf{J}_{dd}^*\end{bmatrix}\begin{bmatrix}\Delta\mathbf{u}\\ \Delta\mathbf{d}\end{bmatrix} \quad (3.2)$$

Here $\Delta\mathbf{u} = \mathbf{u} - \mathbf{u}^*$ and $\Delta\mathbf{d} = \mathbf{d} - \mathbf{d}^*$ represent deviations from the nominal optimal point $(\mathbf{u}^*, \mathbf{d}^*)$. $\mathbf{J}_u^*$ and $\mathbf{J}_d^*$ are first derivatives of J with respect to $\mathbf{u}$ and $\mathbf{d}$, $\mathbf{J}_{uu}^*$, $\mathbf{J}_{ud}^*$ and $\mathbf{J}_{dd}^*$ are second derivatives of J with respect to $\mathbf{u}$, $\mathbf{u}$ and $\mathbf{d}$, and $\mathbf{d}$, respectively at $(\mathbf{u}^*, \mathbf{d}^*)$. The nominal point is assumed to be optimal, which implies that $\mathbf{J}_u^* = 0$. To further simplify notation, we assume that the variables have been shifted so that the nominal optimal point is zero $(\mathbf{u}^*, \mathbf{d}^*) = (0, 0)$ and also $\mathbf{y}^* = 0$, then we have $\mathbf{u} = \Delta\mathbf{u}$, $\mathbf{d} = \Delta\mathbf{d}$ and $\mathbf{y} = \Delta\mathbf{y}$. From the derivation below, we find that the values of $\mathbf{J}_d^*$ and $\mathbf{J}_{dd}^*$ are not needed for finding the optimal $\mathbf{H}$, because they do not affect the optimal input $\mathbf{u}$.

A special case of (3.2) is indirect control, which is further studied for a distillation column in Example 4, where $\mathbf{y}_1$ are the primary variables. Here, the cost function is

$$J = (\mathbf{y}_1 - \mathbf{y}_{1s})^T\mathbf{W}_1^T\mathbf{W}_1(\mathbf{y} - \mathbf{y}_{1s}) \quad (3.3a)$$

where $\mathbf{W}_1$ is a weighting matrix, $\mathbf{y}_{1s}$ are set points for $\mathbf{y}_1$, and with a linear model for $\mathbf{y}_1$

$$\mathbf{y}_1 = \mathbf{G}_1^y\mathbf{u} + \mathbf{G}_{d_1}^y\mathbf{d} \quad (3.3b)$$

where $\mathbf{G}_1^y$ and $\mathbf{G}_{d_1}^y$ are steady state gains, further we get

$$\mathbf{J}_{uu} = \mathbf{G}_1^{yT}\mathbf{W}_1^T\mathbf{W}_1\mathbf{G}_1^y,\ \mathbf{J}_{ud} = \mathbf{G}_1^{yT}\mathbf{W}_1^T\mathbf{W}_1\mathbf{G}_{d_1}^y \quad (3.3c)$$

Measurement model

A linear steady-state model is assumed for the effect of $\mathbf{u}$ and $\mathbf{d}$ on the measurements $\mathbf{y}$

$$\mathbf{y} = \mathbf{G}^y\mathbf{u} + \mathbf{G}_d^y\mathbf{d} = \tilde{\mathbf{G}}^y \begin{bmatrix} \mathbf{u} \\ \mathbf{d} \end{bmatrix} \tag{3.4}$$

In Figure 3.1, $\mathbf{G}^y$ and $\mathbf{G}_d^y$ are transfer functions, but in this paper only steady-state gains in (3.4) are used for selecting $\mathbf{H}$.

Further assumptions

- Any active constraints are controlled and $\mathbf{u}$ spans the remaining unconstrained subspace.
- We want to find as many controlled variables $\mathbf{c}$ as there are degrees of freedom, that is, $n_c = \dim(\mathbf{c}) = \dim(\mathbf{u}) = n_u$. Then $\mathbf{HG}^y$ is a square $n_u \times n_u$ matrix.
- We need at least as many independent measurements $\mathbf{y}$ as there are degrees of freedom $\mathbf{u}$ ($\text{rank}(\mathbf{G}^y) = n_u$) to get offset free control of all CVs ($\mathbf{c}$). This requires $n_y \geq n_u = n_c$.
- We write $\mathbf{d} = \mathbf{W}_d\ \mathbf{d}'$ where $\mathbf{W}_d$ is a diagonal matrix giving the expected magnitude of each disturbance and $\mathbf{d}'$ is of unit magnitude (see below for further definition of "unit magnitude").
- Similarly, $\mathbf{n}^y = \mathbf{W}_{n^y}\ \mathbf{n}^{y'}$ where $\mathbf{W}_{n^y}$ is a diagonal matrix with the magnitude of the noise for each measurement, and the vector $\mathbf{n}^{y'}$ is of unit magnitude (see below).

Problem

For any disturbance $\mathbf{d}$, having inputs $\mathbf{u}$ other than $\mathbf{u}_{\text{opt}}(\mathbf{d})$ will result in a loss. For example, keeping the inputs $\mathbf{u}$ constant at $\mathbf{u}_{\text{opt}}(\mathbf{d}^*)$ when there is a disturbance $\mathbf{d}$ will result in a loss as illustrated in Figure 3.2. In this paper, we use a sub-optimal policy, which is to adjust inputs $\mathbf{u}$ in a feedback fashion (see Figures 3.1 and 3.3) to keep the measured controlled variables $\mathbf{c}_m$ at a constant set point $\mathbf{c}_s = 0$. Mathematically, we have

$$\mathbf{c}_m = \mathbf{H}\underbrace{(\mathbf{y} + \mathbf{n}^y)}_{\mathbf{y}_m} = \mathbf{c}_s = 0 \tag{3.5}$$

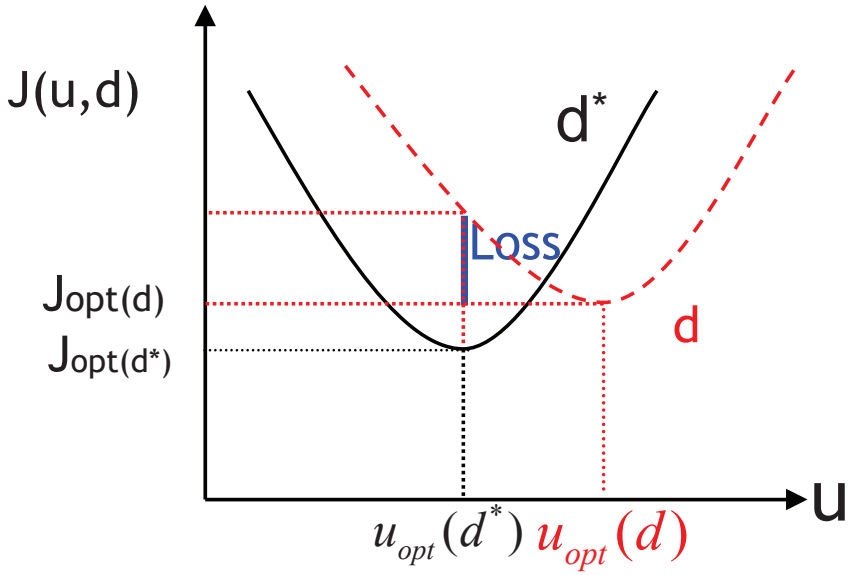

Figure 3.2: Cost function as a function of disturbances $\mathbf{d}^*$ and $\mathbf{d}$ and inputs $\mathbf{u}$; Illustration of loss by keeping input $\mathbf{u}$ constant at $\mathbf{u} = \mathbf{u}_{\text{opt}}(\mathbf{d}^*)$ when there is a disturbance $\mathbf{d}$

.

With this policy, there are two problems of interest. First, to find the "magnitude" of the loss, $L = J(\mathbf{u}, \mathbf{d}) - J_{\text{opt}}(\mathbf{d})$, for a given $\mathbf{H}$ (see solution in Section 3.2.2) and second to find the optimal $\mathbf{H}$ with a minimum loss (see Theorem 2 in Section 3.2.2) for the expected $\mathbf{d}'$ and $\mathbf{n}^{y'}$, when $\mathbf{u}$ is adjusted such that $\mathbf{c}_m = 0$ in (3.5) is satisfied.

The "magnitude" of the loss and the "unit magnitude" of the expected $\mathbf{d}'$ and $\mathbf{n}^{y'}$ still needs to be defined. Two possibilities are considered.

- Worst-case loss, L_{wc}, when the combined normalization vectors for disturbances and measurement noise have 2-norm less than 1,

$$\left\| \begin{bmatrix} \mathbf{d}' \\ \mathbf{n}^{y'} \end{bmatrix} \right\|_2 \leq 1 \tag{3.6}$$

- Average or expected loss, $L_{avg} = \mathcal{E}(L)$, for a normal distributed set

$$\begin{bmatrix} \mathbf{d}' \\ \mathbf{n}^{y'} \end{bmatrix} \in \mathcal{N}(0, 1) \tag{3.7}$$

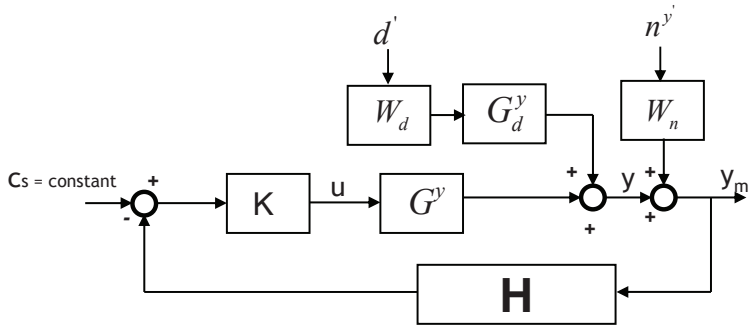

Figure 3.3: Feedback diagram

.

$\mathcal{E}(.)$ is expectation operator.

It is sometimes argued that the worst-case loss is not likely to occur, but this is not really true in this case since we use the combined 2-norm for disturbances and noise in (3.6). This means that the "unlikely" combination with all $\mathbf{d}'$s and $\mathbf{n}^{y'}$s being 1 at the same time will not occur. This is discussed in more detail in the Appendix of (Halvorsen et al., 2003).

3.2.2 Solution to minimum loss problem

The objective is to derive the solution to the above problem. This solution has previously been called the "exact local method" (Halvorsen et al., 2003).

Expression for $\mathbf{u}_{\text{opt}}(\mathbf{d})$

We first want to find the optimal input $\mathbf{u}$ for a given disturbance $\mathbf{d}$. Expanding the gradient $\mathbf{J}_u$ around the nominal optimal point $(\mathbf{u}^*, \mathbf{d}^*) = (0, 0)$ gives

$$\mathbf{J}_u(\mathbf{u}, \mathbf{d}) = \underbrace{\mathbf{J}_u^*(\mathbf{u}^*, \mathbf{d}^*)}_{=0} + \mathbf{J}_{uu}^*\mathbf{u} + \mathbf{J}_{ud}^*\mathbf{d} \tag{3.8}$$

where $\mathbf{J}_u^*(\mathbf{u}^*, \mathbf{d}^*) = 0$ because the nominal point is assumed to be optimal. We assume that we change the input to remain optimal, i.e. we have $\mathbf{u} = \mathbf{u}_{\text{opt}}(\mathbf{d})$ and $\mathbf{J}_u(\mathbf{u}, \mathbf{d}) = 0$, and we get

$$\mathbf{u}_{\text{opt}} = -\mathbf{J}_{uu}^{*^{-1}}\mathbf{J}_{ud}^*\mathbf{d} \tag{3.9}$$

Note that we are considering a quadratic problem (3.2), where the Hessian matrices are assumed constant, i.e. $\mathbf{J}_{uu} = \mathbf{J}^*_{uu}$ and $\mathbf{J}_{ud} = \mathbf{J}^*_{ud}$.

Expression for the loss L in terms of $\mathbf{u} - \mathbf{u}_{\text{opt}}(\mathbf{d})$

Consider a given disturbance $\mathbf{d}$ and a non-optimal input $\mathbf{u}$. A second order Taylor's expansion of the cost J around the "moving" optimum point, $\mathbf{u}_{\text{opt}}(\mathbf{d})$, gives

$$\begin{aligned} J(\mathbf{u},\mathbf{d}) = \underbrace{J(\mathbf{u}_{\text{opt}}(\mathbf{d}),\mathbf{d})}_{J_{\text{opt}}(\mathbf{d})} + \underbrace{\mathbf{J}_{u,opt}}_{=0}(\mathbf{u} - \mathbf{u}_{\text{opt}}(\mathbf{d})) \\ + \frac{1}{2}(\mathbf{u} - \mathbf{u}_{\text{opt}}(\mathbf{d}))^T \mathbf{J}_{uu,opt}(\mathbf{u} - \mathbf{u}_{\text{opt}}(\mathbf{d})) \end{aligned} \tag{3.10}$$

Note that for a truly quadratic problem, this is an exact expression and $\mathbf{J}_{uu,opt} = \mathbf{J}^*_{uu} = \mathbf{J}_{uu}$. Because we are expanding around an optimal point $J_{u,opt} = 0$ and we get the following expression for the loss

$$L(\mathbf{u},\mathbf{d}) = J(\mathbf{u},\mathbf{d}) - J_{\text{opt}}(\mathbf{d}) = \frac{1}{2}\mathbf{z}^T\mathbf{z} = \frac{1}{2}\|\mathbf{z}\|_2^2 \tag{3.11}$$

where we have introduced

$$\mathbf{z} \triangleq \mathbf{J}_{uu}^{1/2}(\mathbf{u} - \mathbf{u}_{\text{opt}}(\mathbf{d})) \tag{3.12}$$

This simple expression for the loss is a key result that allows us to end up with a convex optimization problem.

Optimal sensitivities

Note from (3.9) that we can write $\mathbf{u}_{\text{opt}} = \mathbf{F}^u\mathbf{d}$ where $\mathbf{F}^u = -\mathbf{J}_{uu}^{-1}\mathbf{J}_{ud}$. More generally, we can write

$$\mathbf{y}_{\text{opt}} = \mathbf{F}\mathbf{d} \tag{3.13}$$

where $\mathbf{F}$ is the optimal sensitivity of the outputs (measurements) with respect to the disturbances. Here, $\mathbf{F}$ can be obtained using (3.4) and (3.9),

$$\mathbf{y}_{\text{opt}} = \mathbf{G}^y\mathbf{u}_{\text{opt}} + \mathbf{G}^y_d\mathbf{d} = (-\mathbf{G}^y\mathbf{J}_{uu}^{-1}\mathbf{J}_{ud} + \mathbf{G}^y_d)\mathbf{d}$$

that is,

$$\mathbf{F} = (-\mathbf{G}^y\mathbf{J}_{uu}^{-1}\mathbf{J}_{ud} + \mathbf{G}^y_d) \tag{3.14}$$

However, (3.14) is not generally a robust way to obtain $\mathbf{F}$, for example $\mathbf{J}_{uu}, \mathbf{J}_{ud}$ can be difficult to obtain numerically, and taking the difference in (3.14) can also be unreliable numerically. Thus, for practical use it is usually better to obtain $\mathbf{F}$ directly from its definition, $\mathbf{F} = \frac{d\mathbf{y}_{\text{opt}}}{d\mathbf{d}}$. This typically involves numerical reoptimization for each disturbance.

The loss L as a function of disturbances and noise

We present the derivation of the main result (Halvorsen et al., 2003). We start from the loss expression in (3.11), $L = \frac{1}{2}\|\mathbf{z}\|_2^2$ where $\mathbf{z} = \mathbf{J}_{uu}^{1/2}(\mathbf{u}-\mathbf{u}_{\text{opt}})$. We want to write $\mathbf{z}$ as a function of $\mathbf{d}$ and $\mathbf{n}^y$, given that the input $\mathbf{u}$ should be adjusted to satisfy (3.5). We start by writing $\mathbf{u} - \mathbf{u}_{\text{opt}}$ as a function of $\mathbf{c} - \mathbf{c}_{\text{opt}}$. We have $\mathbf{c} = \mathbf{H}\mathbf{y}$, so

$$\begin{aligned}\mathbf{c} &= \mathbf{H}\mathbf{y} = \mathbf{H}\mathbf{G}^y\mathbf{u} + \mathbf{H}\mathbf{G}_d^y\mathbf{d}\\ \mathbf{c}_{\text{opt}} &= \mathbf{H}\mathbf{y}_{\text{opt}} = \mathbf{H}\mathbf{G}^y\mathbf{u}_{\text{opt}} + \mathbf{H}\mathbf{G}_d^y\mathbf{d}\end{aligned}$$

Thus, $\mathbf{c} - \mathbf{c}_{\text{opt}} = \mathbf{H}\mathbf{G}^y(\mathbf{u} - \mathbf{u}_{\text{opt}})$, or

$$(\mathbf{u} - \mathbf{u}_{\text{opt}}) = (\mathbf{H}\mathbf{G}^y)^{-1}(\mathbf{c} - \mathbf{c}_{\text{opt}}) \tag{3.15a}$$

where $\mathbf{H}\mathbf{G}^y$ is the square gain matrix from the inputs $\mathbf{u}$ to the selected controlled variables $\mathbf{c}$.

The next step is to express $(\mathbf{c} - \mathbf{c}_{\text{opt}})$ as a function of $\mathbf{d}$ and $\mathbf{n}^y$. From (3.13) we have that

$$\mathbf{c}_{\text{opt}} = \mathbf{H}\mathbf{F}\mathbf{d} \tag{3.15b}$$

From (3.5) we have that $\mathbf{H}(\mathbf{y} + \mathbf{n}^y) = \mathbf{c}_s$ (constant), or

$$\mathbf{c} = \mathbf{H}\mathbf{y} = -\mathbf{H}\mathbf{n}^y + \mathbf{c}_s \tag{3.15c}$$

Here, $\mathbf{c}_s = 0$, since we assume the nominal point is optimal. Since the signs for $\mathbf{n}^y$ and $\mathbf{d}$ do not matter for the expressions we derive below (from (3.6) we can have both positive and negative changes), we can write

$$\begin{aligned}\mathbf{u} - \mathbf{u}_{\text{opt}} &= (\mathbf{H}\mathbf{G}^y)^{-1}\mathbf{H}(\mathbf{F}\mathbf{d} + \mathbf{n}^y)\\ &= (\mathbf{H}\mathbf{G}^y)^{-1}\mathbf{H}(\mathbf{F}\mathbf{W}_d\mathbf{d}' + \mathbf{W}_{n^y}\mathbf{n}^{y'})\\ &= (\mathbf{H}\mathbf{G}^y)^{-1}\mathbf{H}\mathbf{Y}\begin{bmatrix}\mathbf{d}'\\ \mathbf{n}^{y'}\end{bmatrix}\end{aligned} \tag{3.15d}$$

where we have introduced

$$\mathbf{Y} = [\mathbf{F}\mathbf{W}_d \quad \mathbf{W}_{n^y}] \tag{3.16}$$

Note that $\mathbf{W}_d$ and $\mathbf{W}_{n^y}$ are usually diagonal matrices, representing the magnitude of the disturbances and measurement noises, respectively.

In summary, we have derived that for the given normalized disturbances $\mathbf{d}'$ and for the given normalized measurement noises $\mathbf{n}^{y'}$ the loss is given by (Halvorsen et al., 2003)

$$L = \frac{1}{2}\mathbf{z}^T\mathbf{z} \tag{3.17}$$

where

$$\mathbf{z} = \mathbf{J}_{uu}^{1/2}(\mathbf{u} - \mathbf{u}_{\text{opt}}) = \underbrace{\mathbf{J}_{uu}^{1/2}(\mathbf{H}\mathbf{G}^y)^{-1}\mathbf{H}\mathbf{Y}}_{\mathbf{M}(\mathbf{H})} \begin{bmatrix} \mathbf{d}' \\ \mathbf{n}^{y'} \end{bmatrix} \tag{3.18}$$

Worst-case and average loss for a given H (analysis using loss method)

The above expressions give the loss for a given $\mathbf{d}'$ and $\mathbf{n}^{y'}$, but the goal is to find the "magnitude" of the loss L for the expected set for example as given in (3.6). Here "magnitude" can be defined in different ways, see (3.6) and (3.7), and for a given $\mathbf{H}$ the worst-case loss (Halvorsen et al., 2003) and average expected loss (Kariwala et al., 2008) are given by

$$L_{wc}(\mathbf{H}) = \frac{1}{2}\bar{\sigma}(\mathbf{M})^2 \tag{3.19}$$

$$L_{avg}(\mathbf{H}) = \mathcal{E}(L) = \frac{1}{2}\|\mathbf{M}\|_F^2 \tag{3.20}$$

where

$$\mathbf{M}(\mathbf{H}) = \mathbf{J}_{uu}^{1/2}(\mathbf{H}\mathbf{G}^y)^{-1}\mathbf{H}\mathbf{Y} \tag{3.21}$$

Here $\bar{\sigma}(\mathbf{M})$ denotes the maximum singular value (induced 2-norm) of the matrix $\mathbf{M}(\mathbf{H})$, and $\|\mathbf{M}\|_F = \sqrt{\sum_{i,j}\mathbf{M}_{ij}^2}$ denotes the Frobenius norm of the matrix $\mathbf{M}$. Use of the norm of $\mathbf{M}$ to analyze the loss is known as the "exact local method" (Halvorsen et al., 2003). Note that these loss expressions are for a given matrix $\mathbf{H}$.

Comment : A uniform distribution for $\mathbf{d}'$ and $\mathbf{n}^{y'}$ is sometimes assumed, resulting in an average loss $\frac{1}{6(n_y+n_d)}\|\mathbf{M}\|_F^2$ (Kariwala et al., 2008). However, as discussed in the Section 3.6.2, this is not meaningful from an engineering point of view.

Null space method and maximum gain rule

Two special methods for analyzing or finding $\mathbf{H}$ can be derived from the expression for $\mathbf{H}$ in (3.21). First, the null space method of selecting $\mathbf{H}$ such that $\mathbf{H}\mathbf{F} = 0$ (Alstad and Skogestad, 2007) follows if we neglect measurement noise such that $\mathbf{Y} = [\mathbf{F}\mathbf{W}_d \quad \underline{\underline{0}}]$, where $\underline{\underline{0}}$ is zero matrix of $n_y \times n_y$ size, and assume that we have enough measurements to make $\mathbf{H}\mathbf{F} = 0$. Second, the approximate maximum gain rule (Skogestad and Postlethwaite, 1996) of maximizing the norm of $\mathbf{S}_1\mathbf{H}\mathbf{G}^y\mathbf{S}_2$ follows from (3.21) if we select the scaling factors as $\mathbf{S}_2 = \mathbf{J}_{uu}^{-1/2}$ and the appropriate $\mathbf{S}_1$ as a diagonal matrix

with the elements of $\mathbf{S}_1^{-1}$ equal to the expected optimal variation in each $\mathbf{c}$ variable (the norm of the corresponding rows in $\mathbf{HY}$).

Loss method for finding optimal H

The objective of this paper is to find methods for obtaining the optimal $\mathbf{H}$ by minimizing either the worst-case loss (3.19) or the average loss (3.20). Fortunately, (Kariwala et al., 2008) proves that the $\mathbf{H}$ that minimizes the average loss in equation (3.20) is super optimal, in the sense that the same $\mathbf{H}$ minimizes the worst-case loss in (3.19). Hence, only minimization of the Frobenius norm in (3.20) is considered in the rest of the paper. Note that square does not effect the optimal solution and can be omitted. In summary, the problem is to find the combination matrix $\mathbf{H}$ that minimizes $\|\mathbf{M}\|_F$:

Theorem 2 Minimum loss method (Alstad et al., 2009). *To minimize the average and worst-case loss, $L_{avg}(\mathbf{H})$ and $L_{wc}(\mathbf{H})$, for expected combined disturbances and noise, find the $\mathbf{H}$ that solves the problem*

$$\min_{\mathbf{H}} \left\| \mathbf{J}_{uu}^{1/2} (\mathbf{H}\mathbf{G}^y)^{-1} \mathbf{H}\mathbf{Y} \right\|_F \tag{3.22}$$

where $\mathbf{Y} = [\mathbf{F}\mathbf{W}_d \quad \mathbf{W}_{n^y}]$.

The objective in (3.22) is to find the non-square $n_c \times n_y$ matrix $\mathbf{H}$.

Here, $\mathbf{H}$ may have a specified structure and we consider the three problems mentioned in the introduction. For the full $\mathbf{H}$ case (Problem 3.1), it may be recast as a convex optimization problem as discussed in Section 3.3. For the measurement selection problem (Problem 3.2), where some columns in $\mathbf{H}$ are zero, convex formulations in each MIQP node are derived in Section 3.4 .

3.3 Convex formulations of minimum loss method (Problem 3.1)

We here consider the standard "full" $\mathbf{H}$ case with no restriction on the structure of the matrix $\mathbf{H}$ (Problem 3.1), that is we want to find optimal combination of all the measurements.

Theorem 3 Convex reformulation for full H case (Alstad et al., 2009). *The problem in equation* (3.22) *may seem non-convex, but for the*

standard case where $\mathbf{H}$ *is a "full" matrix (with no structural constraints), it can be reformulated as a convex constrained quadratic programming problem*

$$\begin{aligned} &\min_{\mathbf{H}} \|\mathbf{HY}\|_F \\ &\text{s.t. } \mathbf{HG}^y = \mathbf{J}_{uu}^{1/2} \end{aligned} \tag{3.23}$$

Proof. From the original problem in equation (3.22), we have that the optimal solution $\mathbf{H}$ is non-unique because if $\mathbf{H}$ is a solution then $\mathbf{H}_1 = \mathbf{DH}$ is also a solution for any non-singular matrix $\mathbf{D}$ of size $n_c \times n_c$. This follows because

$$\mathbf{J}_{uu}^{1/2}(\mathbf{HG}^y)^{-1}\mathbf{HY} = \mathbf{J}_{uu}^{1/2}(\mathbf{HG}^y)^{-1}\mathbf{D}^{-1}\mathbf{DHY} = \mathbf{J}_{uu}^{1/2}(\mathbf{H}_1\mathbf{G}^y)^{-1}\mathbf{H}_1\mathbf{Y}$$

One implication is that we can freely choose $\mathbf{G} = \mathbf{HG}^y$, which is a $n_c \times n_c$ matrix representing the effect of $\mathbf{u}$ on $\mathbf{c}$ ($\mathbf{c} = \mathbf{Gu}$). Thus, in (3.22) we may use the non-uniqueness of $\mathbf{H}$ to set the first part of the expression equal to the identity matrix, which is equivalent to setting $\mathbf{HG}^y = \mathbf{J}_{uu}^{1/2}$. This must be added as a constraint in the optimization as shown in (3.23). □

Theorem 4 Analytical solution *(Alstad et al., 2009)*
For a "full" $\mathbf{H}$ *in* (3.22) *and* (3.23)*, an analytical solution is*

$$\mathbf{H}^T = \left(\mathbf{YY}^T\right)^{-1}\mathbf{G}^y\left(\mathbf{G}^{y^T}\left(\mathbf{YY}^T\right)^{-1}\mathbf{G}^y\right)^{-1}\mathbf{J}_{uu}^{1/2} \tag{3.24}$$

Comment: We also require that $\mathbf{YY}^T$ is full rank, which is always satisfied if we have nonzero measurement noise.

Theorem 5 Simplified analytical solution (new result)
For a full $\mathbf{H}$*, another analytical solution to* (3.22) *is*

$$\mathbf{H}^T = \left(\mathbf{YY}^T\right)^{-1}\mathbf{G}^y\mathbf{Q}_1 \tag{3.25}$$

where $\mathbf{Q}_1$ is any non-singular matrix of $n_c \times n_c$, for example $\mathbf{Q}_1 = \mathbf{I}$.

Proof. This follows trivially from Theorems 3 and 4, since if $\mathbf{H}^T$ is a solution then so is $\mathbf{H}_1^T = \mathbf{H}^T\mathbf{D}^T$ and we simply select

$$\mathbf{D}^T = \mathbf{J}_{uu}^{-1/2}(\mathbf{G}^{y^T}(\mathbf{YY}^T)^{-1}\mathbf{G}^y)\mathbf{Q}_1$$

which is a $n_c \times n_c$ matrix. □

Corollary 1 Important insight (new result) *Theorem 5 gives the very important insight that* $\mathbf{J}_{uu}$ *is not needed for finding the optimal full* $\mathbf{H}$ *in* (3.22) *and* (3.23)*.*

This means that in (3.22) we can replace $\mathbf{J}_{uu}^{1/2}$ by any non-singular matrix $\mathbf{Q}$, and still get an optimal $\mathbf{H}$. This can simplify practical calculations, because $\mathbf{J}_{uu}$ may be difficult to obtain numerically because it involves the second derivative and because $\mathbf{Q}$ may be in some cases be selected for numerical reasons. On the other hand, we have that $\mathbf{F}$, which enters in $\mathbf{Y}$, is relatively straightforward to obtain numerically (de Araújo et al., 2007; Panahi and Skogestad, 2011), because it only needs first derivative, $\mathbf{F} = \frac{d\mathbf{y}_{\text{opt}}}{d\mathbf{d}}$, as mentioned earlier. Although $\mathbf{J}_{uu}$ is not needed for finding the optimal $\mathbf{H}$, it would be required for finding a numerical value for the loss, and it is needed if $\mathbf{H}$ is structured (Problems 3.2 and 3.3) as discussed below.

Vectorized QP formulation: As the numerical software packages, such as Matlab, cannot deal with the matrix formulations, the problem (3.23) is vectorized (see Appendix A). First, the decision matrix

$$\mathbf{H} = \begin{bmatrix} h_{11} & h_{12} & \dots & h_{1n_y} \\ h_{21} & h_{22} & \dots & h_{2n_y} \\ \vdots & \vdots & \ddots & \vdots \\ h_{n_u1} & h_{n_u2} & \dots & h_{n_un_y} \end{bmatrix}$$

is vectorized along the rows of $\mathbf{H}$ to form a long vector

$$\mathbf{h}_\delta = \begin{bmatrix} h_{11} & \dots & h_{1n_y} & h_{21} & \dots & h_{2n_y} & \dots & h_{n_u1} & \dots & h_{n_un_y} \end{bmatrix}^T \in \mathbb{R}^{n_un_y \times 1}$$

The equivalent QP is then formulated as

$$\begin{aligned} &\min_{\mathbf{h}_\delta} \ \mathbf{h}_\delta^T \mathbf{F}_\delta \mathbf{h}_\delta \\ &\text{s.t. } \mathbf{G}_\delta^{y^T} \mathbf{h}_\delta = \mathbf{j}_\delta \end{aligned} \tag{3.26}$$

where $\mathbf{h}_\delta \in \mathbb{R}^{n_un_y \times 1}, \mathbf{j}_\delta \in \mathbb{R}^{n_un_u \times 1}, \mathbf{G}_\delta^{y^T} \in \mathbb{R}^{n_un_u \times n_yn_u}, \mathbf{F}_\delta \in \mathbb{R}^{n_un_y \times n_un_y}$.

3.4 Globally optimal MIQP formulations (Problem 3.2)

We here consider the optimal measurement selection of finding the optimal $\mathbf{H}$ with some zero columns (Problem 3.2). To address the measurement selection, we introduce a binary variable $\sigma_j \in \{0, 1\}$ to complement j^{th} measurement (j^{th} column in $\mathbf{H}$). If measurement j is present in the selected measurements, then $\sigma_j = 1$ and j^{th} column in $\mathbf{H}$ may have non-zero elements, otherwise $\sigma_j = 0$ and j^{th} column in $\mathbf{H}$ has only zero elements. The binary variables column vector for n_y candidate measurements is denoted

as $\boldsymbol{\sigma}_\delta = \begin{bmatrix}\sigma_1 & \sigma_2 & \dots & \sigma_{n_y}\end{bmatrix}^T$. The restrictions on elements in $\mathbf{H}$ based on the the presence or not of the j^{th} candidate measurement are incorporated as mixed integer constraints. Overall, the idea in optimal measurement selection is to use the quadratic programming formulation in Theorem 3, and add additional mixed integer constraints to deal with the measurement selection.

3.4.1 Optimal measurement selection

The mixed integer constraints on the columns in $\mathbf{H}$ are formulated using the standard big-m approach used in MIQP formulations (3.27c) (Hooker and Osorio, 1999) and are added to (3.26). The constraints on the binary variables can be written in the form

$$\mathbf{P}\boldsymbol{\sigma}_\delta = \mathbf{s}$$

For example, in order to select n optimal measurements out of n_y measurements, we have $\sum_j^{n_y} \sigma_j = n$, which can be written in this form with $\mathbf{P} = \underline{1}^T{}_{1\times n_y}$, and $\mathbf{s} = n$, where $\underline{1}$ is a column vector of ones.

Starting from the vectorized formulation in (3.26), we then have the important result that the generalized MIQP problem in the decision variables $\mathbf{h}_\delta$ and $\boldsymbol{\sigma}_\delta$ with big-m constraints becomes

$$\begin{aligned} \min_{\mathbf{h}_\delta, \boldsymbol{\sigma}_\delta} \quad & \mathbf{h}_\delta^T \mathbf{F}_\delta \mathbf{h}_\delta \\ \text{s.t.} \quad & \mathbf{G}_\delta^{\mathrm{y}^{\mathrm{T}}} \mathbf{h}_\delta = \mathbf{j}_\delta \end{aligned} \tag{3.27a}$$

$$\mathbf{P}\boldsymbol{\sigma}_\delta = \mathbf{s} \tag{3.27b}$$

$$\begin{bmatrix} -m \\ -m \\ \vdots \\ -m \end{bmatrix} \sigma_j \le \begin{bmatrix} h_{1j} \\ h_{2j} \\ \vdots \\ h_{n_u j} \end{bmatrix} \le \begin{bmatrix} m \\ m \\ \vdots \\ m \end{bmatrix} \sigma_j, \quad \forall j \in 1, 2, \cdots, n_y \tag{3.27c}$$

where $\mathbf{h}_\delta = \begin{bmatrix} h_{11} & \dots & h_{1n_y} & h_{21} & \dots & h_{2n_y} & \dots h_{n_u 1} & \dots & h_{n_u n_y} \end{bmatrix}^T \in \mathbb{R}^{n_u n_y \times 1}$; $\boldsymbol{\sigma}_\delta = \begin{bmatrix}\sigma_1 & \sigma_2 & \dots & \sigma_{n_y}\end{bmatrix}^T$; $\sigma_j \in \{0, 1\}$. The dimension of matrix $\mathbf{P}$ varies based on the integer constraints we impose, if we impose k number of integer constraints then $\mathbf{P}$ will have a dimension of $k \times n_y$. The constraints in (3.27c) is the standard big-m approach that we used to make the j^{th} column of $\mathbf{H}$ zero when $\sigma_j = 0$ and at the same time to bound the decision variables in $\mathbf{H}$. The m value should be chosen small to reduce the computational time, but it should be sufficiently large to avoid that it becomes

an active constraint. Selecting an appropriate m is problem dependent and appropriate selection of m can become an iterative method and can increase the computational intensiveness of the big-m based MIQP formulations. In such cases, one can use indicator constraints in MIQP problem to set the columns in $\mathbf{H}$ directly to zero, when $\sigma_j = 0$. This can be done by replacing the constraints in (3.27c) with indicator constraints as

$$\text{indicator constraints} : \sigma_j = 0 \implies \begin{bmatrix} h_{1j} \\ h_{2j} \\ \vdots \\ h_{n_u j} \end{bmatrix} = \underline{0}_{n_u \times 1} \quad \forall j \in 1, 2, \cdots, n_y \tag{3.28}$$

where $\underline{0}$ is a column vector of zeros. For MIQP, theoretically, indicator constraint approach (3.28) would be faster than using big-m approach (3.27c). This is because in MIQP, indicator constraint approach (3.28) solves an equality constrained QP at each node, whereas big-m approach (3.27c) solves an inequality constrained QP.

For the solution of the MIQP problem with (3.27c) or (3.28), Theorem 3 applies. This statement is proven as follows : At each node in the MIQP search tree, we could use Theorem 3. This will preserve the loss ordering between different nodes in the MIQP search tree, because in Theorem 3, meeting the constraint $\mathbf{HG}^y = \mathbf{J}_{uu}^{1/2}$ implies $\mathbf{J}_{uu}^{1/2}(\mathbf{HG}^y)^{-1} = \mathbf{I}$ and the loss value in (3.22) is equal to $\|\mathbf{HY}\|_F$.

3.4.2 Specific cases

We consider five specific cases of Problem 3.2 and show how they can be solved using the MIQP formulation in (3.27). The integer constraint in (3.27b) is modified for each case. Note that Cases 2.1,2.2 and 2.3 can alternatively be solved using the branch and bound approaches (Kariwala and Cao, 2010). However, Cases 3.2.4 and 3.2.5 can only be solved using our MIQP formulation.

Case 3.2.1 Given subset of measurements. For example, assume we have two inputs and 5 measurements of which we will not use measurements 1 and 3, then $\mathbf{H} = \begin{bmatrix} 0 & h_{12} & 0 & h_{14} & h_{15} \\ 0 & h_{22} & 0 & h_{24} & h_{25} \end{bmatrix}$. The resulting

constraints can be written in the form in (3.27b) with

$$\mathbf{P} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \ \mathbf{s} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

This is a very simple case, and we may use Theorem 3, which implies that $\mathbf{J}_{uu}$ is *not* needed. The fact that Theorem 3 hold is quite obvious since it corresponds to simply deleting some measurements (deleting rows in $\mathbf{G}^y$ and $\mathbf{Y}$), and keeping $\mathbf{H}$ full for the remaining measurements.

Case 3.2.2 Optimal subset of measurements. Here the objective is to select a certain number (n) of measurements (i.e. $n_y - n$ columns in $\mathbf{H}$ are zero). The constraint in the binary variables is

$$\sum_{j=1}^{n_y} \sigma_j = n \tag{3.29}$$

which can be written in the form in (3.27b) with

$$\mathbf{P} = \underline{1}^T{}_{1\times n_y}, \mathbf{s} = n$$

where $\underline{1}$ is a column vector of ones.

Case 3.2.3 Best individual measurements for decentralized control. This is the case where we want to select $n = n_c$ measurements, which is the minimum feasible number of measurements, if we want offset free control of $\mathbf{c} = \mathbf{H}\mathbf{y}$. For example, one candidate $\mathbf{H}$ is

$$\mathbf{H} = \begin{bmatrix} h_{11} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & h_{24} & 0 \end{bmatrix} \tag{3.30}$$

The constraints to be used in (3.27b) are $\sum_{j=1}^{n_y} \sigma_j = n_u = n_c$ and in addition the off diagonal elements for the selected n_c measurements should be zero (for this candidate $\mathbf{H}$ the selected measurements are 1, 4 and the off-diagonal elements h_{21} and h_{14} are zero).

Fortunately, Theorem 3 which requires $\mathbf{H}$ to be a full matrix may be used at each node in the MIQP, because the last restriction (off-diagonal elements are zero) may be omitted. The reason is that we can first find the optimal measurement subset for this selected n_c measurements, for example, $\mathbf{H} = \begin{bmatrix} h_{11} & 0 & 0 & h_{14} & 0 \\ h_{21} & 0 & 0 & h_{24} & 0 \end{bmatrix}$, and we can

then use the extra degrees of freedom $\mathbf{D}$ to make the off diagonal elements in $\mathbf{H}$ zero.

To prove this, let $\mathbf{H}_{nc}$ be the optimal solution for the best n_c measurements combination matrix, for example, $\mathbf{H}_{nc} = \begin{bmatrix} h_{11} & h_{14} \\ h_{21} & h_{24} \end{bmatrix}$. The objective function is unaffected by $\mathbf{D}$, so as in the proof of Theorem 3 we choose $\mathbf{D} = \mathbf{H}_{nc}^{-1}$, to arrive at a diagonal $\mathbf{H}$ as in (3.30).

Case 3.2.4 Restriction on measurements from different process sections. For example, consider a process with n_s sections with n_{y_k} measurements in section k (i.e. the total number of available measurements is $n_y = \sum_{k=1}^{n_s} n_{y_k}$). If we want to select r_k measurements from each section k, the constraints (3.27b) become

$$\sum_{j=1}^{n_{y_k}} \sigma_{(\sum_{p=1}^{k-1} n_{yp}+j)} = r_k, \quad \forall k \in 1, 2, \ldots, n_s \tag{3.31}$$

and Theorem 3 applies for the MIQP formulation.

Case 3.2.5 Adding extra measurements to a given set of measurements. This case may be very important in practice. For example, consider a process with $n_y = 5$ measurements, where we have decided to use the measurements $\{2, 3\}$, and in addition want 2 other measurements (total 4 measurements). These constraints can be written

$$\begin{aligned} \sigma_j &= 1, \quad \forall j = 2, 3 \\ \sum_{j=1}^{n_y} \sigma_j &= 4 \end{aligned} \tag{3.32}$$

which can be written in the form (3.27b) with

$$\mathbf{P} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix}, \ \mathbf{s} = \begin{bmatrix} 1 \\ 1 \\ 4 \end{bmatrix}$$

and Theorem 3 applies at each MIQP node.

All of the above five cases belong to the optimal measurement selection (Problem 3.2) and can be easily solved using MIQP formulations. This is discussed in more details for the examples below. Note that the Cases 3.2.4 and 3.2.5 cannot be dealt by BAB methods (Kariwala and Cao, 2010), at least not without changing the algorithms.

3.5 Examples (Problem 3.2)

3.5.1 Example 1: measurement selection for toy problem (Case 3.2.2)

To illustrate the problem formulation for (3.27) for Case 3.2.2, consider a "toy problem" from Halvorsen et al. (2003) which has two inputs $\mathbf{u} = [u_1 \quad u_2]^T$, one disturbance d and two measured outputs $\mathbf{z} = [z_1 \quad z_2]^T$. The cost function is

$$J = (z_1 - z_2)^2 + (z_1 - d)^2$$

where the outputs depend linearly on $\mathbf{u}$, d as

$$\mathbf{z} = \mathbf{G}^z \mathbf{u} + \mathbf{G}_d^z d$$

with $\mathbf{G}^z = \begin{bmatrix} 11 & 10 \\ 10 & 9 \end{bmatrix}$; $\mathbf{G}_d^z = \begin{bmatrix} 10 \\ 9 \end{bmatrix}$. The disturbances are of magnitude 1 and the measurements noise is at magnitude 0.01.

At the optimal point we have $z_1 = z_2 = d$ and $J_{\text{opt}}(d) = 0$. Both the inputs and outputs are included in the candidate set of measurements

$$\mathbf{y} = \begin{bmatrix} z_1 \\ z_2 \\ u_1 \\ u_2 \end{bmatrix}$$

and we have $n_y = 4, n_u = 2$. This gives

$$\mathbf{G}^y = \begin{bmatrix} 11 & 10 \\ 10 & 9 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}, \ \mathbf{G}_d^y = \begin{bmatrix} 10 \\ 9 \\ 0 \\ 0 \end{bmatrix}$$

Furthermore,

$$\mathbf{J}_{uu} = \begin{bmatrix} 244 & 222 \\ 222 & 202 \end{bmatrix}, \ \mathbf{J}_{ud} = \begin{bmatrix} 198 \\ 180 \end{bmatrix}$$

$$\mathbf{W}_d = 1, \ \mathbf{W}_{n^y} = 0.01 \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

and $\mathbf{J}_{uu}^{1/2} = \begin{bmatrix} 11.59 & 10.46 \\ 10.46 & 9.62 \end{bmatrix}$. The resulting sensitivity matrix is

$$\mathbf{Y} = [\mathbf{F}\mathbf{W}_d \quad \mathbf{W}_{n^y}] = \begin{bmatrix} -1 & 0.01 & 0 & 0 & 0 \\ -1 & 0 & 0.01 & 0 & 0 \\ 9 & 0 & 0 & 0.01 & 0 \\ -9 & 0 & 0 & 0 & 0.01 \end{bmatrix}$$

After vectorization (see Appendix A) we generate the matrices in (3.26). The resulting matrices to be used in MIQP problem (3.27) are

$$\mathbf{F}_\delta = \begin{bmatrix} 2 & 2 & -18 & 18 & 0 & 0 & 0 & 0 \\ 2 & 2 & -18 & 18 & 0 & 0 & 0 & 0 \\ -18 & -18 & 162 & -162 & 0 & 0 & 0 & 0 \\ 18 & 18 & -162 & 162 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 2 & -18 & 18 \\ 0 & 0 & 0 & 0 & 2 & 2 & -18 & 18 \\ 0 & 0 & 0 & 0 & -18 & -18 & 162 & -162 \\ 0 & 0 & 0 & 0 & 18 & 18 & -162 & 162 \end{bmatrix} \in \mathbb{R}^{8\times 8}$$

$$\mathbf{G}_\delta^{y^T} = \begin{bmatrix} 11 & 10 & 1 & 0 & 0 & 0 & 0 & 0 \\ 10 & 9 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 11 & 10 & 1 & 0 \\ 0 & 0 & 0 & 0 & 10 & 9 & 0 & 1 \end{bmatrix} \in \mathbb{R}^{4\times 8}, \quad \mathbf{j}_\delta = \begin{bmatrix} 11.59 \\ 10.46 \\ 10.46 \\ 9.62 \end{bmatrix} \in \mathbb{R}^{4\times 1}.$$

To obtain the optimal $n < 4$ measurement subset the constraint (3.27b) is

$$\sum_{j=1}^{n_y} \sigma_j = n$$

We used $m = 120$ for the big-m in (3.27) and with $n = 3$ we find by solving MIQP problem that the optimal solution is $\mathbf{H} = \begin{bmatrix} 1.02 & 0 & 0.40 & 0.28 \\ 0.76 & 0 & 2.06 & 1.98 \end{bmatrix}$, that is measurement 2 is not used. We can always choose the degrees of freedom in the matrix $\mathbf{D}$, for example, to have identity in measurements 1 and 3 to get, for example, $\mathbf{H} = \begin{bmatrix} 1 & 0 & 0 & -0.11 \\ 0 & 0 & 1 & 1 \end{bmatrix}$. The minimized loss (3.20) as a function of the number of measurements n is shown in Figure 3.4. As expected, the loss is reduced as we use more measurements, but the reduction in loss is very small when we increase the number of measurements from 3 to 4. Based on Figure 3.4, we conclude that using CVs as a combination of a 3 measurement subset is the best for this toy problem.

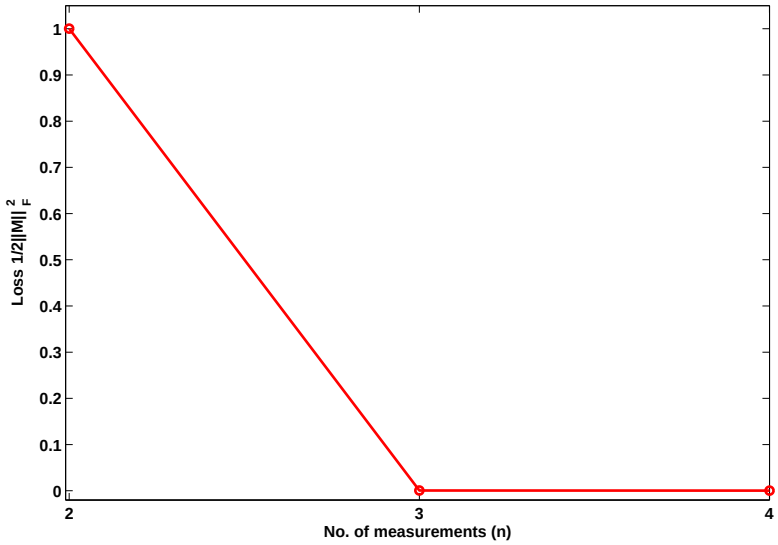

Figure 3.4: The loss vs the number of included measurements (n) for "toy problem"

.

3.5.2 Example 2: measurement selection for evaporator process (Case 3.2.2)

The main purpose of this example is to evaluate the MIQP method (3.27) for Case 3.2.2 on a simple but realistic process. We consider the evaporator example of Newell and Lee (1989) (Figure 3.5) as modified by Kariwala et al. (2008). The process has 2 steady-state degrees of freedom (inputs), 10 candidate measurements and 3 disturbances.

$$\mathbf{u} = [F_{200} \quad F_1]^T$$
$$\mathbf{y} = [P_2 \quad T_2 \quad T_3 \quad F_2 \quad F_{100} \quad T_{201} \quad F_3 \quad F_5 \quad F_{200} \quad F_1]^T$$
$$\mathbf{d} = [X_1 \quad T_1 \quad T_{200}]^T$$

Note that we as usual have included the inputs in the candidate measurements. The economic objective is to maximize the operating profit [$/$h$], formulated as minimization of the negative profit (Kariwala et al., 2008).

$$J = 600F_{100} + 0.6F_{200} + 1.009(F_2 + F_3) + 0.2F_1 - 4800F_2 \tag{3.33}$$

The objective in self-optimizing control is to find optimal CVs that minimize the loss, $L = J - J_{\text{opt}}(\mathbf{d})$, in presence of disturbances and implementation errors. We formulated the problem (3.27) for this evaporator example and solved the MIQP to find the optimal CVs as the combinations of the best measurement subset size from 2 to 10. The YALMIP toolbox (Lofberg, 2004) is used to solve the MIQP problem with $m = 200$ in the big-m constraints in (3.27). To compare, the same problem was also solved by the downwards branch and bound (Downwards BAB) method and the partial bidirectional branch bound (PB^3) method (Kariwala and Cao, 2009). The three methods gave the same results and the loss as a function of the number of measurements (n) used is shown in Figure 3.6. The corresponding optimal measurements sets for the 9 subsets are given in Table 3.1. We note that F_{200} is included in all cases. From Figure 3.6, we see that the loss decreases rapidly when the number of measurements is increased from 2 to 3, but from 3 measurements and on the loss decrease is smaller. Based on Figure 3.6, Table 3.1 and acceptable loss CVs can be found as combinations of optimal measurement subsets for this 10-measurement evaporator example.

The average computational times (CPU time) using a Windows XP SP2 notebook with Intel ®Core$^{\text{TM}}$ Duo Processor T7250 (2.00 GHz, 2M Cache, 800 MHz FSB) using MATLAB ®R2009a for the MIQP, Downwards BAB, PB^3 methods and in addition the exhaustive search method are also tabulated in Table 3.1. Note that the exhaustive search was not actually

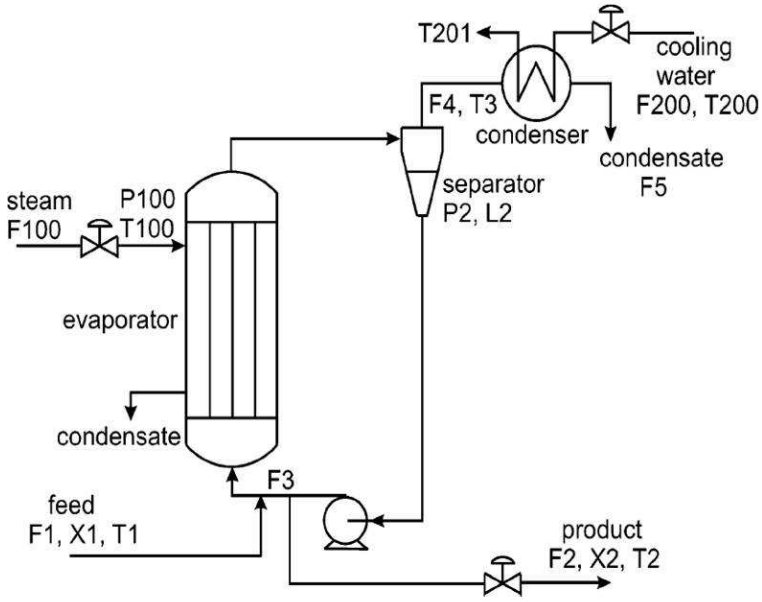

Figure 3.5: Evaporator process

performed and the given CPU time is an estimate based on assuming 0.001 s for each evaluation.

From Table 3.1, it can be seen that the MIQP method finds the optimal solution about one order of magnitude faster than the exhaustive search method, whereas the PB^3 and Downwards BAB methods are even one order of magnitude faster than MIQP. In conclusion, even though the MIQP method is not as fast as that of Downwards BAB and PB^3 methods; it is still acceptable as the optimal CVs selection is performed off-line. The advantage of MIQP method is that the method is simple, intuitive and can easily incorporate structural constraints which cannot be included with the BAB methods. This is considered in the next example.

3.5.3 Example 3: evaporator process with structural constraints (Case 3.2.4)

This example considers optimal measurement selection using MIQP formulations with the additional restrictions (3.31). As above, there are 3 temperature measurements, 6 flow measurements and 1 pressure measurement. The task is to use only 5 out of 10 measurements, more specifically, we want to use 1 pressure (among 1), 2 temperatures (among 3) and 2 flows (among

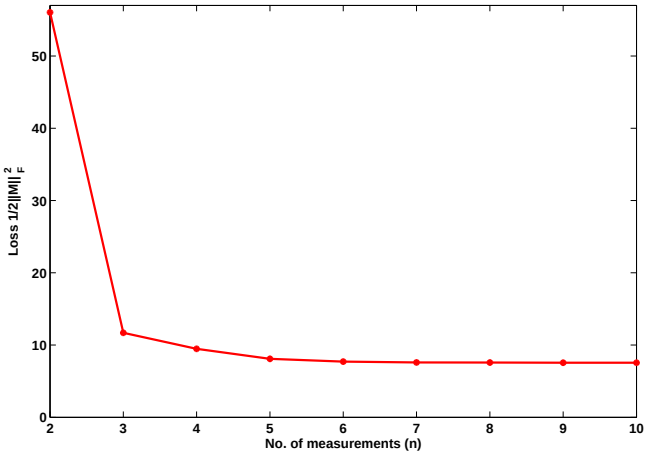

Figure 3.6: Evaporator: loss vs the number of included measurements (n)

6). These constraints can easily be incorporated in the MIQP formulations, whereas these can not be incorporated directly in the Downwards BAB and PB[3] methods. For the constraint (3.27b) we have

$$\mathbf{P} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 1 & 1 \end{bmatrix}, \ \mathbf{s} = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$$

The optimal loss with these structural constraints is 12.9096 and the optimal measurement set is $[F_2 \quad F_{100} \quad T_{201} \quad T_2 \quad P_2]$. To compare the loss with five measurements without any structural requirements is 8.0960 and the optimal measurements are $[F_2 \quad F_{100} \quad F_3 \quad F_{200} \quad T_{201}]$.

3.5.4 Example 4: measurement selection for distillation column (Case 3.2.2)

This example is included to apply the MIQP (3.27) formulations on a case with a large number of measurements and to highlight the computational effectiveness of the developed methods over the exhaustive search methods. We also include the computational effectiveness of both big-m approach (3.27c) and indicator constraint approach (3.28) for MIQP (3.27). We consider indirect composition control of a binary distillation column with 41 stages (Skogestad, 1997; Hori and Skogestad, 2008) and reflux (L) and boil-up (V) as the remaining unconstrained steady state degrees of freedom ($\mathbf{u}$).

Table 3.1: Evaporator example: optimal measurement sets as a function of the number of measurements with associated losses and computational times

No. Meas n	Optimal Measurements	Loss* $\frac{1}{2}\|\mathbf{M}\|_F^2$	CPU time (sec) MIQP	Downwards BAB	PB[3]	Exhaustive
2	$[F_3 \quad F_{200}]$	56.0260	0.0235	0.0028	0.0023	0.045
3	$[F_2 \quad F_{100} \quad F_{200}]$	11.7014	0.0350	0.0013	0.0028	0.12
4	$[F_2 \quad T_{201} \quad F_3 \quad F_{200}]$	9.4807	0.0400	0.0016	0.0025	0.21
5	$[F_2 \quad F_{100} \quad T_{201} \quad F_3 \quad F_{200}]$	8.0960	0.0219	0.0011	0.0014	0.252
6	$[F_2 \quad F_{100} \quad T_{201} \quad F_3 \quad F_5 \quad F_{200}]$	7.7127	0.0204	0.0016	0.0017	0.21
7	$[P_2 \quad F_2 \quad F_{100} \quad T_{201} \quad F_3 \quad F_5 \quad F_{200}]$	7.5971	0.0289	0.0009	0.0016	0.12
8	$[P_2 \quad T_2 \quad F_2 \quad F_{100} \quad T_{201} \quad F_3 \quad F_5 \quad F_{200}]$	7.5756	0.0147	0.0005	0.0009	0.045
9	$[P_2 \quad T_2 \quad F_2 \quad F_{100} \quad T_{201} \quad F_3 \quad F_5 \quad F_{200} \quad F_1]$	7.5617	0.0110	0.0008	0.0009	0.01
10	$[P_2 \quad T_2 \quad T_3 \quad F_2 \quad F_{100} \quad T_{201} \quad F_3 \quad F_5 \quad F_{200} \quad F_1]$	7.5499	0.0008	0.0011	0.0009	0.001

*The results are the same as in (Kariwala et al., 2008), but the loss given in (Kariwala et al., 2008) is a factor $3(n + n_d)$ smaller, see Section 3.6.2.

The considered disturbances are in feed flow rate (F), feed composition (z_F) and liquid fraction (q_F), which can vary between $1\pm0.2, 0.5\pm0.1$ and 1 ± 0.1, respectively. As online composition measurements are assumed unavailable, we use stage temperatures inside the column to control the compositions indirectly. The boiling points difference between light key component (L) and heavy key component (H) is 10 ^oC. We assume constant relative volatility of the components, constant pressure, no vapour hold up, equilibrium on each stage and constant molar flow rate. Under these assumptions only mass and component balances are included in this binary distillation column model and temperatures are approximated as linear functions of mole fractions. The temperature T_i (^oC) on stage i is calculated as a simple linear function of the liquid composition x_i on each stage (Skogestad, 1997).

$$T_i = 0x_i + 10(1 - x_i) \tag{3.34}$$

The candidate measurements are the 41 stage temperatures which are measured with an accuracy of $\pm0.5^oC$. Note that we do *not* include the inputs (flows L and V) in the candidate measurements for this example because we would like to use only temperature combinations for control. The cost function J for the indirect composition control problem is the relative steady-state composition deviation,

$$J = \left(\frac{x^H_{top} - x^H_{top,s}}{x^H_{top,s}}\right)^2 + \left(\frac{x^L_{btm} - x^L_{btm,s}}{x^L_{btm,s}}\right)^2 \tag{3.35}$$

where x^H_{top} and x^L_{btm} denote the heavy key component (H) composition in top product and light key component (L) composition in bottom product

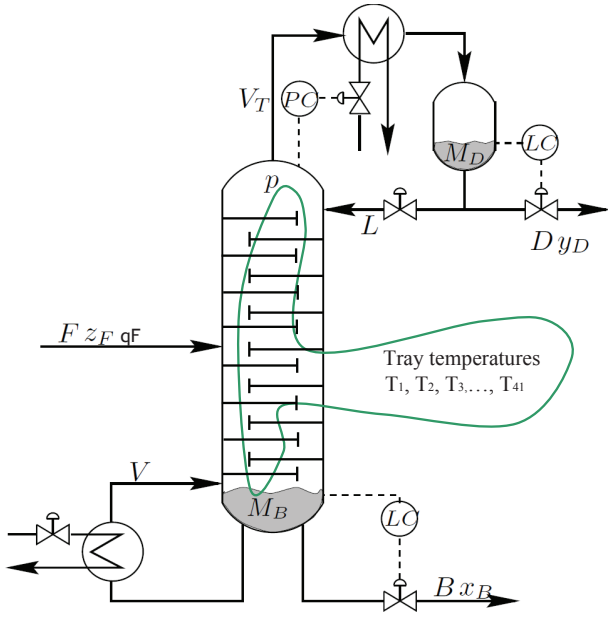

Figure 3.7: Distillation column using LV-configuration

and $x^H_{top} = x^L_{btm} = 0.01$(99% purity). The specification or set point value is denoted with subscript 's' (Hori and Skogestad, 2008). This cost can be written in the general form in (3.3).

The MIQP formulation described in Case 3.2.2 in Section 3.4 is used to find 2 CVs as the optimal subset combinations of 2 to 41 stage temperatures. An MIQP is set up for this distillation column with the choice $m = 2$ for the big-m constraints in equation (3.27). To obviate the need to select an appropriate m, another MIQP is set up by replacing big-m constraints (3.27c) with indicator constraint approach (3.28). The constraint in (3.27b) becomes $\sum_{j=1}^{n_y} \sigma_j = n$, where n varies from 2 to 41. The IBM ILOG Optimizer CPLEX solver is used to solve the MIQP problem. The minimized loss function with the number of measurements is shown in Figure 3.8.

The optimal controlled variables (measurement combination matrix $\mathbf{H}$) for the cases with 2, 3, 4 and 41 measurements are shown in Table 3.2. For the case with 2 measurements, we just give the measurement, and not the combination, because we can always choose the $\mathbf{D}$ matrix to make, for example, $\mathbf{H} = \mathbf{I}$ (identity). For the case with 3 and 4 measurements, we choose to use the degrees of freedom in $\mathbf{D}$ to make selected elements in $\mathbf{H}$ equal to 1.

The same problem was also solved by the downwards branch and bound

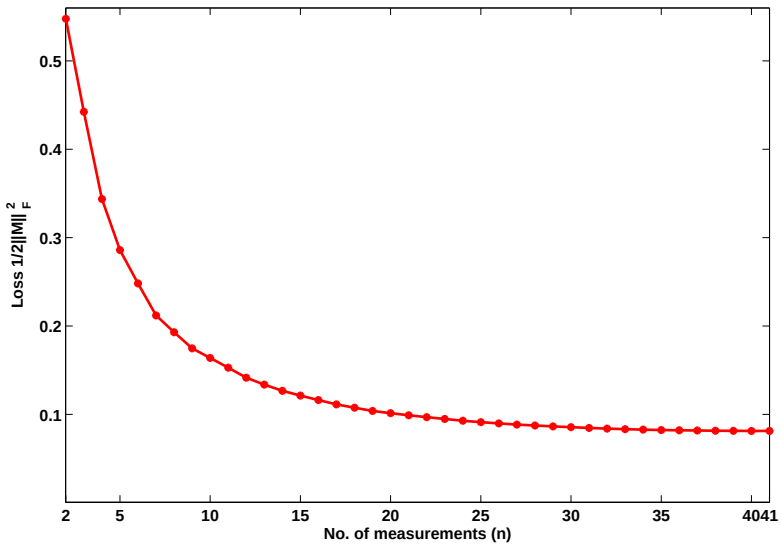

Figure 3.8: Distillation column: loss vs the number of included measurements (n)

and partial bidirectional branch bound methods (Kariwala and Cao, 2009). The computational times (CPU time) taken by MIQP with big-m approach, MIQP with indicator constraint approach, Downward BAB and PB^3 methods and also the exhaustive search method are compared in Figure 3.9. Note that exhaustive search is not performed and instead we give an estimate assuming 0.01 s for each evaluation. From Figure 3.9, it can be seen that the MIQP finds the optimal solution 6 orders of magnitude faster than the exhaustive search methods. Contrary to theory, MIQP with indicator constraints take slightly higher computational times than MIQP with big-m approach, this could be due to the branching strategy used in CPLEX solver resulting in exploration of higher number of nodes. On an average, the MIQP with the big-m or the indicator constraint approach is about 1 order of magnitude slower than the PB^3 and Downwards BAB methods. The MIQP method is relatively quick for measurement subset sizes between 25 and 41, but slower for subset sizes from 10 to 23. This is reasonable because subset sizes (10 to 23) have a very high number of possibilities ($\binom{41}{10}$ to $\binom{41}{23}$). In conclusion, even though the MIQP methods are not as computationally attractive as Downwards BAB and PB^3 methods, the differences are not excessive.

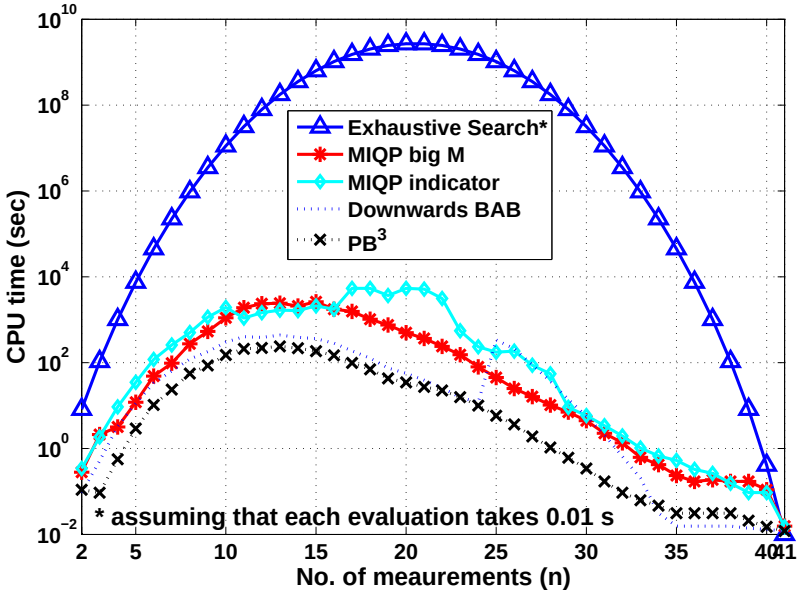

Figure 3.9: Distillation column: CPU time requirement for computations in Figure 3.8

.

Table 3.2: Distillation column example: optimal measurements and optimal controlled variables with loss

No. Meas n	$\mathbf{c}'s$ as combinations of measurements	Loss $\frac{1}{2}\|\mathbf{M}\|_F^2$
2	$c_1 = T_{12}$ $c_2 = T_{30}$	0.5477
3	$c_1 = T_{12} + 0.0446T_{31}$ $c_2 = T_{30} + 1.0216T_{31}$	0.4425
4	$c_1 = 1.0316T_{11} + T_{12} + 0.0993T_{31}$ $c_2 = 0.0891T_{11} + T_{30} + 1.0263T_{31}$	0.3436
41	$c_1 = f(T_1, T_2, \ldots, T_{41})$ $c_2 = f(T_1, T_2, \ldots, T_{41})$	0.0813

3.5.5 Example 5: measurement selection for Kaibel column (Cases 3.2.4 and 3.2.5)

The Kaibel column example is included to show the optimal measurement selection using MIQP formulations with additional restrictions as given in (3.31) and (3.32). The 4-product Kaibel column shown in Figure 3.10 has high energy saving potential (Halvorsen and Skogestad, 2003), but presents a difficult control problem. The given 4-product Kaibel column arrangement separates a mixture of methanol (A), ethanol (B), propanol (C), butanol (D) into almost pure components. The economic objective function J is to minimize the impurities in the products.

$$J = D(1 - x_{A,D}) + S_1(1 - x_{B,S_1}) + S_2(1 - x_{C,S_2}) + B(1 - x_{D,B}) \quad (3.36)$$

where D, S_1, S_2 and B are the distillate, side product 1, side product 2 and bottom flow rates (mol/min) respectively. $x_{i,j}$ is mole fraction of component i in product j.

The Kaibel column has 4 inputs (L, S_1, S_2, R_L) and 71 temperature measurements (7 sections with each section having 10 tray temperatures plus 1 temperature for reboiler), which we included as the candidate measurements $(\mathbf{y})$ and are measured with an accuracy of $\pm 1^oC$. The considered disturbances are in vapor boil up (V), vapor split (R_V), feed flow rate (F), mole fraction of A in feed stream (z_A), mole fraction of B in feed stream (z_B), mole fraction of C in feed stream (z_C) and liquid fraction of the feed stream (q_F), which vary between $3 \pm 0.25, 0.4 \pm 0.1, 1 \pm 0.25, 0.25 \pm 0.05, 0.25 \pm$

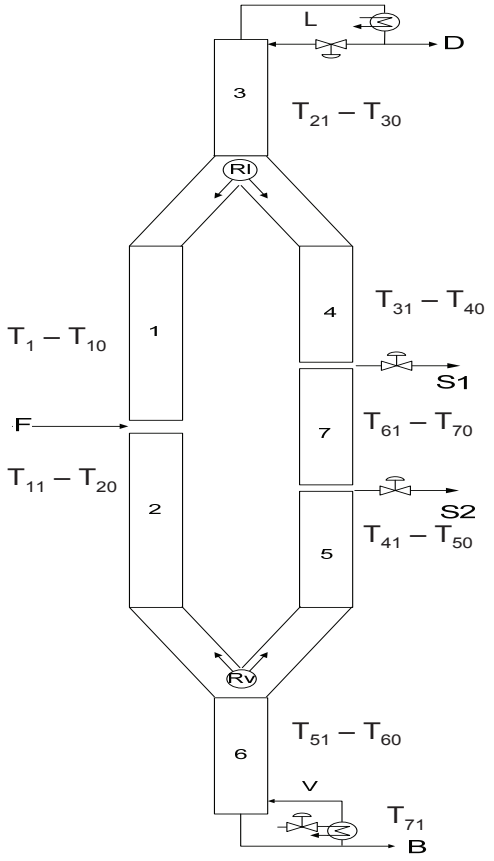

Figure 3.10: The 4-product Kaibel column

$0.05, 0.25 \pm 0.05$ and 0.9 ± 0.05, respectively. The reader is referred to Strandberg (2006) for further details on this example.

We consider the selection of the control variables as individual measurements or combinations of a measurement subset with measurements from specified sections of the column as structural constraints. Such structural constraints may be important for dynamic reasons, for example, at least one temperature in the prefractionator should be used in the regulatory layer (Strandberg, 2006). The 4-product Kaibel column is divided into 4 segments with 20, 20, 10 and 21 measurements, respectively. The measurements in the four segments are $T_1 - T_{20}$, $T_{21} - T_{40}$, $T_{61} - T_{70}$ and $T_{41} - T_{60}$ plus T_{71}, respectively (Figure 3.10). Note that segment 4 includes reboiler

temperature T_{71}. The candidate measurements $\mathbf{y}$ and given inputs $\mathbf{u}$ are

$$\mathbf{y} = [T_1 \quad T_2 \quad T_3 \quad \cdots \quad T_{71}]^T$$
$$\mathbf{u} = [L \quad S_1 \quad S_2 \quad R_L]^T$$

We formulate an MIQP using (3.27) to find four CVs for the following three cases

(i) Optimal combinations of 4, 5, 6 and 71 measurements with no constraint on sections (Case 3.2.2)

(ii) Single measurements from each of the four segments (Case 3.2.4)

(iii) Including extra measurements to a given set of measurements (Case 3.2.5). In this case, $\{T_{12}, T_{25}, T_{45}, T_{62}\}$ are taken as the given set of measurements, which could have been selected based on considerations for stabilizing the column profiles.

The constraint for (i) is

$$\sum_{j=1}^{n_y} \sigma_j = n$$

for $n = 4, 5, 6$ and 71. This can alternatively be written in the general form in (3.27b) with

$$\mathbf{P} = \underline{1}^T{}_{1\times n_y}, \mathbf{s} = n$$

where $\underline{1}$ is a column vector of ones and n is 4, 5, 6 and 71.

The constraints for (ii) can be written in the general form (3.27b) with

$$\mathbf{P} = \begin{bmatrix} \underline{1}^T{}_{1\times 20} & \underline{0}^T{}_{1\times 20} & \underline{0}^T{}_{1\times 20} & \underline{0}^T{}_{1\times 10} & 0 \\ \underline{0}^T{}_{1\times 20} & \underline{1}^T{}_{1\times 20} & \underline{0}^T{}_{1\times 20} & \underline{0}^T{}_{1\times 10} & 0 \\ \underline{0}^T{}_{1\times 20} & \underline{0}^T{}_{1\times 20} & \underline{1}^T{}_{1\times 20} & \underline{0}^T{}_{1\times 10} & 1 \\ \underline{0}^T{}_{1\times 20} & \underline{0}^T{}_{1\times 20} & \underline{0}^T{}_{1\times 20} & \underline{1}^T{}_{1\times 10} & 0 \end{bmatrix}, \ \mathbf{s} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

where $\underline{1}$ is a column vector of ones and $\underline{0}$ is a column vector of zeros.

(iii) We consider including 1, 2 and 3 extra measurements to the given set $\{T_{12}, T_{25}, T_{45}, T_{62}\}$. The constraints for this case are

$$\sigma_j = 1, \quad \forall j = 12, 25, 45, 62$$
$$\sum_{j=1}^{71} \sigma_j = n$$

where $n = 5, 6$ or 7.

Table 3.3: Kaibel column: optimal measurement sets and loss using optimal combination of these measurements

Case	No. Meas n	Optimal measurements	Loss $\frac{1}{2}\|\mathbf{M}\|_F^2$	CPU time (min)
(i)	4	$[T_{12} \quad T_{40} \quad T_{51} \quad T_{66}]$	11.6589	34.23
(i)	5	$[T_{12} \quad T_{51} \quad T_{62} \quad T_{65} \quad T_{66}]$	2.9700	120
(i)	6	$[T_{12} \quad T_{20} \quad T_{23} \quad T_{57} \quad T_{60} \quad T_{64}]$	1.0140	120
(i)	71	$[T_1 \quad T_2 \quad \ldots \quad T_{71}]$	0.0101	0.0007
(ii)	4*	$[T_{12} \quad T_{40} \quad T_{51} \quad T_{66}]$	11.6589	1.19
(iii)	4†	$[T_{12} \quad T_{25} \quad T_{45} \quad T_{62}]$	1328.6691	0.0005
(iii)	5**	$[T_{12} \quad T_{25} \quad T_{45} \quad T_{62} \quad T_{69}]$	65.7180	0.096
(iii)	6**	$[T_{12} \quad T_{25} \quad T_{45} \quad T_{55} \quad T_{62} \quad T_{71}]$	3.5646	0.19
(iii)	7**	$[T_{12} \quad T_{25} \quad T_{45} \quad T_{51} \quad T_{62} \quad T_{65} \quad T_{67}]$	0.9450	2.21

* (ii) Case 3.2.4; **(iii) Case 3.2.5 ; †given non-optimal measurement set

The optimal measurements sets for cases (i),(ii),(iii) together with the loss and computational times are reported in Table 3.3. Note that for Case (i) with 5, 6 measurements, the reported solutions are not optimal solutions as the computational time required for these cases exceeded the set maximum computational time limit of 120 min. The measurements sets for $n = 4$ are the are same for (i) and (ii) because it happens that the optimal measurements in Case (i) have the desired distribution. However, the computational time is about 30 times higher for Case (i) as the number of possibilities is higher in (i) than in (ii). For Case (iii), the loss decreases as we add 1, 2, and 3 extra measurements to the given set.

3.6 Discussion

3.6.1 Structured H with specified zero elements (Problem 3.3)

Unfortunately, the convex formulation in Theorem 3 used in the above examples, does not generally apply when specified elements in $\mathbf{H}$ are zero. Some examples are

(I) **Decentralized structure**. This is the case, where we want to combine measurements from a individual unit/section alone in a plant, so the measurement sets are disjoint. This can be viewed as selecting CVs for individual units/sections in the plant. As an example, consider a process with 2 inputs (degrees of freedom) and 5 measurements with 2 disjoint measurement sets {1,2,3}, {4,5}; the structure

is

$$\mathbf{H}_I = \begin{bmatrix} h_{11} & h_{12} & h_{13} & 0 & 0 \\ 0 & 0 & 0 & h_{24} & h_{25} \end{bmatrix}$$

(II) **Triangular structure**. More generally, $\mathbf{H}$ may have a triangular structure. As an example, consider a process with 2 degrees of freedom and 5 measurements with partially disjoint measurement sets as $\{1, 2, 3, 4, 5\}$ for one CV and $\{4, 5\}$ for another CV, the structure is

$$\mathbf{H}_{II} = \begin{bmatrix} h_{11} & h_{12} & h_{13} & h_{14} & h_{15} \\ 0 & 0 & 0 & h_{34} & h_{35} \end{bmatrix}$$

Since Theorem 3 does **not** hold for these cases with specified structures, we need to solve non-convex problems. This is outside the scope of this paper, where convex formulations are considered.

3.6.2 Use of average loss $\frac{1}{2}\|\mathbf{M}\|_F^2$

For the measurement selection problem, using an uniform distribution for $\mathbf{d}'$ and $\mathbf{n}^{y'}$ with $\left\| \begin{bmatrix} \mathbf{d}' \\ \mathbf{n}^{y'} \end{bmatrix} \right\|_2 \leq 1$ results in the average loss $\hat{L}_{avg} = \frac{1}{6(n_y+n_d)}\|\mathbf{M}\|_F^2$ (Kariwala et al., 2008). Although this loss expression is mathematically correct, the use of a uniform distribution is not meaningful from an engineering point of view. Specifically, the reduction in the loss by the factor $3(n_y + n_d)$ is not meaningful. To illustrate this, note that we can add dummy measurements and thus set n_y to any number, and then choose to not use these dummy measurements when selecting $\mathbf{c} = \mathbf{H}\mathbf{y}$, simply by setting the corresponding columns in $\mathbf{H}$ to zero. As the Frobenius norm of a matrix is the same if we add columns of zeros, $\|\mathbf{M}\|_F$ will be unchanged, but n_y increases and the loss $\hat{L}_{avg}$ decreases. Since the loss should not change by adding dummy measurements that we do not use, the use of uniform distribution of the two-norm is not physically meaningful. Hence, in this paper, we choose to use the more common normal distribution for $\mathbf{d}'$ and $\mathbf{n}^{y'}$ which gives the average loss (expected loss) $L_{avg} = \frac{1}{2}\|\mathbf{M}\|_F^2$ in (3.20).

3.7 Conclusions

The problem of finding optimal CV measurement combinations that minimize the loss from optimal operation is solved. The optimal CV selection problem from self optimizing control framework is reformulated as a QP and the optimal CV selection for measurement subsets is formulated as an MIQP

problem. The developed MIQP based method allows for additional structural constraints compared to the bidirectional branch and bound methods reported in literature. The MIQP based method was found to use about 10 times more CPU time than the bidirectional branch and bound methods, but this is acceptable as the optimal CV selection problem is done offline. In addition, the MIQP method can be used on some problems where the branch and bound methods do not apply, as shown for the Kaibel column example.

Bibliography

Alstad, V., Skogestad, S., 2007. Null space method for selecting optimal measurement combinations as controlled variables. Ind. Eng. Chem. Res. 46, 846–853.

Alstad, V., Skogestad, S., Hori, E., 2009. Optimal measurement combinations as controlled variables. Journal of Process Control 19 (1), 138–148.

Ariyur, K. B., Krstic, M., 2003. Real-Time Optimization by Extremum-Seeking Control. Wiley-Interscience.

de Araújo, A. C., Govatsmark, M., Skogestad, S., 2007. Application of plantwide control to the hda process. I - steady-state optimization and self-optimizing control. Control Engineering Practice 15 (10), 1222 – 1237.

Engell, S., 2007. Feedback control for optimal process operation. Journal of Process Control 17 (3), 203 – 219, special Issue ADCHEM 2006 Symposium.

Forbes, J. F., Marlin, T. E., 1996. Design cost: A systematic approach to technology selection for model-based real-time optimization systems. Computers & Chemical Engineering 20 (6-7), 717 – 734, fifth International Symposium on Process Systems Engineering.

Foss, A., 1973. Critique of chemical process control theory. AIChE Journal 19, 209–214.

Guay, M., Zhang, T., 2003. Adaptive extremum seeking control of nonlinear dynamic systems with parametric uncertainties. Automatica 39 (7), 1283 – 1293.

Halvorsen, I. J., Skogestad, S., 2003. Minimum energy consumption in multicomponent distillation. 3. more than three products and generalized petlyuk arrangements. Industrial & Engineering Chemistry Research 42 (3), 616–629.

Halvorsen, I. J., Skogestad, S., Morud, J. C., Alstad, V., 2003. Optimal selection of controlled variables. Ind. Eng. Chem. Res. 42.

Heldt, S., 2010. Dealing with structural constraints in self-optimizing control engineering. Journal of Process Control 20 (9), 1049 – 1058.

Hooker, J. N., Osorio, M. A., October 1999. Mixed logical-linear programming. Discrete Appl. Math. 96-97, 395–442.

Hori, E. S., Skogestad, S., 2008. Selection of controlled variables: Maximum gain rule and combination of measurements. Industrial & Engineering Chemistry Research 47 (23), 9465–9471.

Kadam, J. V., Marquardt, W., Srinivasan, B., Bonvin, D., 2007. Optimal grade transition in industrial polymerization processes via NCO tracking. AIChE Journal 53 (3), 627–639.

Kariwala, V., 2007. Optimal measurement combination for local self-optimizing control. Industrial & Engineering Chemistry Research 46 (11), 3629–3634.

Kariwala, V., Cao, Y., 2009. Bidirectional branch and bound for controlled vaiable selection. Part II: Exact local method for self-optimizing control. Computers and Chemical Engineering 33, 1402–1414.

Kariwala, V., Cao, Y., 2010. Bidirectional branch and bound for controlled vaiable selection. Part III: Local average loss minimization. IEEE Transactions on Industrial Informatics 6, 54–61.

Kariwala, V., Cao, Y., Janardhanan, S., 2008. Local self-optimizing control with average loss minimization. Ind. Eng. Chem. Res. 47, 1150–1158.

Kassidas, A., Patry, J., Marlin, T., 2000. Integrating process and controller models for the design of self-optimizing control. Computers & Chemical Engineering 24 (12), 2589 – 2602.

Lofberg, J., sept. 2004. Yalmip : A toolbox for modeling and optimization in matlab. In: Computer Aided Control Systems Design, 2004 IEEE International Symposium on. pp. 284 –289.

Morari, M., Stephanopoulos, G., Arkun, Y., 1980. Studies in the synthesis of control structures for chemical processes. Part I: formulation of the problem. process decomposition and the classification of the control task. analysis of the optimizing control structures. AIChE Journal 26 (2), 220–232.

Narraway, L., Perkins, J., Barton, G., 1991. Interaction between process design and process control: economic analysis of process dynamics. Journal of Process Control 1 (5), 243 – 250.

Narraway, L. T., Perkins, J. D., 1993. Selection of process control structure based on linear dynamic economics. Industrial & Engineering Chemistry Research 32 (11), 2681–2692.

Newell, R. B., Lee, P., 1989. Applied process control : A case study. Prentice-Hall of Australia, New York ; Sydney.

Panahi, M., Skogestad, S., 2011. Economically efficient operation of CO2 capturing process part I: Self-optimizing procedure for selecting the best controlled variables. Chemical Engineering and Processing: Process Intensification 50 (3), 247 – 253.

Skogestad, S., 1997. Dynamics and control of distillation columns: A tutorial introduction. Chemical Engineering Research and Design 75 (6), 539 – 562, distillation.

Skogestad, S., 2000. Plantwide control: The search for the self-optimizing control structure. Journal of Process Control 10, 487–507.

Skogestad, S., Postlethwaite, I., 1996. Multivariable Feedback Control, 1. Edition. Wiley.

Srinivasan, B., Bonvin, D., Visser, E., Palanki, S., 2003. Dynamic optimization of batch processes: II. Role of measurements in handling uncertainty. Computers & Chemical Engineering 27 (1), 27 – 44.

Strandberg, Jens; Skogestad, S., 2006. Stabilizing operation of a 4-product integrated kaibel column. Institution of Chemical Engineers Symposium Series 152, 636–647.

van de Wal, M., de Jager, A., 2001. A review of methods for input/output selection. Automatica 37 (4), 487–510.

Vasudevan, S., Rangaiah, G. P., Konda, N. V. S. N. M., Tay, W. H., 2009. Application and evaluation of three methodologies for plantwide control of the styrene monomer plant. Industrial & Engineering Chemistry Research 48 (24), 10941–10961.

Chapter 4

Convex approximation methods for optimal controlled variables with structural constraints in Self-optimizing control

Based on the published conference papers in
American Control Conference, 2011, San Francisco, USA. pp. 342–347 &
IFAC World Congress, 2011, Milano, Italy. pp. 4977–4982

Control structure selection is vital to keep the process operation optimal in the presence of disturbances. In this paper we briefly review the controlled variable selection, $\mathbf{c} = \mathbf{Hy}$, with the aim to minimize the loss from optimal operation. Selecting $\mathbf{c}'s$ that obey structural constraints are important for dynamic reasons and for ease in practical implementation. The structural constraints are (i) to find $\mathbf{c}'s$ as combinations of the same measurement subsets; (ii) to find $\mathbf{c}'s$ as combinations of measurements with (decentralized) block diagonal/triangular $\mathbf{H}$. Structural constraints of first kind are reformulated to convex quadratic optimization problems and Mixed Integer Quadratic Programming methods are developed to select optimal measurements to arrive at globally optimal $\mathbf{H}$, but the second kind are non-convex. Hence, we propose a few new ideas and convex approximation methods for the second type. The proposed methods are evaluated on random cases, an evaporator case study and a binary distillation column case study with 41 stages and are observed to provide good upper bounds.

4.1 Introduction

Control structure selection deals with the selection of controlled variables (CV/outputs) and manipulated variables (MV/inputs), and the pairings or interconnections of these variables (Foss, 1973; Skogestad, 2000). Generally, the controlled variables ($\mathbf{c}$) are selected as individual measurements or combinations of measurements.

$$\mathbf{c} = \mathbf{H}\mathbf{y} \tag{4.1}$$

where $\mathbf{c} \in \mathbb{R}^{n_c}$ are the controlled variables, $\mathbf{u} \in \mathbb{R}^{n_u}$ are the manipulated variables, $\mathbf{y} \in \mathbb{R}^{n_y}$ are the measurements and $\mathbf{H} \in \mathbb{R}^{n_c \times n_y}$ is the measurement combination matrix, which is to be selected.

The overall goal of control structure design is to reflect the business objectives. In this paper, the focus is on selecting CV ($\mathbf{c}$) to aid the process plant to operate optimally even in the presence of disturbances. A comprehensive review of input/output selection methods was provided by (van de Wal and de Jager, 2001), but these focused on controllability issues and failed to account for the business objectives, like minimizing the cost (J). A comprehensive review of heuristic and mathematical methods for plantwide control are presented (Larsson and Skogestad, 2000).

The idea in self-optimizing control (SOC) is to use the degrees of freedom in selecting $\mathbf{c}$ to get some degree of "self-optimization" into the fast control layer, such that less frequent updates of $\mathbf{c}_s$ are required by the optimization layer. The ideas of "self-optimizing control" dates back to (Morari et al., 1980), who stated that "we want to find a function $\mathbf{c}$ of the process variables which when held constant, leads automatically to the optimal adjustments of the manipulated variables, and with it, the optimal operating condition". A few other alternatives of optimal operation are real time optimization (Forbes and Marlin, 1996), necessary conditions of Optimality tracking (Srinivasan et al., 2003; Kadam et al., 2007), extremum seeking control (Ariyur and Krstic, 2003; Guay and Zhang, 2003) and optimizing controllers (Kassidas et al., 2000; Engell, 2007). However, SOC is based on pseudo-steady state approximation of process that uses feedback policy to keep $\mathbf{c}$ at constant set point $\mathbf{c}_s$ to counteract the disturbances effectively and reduces the frequency of optimization. In this context SOC can be viewed as a complement. This is illustrated in Figure 4.1.

Mathematically, the optimal $\mathbf{H}$ that minimizes the average or worst-case steady state loss from optimum may be obtained by solving the following steady-state optimization problem (see theorem 6 for details)(Halvorsen

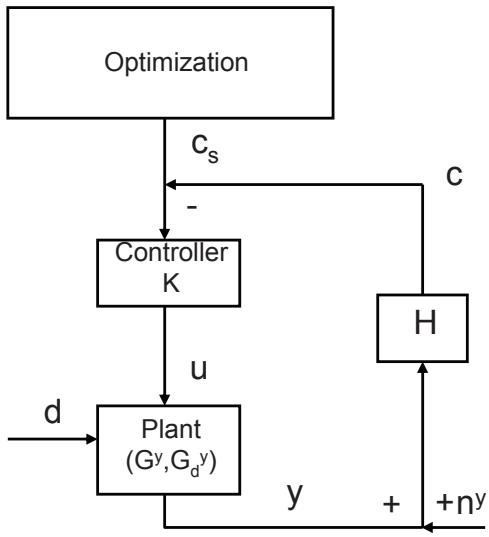

Figure 4.1: Feedback implementation of optimal operation with separate layers for optimization and control

.

et al., 2003; Kariwala et al., 2008)

$$\min_{\mathbf{H}} \|\mathbf{J}_{uu}^{1/2}(\mathbf{H}\mathbf{G}^y)^{-1}\mathbf{H}\mathbf{Y}\|_F \tag{4.2}$$

where $\mathbf{Y} = [\mathbf{F}\mathbf{W}_d \ \mathbf{W}_{n^y}]$, $\mathbf{F} = \frac{d\mathbf{y}_{opt}}{d\mathbf{d}}$ is the optimal sensitivity matrix with respect to disturbances, $\mathbf{W}_d$ and $\mathbf{W}_{n^y}$ are diagonal matrices with elements equal to the expected magnitude of disturbances and measurement noises (errors), $\mathbf{G}^y$ is the measurement gain matrix and $\mathbf{J}_{uu}$ is the Hessian of the cost function J with respect to the degrees of freedom $\mathbf{u}$.

In general, (4.2) is a non-convex optimization problem in the decision variable $\mathbf{H}$. However, in the standard case when $\mathbf{H}$ is a "full" matrix, it may be reformulated as a convex problem. This follows because the optimal $\mathbf{H}$ is not unique and we have enough "extra" degrees of freedom in $\mathbf{H}$ to impose a constraint on the matrix $\mathbf{H}\mathbf{G}^y$ and we get an equivalent quadratic programming (QP) problem which is convex (see theorem 7) (Alstad et al., 2009).

$$\begin{aligned} &\min_{\mathbf{H}} \|\mathbf{H}\mathbf{Y}\|_F \\ &\text{s.t. } \mathbf{H}\mathbf{G}^y = \mathbf{J}_{uu}^{1/2} \end{aligned} \tag{4.3}$$

However, in real applications we may want to impose limitations on the structure of **H**, that is, we may require some elements in **H** to be zero. For example, for dynamic reasons we may want to combine measurements from given process section, and we require a (decentralized) block diagonal (BD) or triangular (T) **H**.

$$\mathbf{H}_{BD} = \begin{bmatrix} \mathbf{H}_1 & 0 & \cdots & 0 \\ 0 & \mathbf{H}_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{H}_{n_{iu}} \end{bmatrix} \tag{4.4}$$

$$\mathbf{H}_{T} = \begin{bmatrix} \mathbf{H}_{11} & \mathbf{H}_{12} & \cdots & \mathbf{H}_{1n_{iu}} \\ 0 & \mathbf{H}_{22} & \cdots & \cdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{H}_{n_{iu}n_{iu}} \end{bmatrix} \tag{4.5}$$

In such cases, because of all the zeros in **H**, we do not have enough "extra" degrees of freedom in **H** to impose the constraint $\mathbf{HG}^y = \mathbf{J}_{uu}^{1/2}$. Instead, we discuss in this paper how to introduce various convex approximations, for example by having $\mathbf{HG}^y$ matching selected elements in $\mathbf{J}_{uu}^{1/2}$. In this case, the term $\mathbf{J}_{uu}^{1/2}(\mathbf{HG}^y)^{-1}$ in (4.2) is not truly the identity matrix, so minimizing $\|\mathbf{HY}\|_F$ with this "partial" constraint will result in a sub optimal **H** (upper bound).

To sum up, in terms of finding the optimal solution **H** in (4.2), we may consider four problems, of which the last two are the focus in this paper:

Problem 4.1 Full **H**, where the CV are combinations of all measurements **y**. This is a convex QP problem (4.3) and is solved (Alstad et al., 2009)

Problem 4.2 Full **H** with optimal measurements selection, where there are some zero columns in **H**. This may be solved using a partial branch and bound method PB^3 (Kariwala and Cao, 2009, 2010) or alternatively a mixed integer quadratic programming (MIQP) (Yelchuru et al., 2010). These methods are all convex.

Problem 4.3 Structured **H** with some specified zero elements in **H** (see (4.4),(4.5)). This results in a non-convex nonlinear programming (NLP) problem.

Problem 4.4 Structured **H** with measurements selection (there are specified zero elements and some zero columns in **H**). This results in a non-convex mixed integer nonlinear programming (MINLP) problem

Problems 4.3 and 4.4 are non-convex and cannot be addressed with both PB^3 (Kariwala and Cao, 2010) or MIQP methods (Yelchuru et al., 2010). An iterative method has been proposed to obtain an upper bound for the Problems 4.3 and 4.4 (Heldt, 2010), but this method is also non-convex.

This paper is organized as follows: In Section4.2, we review how to transform the original problem (4.2) to a convex QP (4.3) for the case when **H** is a full matrix (Problem 4.1). The proof is included because it provides the starting point for the subsequent convex approximations in Section 4.3 (Problem 4.3). In Section 4.4, we briefly review the MIQP formulations for CV selection (Problem 4.2) and the new MIQP methods to address Problem 4.4. In Section 4.5, the developed methods are evaluated on some artificial random examples, on an evaporator case study and on a binary distillation column case study with 41 stages and the results are discussed. The conclusions are given in Section 4.6.

4.2 Convex formulations of minimum loss method (Problem 4.1)

Consider the feedback system in Figure 4.2, where the input **u** (degrees of freedom) is adjusted to keep the variables $\mathbf{c} = \mathbf{Hy}$ at a constant set point in spite of disturbances. We consider only the (pseudo)-steady state behavior where perfect control of **c** is possible if the controller has integral action. The objective is to select **H** such that this control policy minimizes the steady-state loss $L = J(\mathbf{u}, \mathbf{d}) - J_{opt}(\mathbf{d})$ for the expected disturbances. Here, $J(\mathbf{u}, \mathbf{d})$ is the cost function and $\mathbf{J}_{uu}$ is its Hessian.

Theorem 6 Minimum loss method (exact local method) (Halvorsen et al., 2003; Kariwala et al., 2008; Alstad et al., 2009) *To minimize the average and worst-case loss for expected combined disturbances and noise, (*$\|[\mathbf{d}' \ \mathbf{n}^{y'}]^T\|_2 \leq 1$*), find the* **H** *that solves the problem*

$$\min_{\mathbf{H}} \left\| \mathbf{J}_{uu}^{1/2} (\mathbf{H}\mathbf{G}^y)^{-1} \mathbf{H}\mathbf{Y} \right\|_F \tag{4.6}$$

where $\mathbf{Y} = [\mathbf{F}\mathbf{W}_d \quad \mathbf{W}_{n^y}]$.

We first consider the standard "full" **H** case with no restriction on the structure of the matrix **H** (Problem 4.1), that is we want to find optimal combination of all the measurements.

Theorem 7 Reformulation as a convex problem *(Alstad et al., 2009) The problem in equation* (4.6) *may seem non-convex, but for the standard*

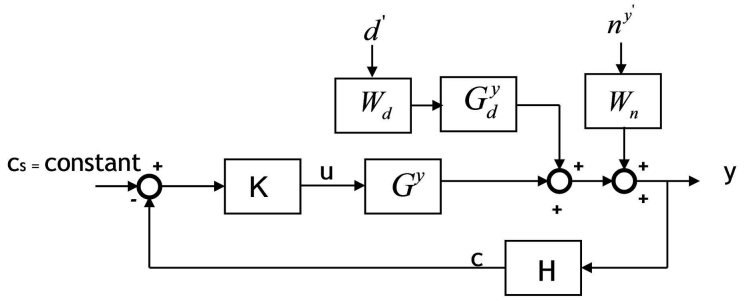

Figure 4.2: Feedback diagram

.

case where $\mathbf{H}$ *is a "full" matrix (with no structural constraints), it can be reformulated as a convex constrained quadratic programming problem.*

$$\begin{aligned} &\min_{\mathbf{H}} \|\mathbf{HY}\|_F \\ &\text{s.t. } \mathbf{HG}^y = \mathbf{J}_{uu}^{1/2} \end{aligned} \tag{4.7}$$

Proof. From the original problem in equation (4.6), we have that the optimal solution $\mathbf{H}$ is non-unique because if $\mathbf{H}$ is a solution then $\mathbf{H}_1 = \mathbf{DH}$ is also a solution for any "full" non-singular matrix $\mathbf{D}$ of size $n_c \times n_c$. This follows because

$$\mathbf{J}_{uu}^{1/2}(\mathbf{HG}^y)^{-1}\mathbf{HY} = \mathbf{J}_{uu}^{1/2}(\mathbf{HG}^y)^{-1}\mathbf{D}^{-1}\mathbf{DHY} = \mathbf{J}_{uu}^{1/2}(\mathbf{H}_1\mathbf{G}^y)^{-1}\mathbf{H}_1\mathbf{Y}$$

One implication is that we can freely choose $\mathbf{G} = \mathbf{HG}^y$, which is a $n_c \times n_c$ matrix representing the effect of $\mathbf{u}$ on $\mathbf{c}$ ($\mathbf{c} = \mathbf{Gu}$). Thus, in (4.6) we may use the non-uniqueness of $\mathbf{H}$ to set the first part of the expression equal to the identity matrix, which is equivalent to setting $\mathbf{HG}^y = \mathbf{J}_{uu}^{1/2}$. This identity must then be added as a constraint in the optimization as shown in (4.7). □

As present numerical software packages such as Matlab cannot deal directly with the matrix formulation in (4.7), the decision matrix

$$\mathbf{H} = \begin{bmatrix} h_{11} & h_{12} & \dots & h_{1n_y} \\ h_{21} & h_{22} & \dots & h_{2n_y} \\ \vdots & \vdots & \ddots & \vdots \\ h_{n_u1} & h_{n_u2} & \dots & h_{n_un_y} \end{bmatrix}$$

is vectorized along the rows of $\mathbf{H}$ to form a long vector

$$\mathbf{h}_\delta = \begin{bmatrix} h_{11} & \dots & h_{1n_y} & h_{21} & \dots & h_{2n_y} & \dots & h_{n_u1} & \dots & h_{n_un_y} \end{bmatrix}^T$$

The equivalent QP is then formulated as (see Appendix A)

$$\begin{aligned} &\min_{\mathbf{h}_\delta} \ \mathbf{h}_\delta^T \mathbf{F}_\delta \mathbf{h}_\delta \\ &\text{s.t. } \mathbf{G}_\delta^{y^T} \mathbf{h}_\delta = \mathbf{j}_\delta \end{aligned} \tag{4.8}$$

where $\mathbf{h}_\delta \in \mathbb{R}^{n_u n_y \times 1}, \mathbf{j}_\delta \in \mathbb{R}^{n_u n_u \times 1}, \mathbf{G}_\delta^{y^T} \in \mathbb{R}^{n_u n_u \times n_y n_u}, \mathbf{F}_\delta \in \mathbb{R}^{n_u n_y \times n_u n_y}$.

4.3 Convex approximations for structured H (Problem 4.3)

We consider the problem

$$\begin{aligned} &\min_{\mathbf{H}} \|\mathbf{J}_{uu}^{1/2} (\mathbf{H}\mathbf{G}^y)^{-1} \mathbf{H}\mathbf{Y}\|_F \\ &\text{s.t.} \mathbf{H} = [\text{particular structure}] \end{aligned} \tag{4.9}$$

where, for example, $\mathbf{H}$ may have a block diagonal or triangular structure as given in (4.4) or (4.5). Unfortunately, (4.9) cannot be reformulated into a convex QP as in (4.7) because we do not have enough degrees of freedom in $\mathbf{D}$ to make $\mathbf{D}\mathbf{H}\mathbf{G}^y = \mathbf{J}_{uu}^{1/2}$, which requires that $\mathbf{D}$ can be any full matrix. The reason is that we need $\mathbf{H}_1 = \mathbf{D}\mathbf{H}$ to have a particular structure, which implies that $\mathbf{D}$ must have a structure corresponding to $\mathbf{H}$. For example, if $\mathbf{H}$ is block diagonal then $\mathbf{D}$ must be block-diagonal, and if $\mathbf{H}$ is triangular then $\mathbf{D}$ must be triangular. Hence for Problem 4.3, a non-convex problem (4.9) need to be solved.

Nevertheless, using the ideas from Theorem 7, we will derive convex approximations for (4.9) (Problem 4.3). The idea is to make use of the extra degrees of freedom in $\mathbf{D}$ as given by the requirement

$$\text{structure } \mathbf{D}\mathbf{H} = \text{structure } \mathbf{H}$$

where $\mathbf{H}$ has a given structure.

In addition, there are degrees of freedom in selecting $\mathbf{u}$, which may be used. These degrees of freedom are related to the fact that the solution is unchanged if we redefine the inputs. Let

$$\mathbf{u}_1 = \mathbf{D}_u{}^{-1}\mathbf{u} \text{ or } \mathbf{u} = \mathbf{D}_u \mathbf{u}_1 \tag{4.10}$$

where $\mathbf{D}_u$ is any non-singular $n_u \times n_u$ matrix. In terms of the new input variables $\mathbf{u}_1$, the following matrices will change

$$\begin{aligned} \mathbf{G}^{y^1} &= \mathbf{G}^y \mathbf{D}_u \\ \mathbf{J}_{u_1 u_1} &= \mathbf{D}_u{}^T \mathbf{J}_{uu} \mathbf{D}_u \end{aligned} \tag{4.11}$$

The matrix $\mathbf{F}$ is unchanged. The degrees of freedom $\mathbf{D}_u$ were not used in the full $\mathbf{H}$ case (Problem 4.1) because it was sufficient to use $\mathbf{D}$ to get a convex problem formulation. With the degrees of freedom in $\mathbf{D}$ and $\mathbf{D}_u$, the problem (4.6) becomes

$$\min_{\mathbf{H},\mathbf{D},\mathbf{D}_u} \|(\mathbf{D}_u^T\mathbf{J}_{uu}\mathbf{D}_u)^{1/2}(\mathbf{D}\mathbf{H}\mathbf{G}^y\mathbf{D}_u)^{-1}\mathbf{D}\mathbf{H}\mathbf{Y}\|_F \tag{4.12}$$

where $\mathbf{D}$ has a certain structure and $\mathbf{D}_u$ is a full matrix. However, note that the solution of this problem is identical to (4.6) and we will use the extra degrees of freedom in (4.12) to derive convex approximations. We will mainly focus on the use of the degrees of freedom in $\mathbf{D}$. The degree of freedom in $\mathbf{D}_u$ will mainly be used to make the resulting optimization problem well posed.

The idea as in Theorem 7 is to exclude the matrix $\mathbf{J}_{uu}^{1/2}(\mathbf{H}\mathbf{G}^y)^{-1}$ in front of $\mathbf{H}\mathbf{Y}$ (4.9). However, when $\mathbf{H}$ has a particular structure, we do not generally have enough degrees of freedom to make $\mathbf{J}_{uu}^{1/2}(\mathbf{H}\mathbf{G}^y)^{-1} = \mathbf{I}$ or equivalently $\mathbf{H}\mathbf{G}^y = \mathbf{J}_{uu}^{1/2}$. To proceed, we have considered the following three convex approximation methods.

Method 1 Use the number of non-zero (n_{nz}) elements in $\mathbf{D}$ (that preserve the particular structure in $\mathbf{H}, \mathbf{H}_1 = \mathbf{D}\mathbf{H}$) to match up to n_{nz} number of elements in $\mathbf{H}\mathbf{G}^y$ to $\mathbf{J}_{uu}^{1/2}$ (Yelchuru and Skogestad, 2011) and minimize $\|\mathbf{H}\mathbf{Y}\|_F$.

Method 2 Introduce an inequality constraint $\mathbf{H}\mathbf{G}^y \leq \mathbf{J}_{uu}^{1/2}$ instead of equality constraint in (4.7) and minimize $\|\mathbf{H}\mathbf{Y}\|_F$. This assumes that $\mathbf{J}_{uu}^{1/2}$ has some negative elements such that the trivial solution $\mathbf{H} = 0$ is avoided. If $\mathbf{J}_{uu}^{1/2}$ does not have negative elements, then the inputs need to be modified as in (4.10) and (4.11).

Method 3 Impose a constraint to let $\mathbf{J}_{uu}^{1/2}(\mathbf{H}\mathbf{G}^y)^{-1}$ have a structure similar to the $\mathbf{D}$ that preserves the structure in $\mathbf{D}\mathbf{H}$ and minimize $\|\mathbf{H}\mathbf{Y}\|_F$.

These three convex approximation methods have been observed to provide good upper bounds to the Problem 4.3 and in particular Method 1 has been found to work well. These three methods are tested for various random cases with particular structure in (4.4) and are discussed in Section 4.5.1. Even though the Method 3 give a reasonable upper bound to Problem 4.3, we consider only convex approximation methods 1 and 2 for Problem 4.4 later.

4.3.1 Convex approximation method 1: matching the elements in $\mathbf{HG}^y$ to $\mathbf{J}_{uu}^{1/2}$

The optimal solution to equation (4.9) is non-unique, so if $\mathbf{H}$ is a solution then $\mathbf{H}_1 = \mathbf{DH}$ is also a solution for any non-singular matrix $\mathbf{D}$ of $n_c \times n_c$ size that preserves the particular structure of $\mathbf{H}$. For example, for a block diagonal $\mathbf{H}$ (4.4), a block diagonal $\mathbf{D}$ matrix preserves the structure in $\mathbf{H}$ and $\mathbf{H}_1 = \mathbf{DH}$. We denote the number of non-zero elements in extra degrees of freedom $\mathbf{D}$ by n_{nz}. Then n_{nz} non-zero elements of $\mathbf{D}$ can be used to match up to n_{nz} elements of $\mathbf{HG}^y$ to elements of $\mathbf{J}_{uu}^{1/2}$. To avoid a trivial solution where $\mathbf{H} = 0$, we make sure that all elements in $\mathbf{J}_{uu}$ are non-zero. This may be done by using the degrees of freedom in $\mathbf{D}_u$. The choice of $\mathbf{D}_u$ could have been used even more systematically, but this has so far not been done.

The $\mathbf{HG}^y$ matrix should have full rank ($n_c = n_u$) as its inverse should exist for the loss (4.9) evaluation. Hence, to have $\mathbf{HG}^y$ as full rank matrix, we can match between n_u and n_{nz} number of elements and the selection of elements to be matched is a combinatorial problem.

To facilitate the analysis, we introduce $\boldsymbol{\beta}_\delta = [\beta_1 \quad \beta_2 \quad \dots \quad \beta_{n_u n_u}]^T$, $\beta_l \in \{0, 1\}$, binary variables vector to complement $n_u n_u$ number of elements in column wise vectorized $\mathbf{HG}^y$ matrix (i.e. $vec(\mathbf{HG}^y)$). The l^{th} element is represented by $|_l$ and β_l is used to complement it. Whenever we match an element l in $vec(\mathbf{HG}^y)$ to $vec(\mathbf{J}_{uu}^{1/2})$, the associated binary variable β_l is 1, and vice versa. We use the non-zero elements in $\mathbf{D}$ to match between n_u and n_{nz} elements of $vec(\mathbf{HG}^y)$ to $vec(\mathbf{J}_{uu}^{1/2})$ and $\sum_{l=1}^{n_u n_u} \beta_l$ is between n_u and n_{nz}. The unmatched elements in $vec(\mathbf{HG}^y)$ can vary between $-b$ to b, and these are formulated (4.14b) using big-m approach (Hooker and Osorio, 1999).

Based on the particular structure in $\mathbf{H}$, for a selected non-zero element in $\mathbf{D}$, the elements of $\mathbf{HG}^y$ that can be matched to $\mathbf{J}_{uu}^{1/2}$ are restricted. For illustration, consider an example of a process with 5 measurements and 2 inputs. Let the gain from $\mathbf{u}$ to $\mathbf{y}$ be $\mathbf{G}^y$ and consider a block diagonal $\mathbf{H}$ with disjoint measurement sets {1,2,3},{4,5}, then

$$\mathbf{G}^y = \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \\ g_{31} & g_{32} \\ g_{41} & g_{42} \\ g_{51} & g_{52} \end{bmatrix}, \quad \mathbf{H} = \begin{bmatrix} h_{11} & h_{12} & h_{13} & 0 & 0 \\ 0 & 0 & 0 & h_{24} & h_{25} \end{bmatrix} \tag{4.13a}$$

and a diagonal matrix $\mathbf{D} = \begin{bmatrix} d_{11} & 0 \\ 0 & d_{22} \end{bmatrix}$ can preserve the structure in $\mathbf{H}$ and $\mathbf{H}_1 = \mathbf{DH}$.

$$\mathbf{H}_1 = \mathbf{DH} = \begin{bmatrix} d_{11}h_{11} & d_{11}h_{12} & d_{11}h_{13} & 0 & 0 \\ 0 & 0 & 0 & d_{22}h_{24} & d_{22}h_{25} \end{bmatrix} \tag{4.13b}$$

and the associated

$$\mathbf{HG}^y = \begin{bmatrix} h_{11}g_{11} + h_{12}g_{21} + h_{13}g_{31} & h_{11}g_{12} + h_{12}g_{22} + h_{13}g_{32} \\ h_{24}g_{41} + h_{25}g_{51} & h_{24}g_{42} + h_{25}g_{52} \end{bmatrix} \tag{4.13c}$$

and

$$\begin{aligned} \mathbf{H}_1\mathbf{G}^y &= \mathbf{DHG}^y \\ &= \begin{bmatrix} d_{11}(h_{11}g_{11} + h_{12}g_{21} + h_{13}g_{31}) & d_{11}(h_{11}g_{12} + h_{12}g_{22} + h_{13}g_{32}) \\ d_{22}(h_{24}g_{41} + h_{25}g_{51}) & d_{22}(h_{24}g_{42} + h_{25}g_{52}) \end{bmatrix} \end{aligned} \tag{4.13d}$$

The non-zero elements in $\mathbf{D}$ are d_{11} and d_{22}. From (4.13d), the non-zero element d_{11} can only be used to match either $vec(\mathbf{HG}^y)|_1$ or $vec(\mathbf{HG}^y)|_3$ and the non-zero element d_{22} can only be used to match either $vec(\mathbf{HG}^y)|_2$ or $vec(\mathbf{HG}^y)|_4$. These would result in mixed integer constraints (4.14b).

Starting from (4.7) and incorporating the element matching constraints with particular structure constraint on $\mathbf{H}$ result in MIQP formulation

$$\min_{\mathbf{H},\boldsymbol{\beta}_\delta} \|\mathbf{HF}\|_F \tag{4.14a}$$

$$\begin{aligned} \text{s.t.} - b(1-\beta_l) \le vec(\mathbf{HG}^y - \mathbf{J}_{uu}^{1/2})|_l \le b(1-\beta_l),\ \forall l = 1, 2, \cdots, n_u n_u \\ n_u \le \sum_{l=1}^{n_u n_u} \beta_l \le n_{nz} \\ n_{u_k} \le \sum_{p=0}^{n_u-1} \sum_{j=\sum_k n_{u_{k-1}}+1}^{\sum_k n_{u_k}} \beta_{n_u p+j} \le n_{nz_k},\ \forall k = 1, 2, \ldots, \text{number of blocks} \end{aligned} \tag{4.14b}$$

$$\mathbf{H} = [\text{particular structure}] \tag{4.14c}$$

where n_{u_k},n_{nz_k} are the number of inputs, number of non-zero elements in $\mathbf{D}$ in block k respectively.

Note that quadratic programming problem that need to be solved at each node in MIQP (4.14) search tree is a convex approximation to (4.9).

The convex approximations arise due to the less degrees of freedom we have available in $\mathbf{D}$ that preserve the particular structure in $\mathbf{H}$ and $\mathbf{H}_1 = \mathbf{DH}$ and causes the sub optimality in (4.14). This convex approximation will give an upper bound for (4.9). The formulation in (4.14) is vectorized (see Appendix A) to result in controlled variables $\mathbf{c}'s$ with particular structure in $\mathbf{H}$ as

$$\min_{\mathbf{h}_\delta, \boldsymbol{\beta}_\delta} \ \mathbf{h}_\delta^T \mathbf{F}_\delta \mathbf{h}_\delta \quad \text{s.t.} \tag{4.15a}$$

$$-b(1-\beta_l) \leq (\mathbf{G}_\delta^{y^T} \mathbf{h}_\delta - \mathbf{j}_\delta)|_l \leq b(1-\beta_l), \ \forall l = 1, 2, \cdots, n_u n_u$$

$$n_u \leq \sum_{l=1}^{n_u n_u} \beta_l \leq n_{nz}$$

$$n_{u_k} \leq \sum_{p=0}^{n_u - 1} \sum_{j=\sum_k n_{u_{k-1}}+1}^{\sum_k n_{u_k}} \beta_{n_u p + j} \leq n_{nz_k}, \ \forall k = 1, 2, \ldots, \text{number of blocks} \tag{4.15b}$$

$$\mathbf{h}_\delta(\text{ind}) = 0, \ \text{ind is for 0 in particular structure } \mathbf{H} \tag{4.15c}$$

where

$$\mathbf{h}_\delta = \begin{bmatrix} h_{11} & \ldots h_{1n_y} & h_{21} & \ldots h_{2n_y} & \ldots h_{n_u 1} & \ldots h_{n_u n_y} \end{bmatrix}^T \in \mathbb{R}^{n_u n_y \times 1}$$

$\boldsymbol{\beta}_\delta = [\beta_1 \quad \beta_2 \quad \ldots \quad \beta_{n_u n_u}]^T$, $\beta_l \in \{0, 1\}$. n_{u_k},n_{nz_k} are the number of inputs, number of non-zero elements in $\mathbf{D}$ in block k respectively. The constraints in (4.15b) are to bound the unmatched elements of $vec(\mathbf{HG}^y)$ between $-b$ and b as the big-m constraints.

4.3.2 Convex approximation method 2: relaxing the equality constraint to $\mathbf{HG}^y \leq \mathbf{J}_{uu}^{1/2}$

In this method, the affine constraint $\mathbf{HG}^y = \mathbf{J}_{uu}^{1/2}$ in $\mathbf{H}$ is relaxed to inequality constraint $\mathbf{HG}^y \leq \mathbf{J}_{uu}^{1/2}$ (element wise), where the degrees of freedom in $\mathbf{D}_u$ are used to make sure that $\mathbf{J}_{uu}^{1/2}$ to contain negative elements in each row. Negative elements in each row are required to obviate the trivial solution. Then the convex approximation to (4.9) can be written as

$$\begin{aligned} &\min_{\mathbf{H}} \|\mathbf{HY}\|_F \\ &\text{s.t. } \mathbf{HG}^y \leq \mathbf{J}_{uu}^{1/2} \\ &\quad \mathbf{H} = [\text{particular structure}] \end{aligned} \tag{4.16}$$

The sub optimality in (4.16) from (4.9) is due to relaxation of equality constraint to inequality constraint. The formulation in (4.16) is vectorized (see Appendix A) to result in a formulation in (4.17).

$$\begin{aligned} &\min_{\mathbf{h}_\delta} \ \mathbf{h}_\delta^T \mathbf{F}_\delta \mathbf{h}_\delta \\ &\text{s.t. } \mathbf{G}_\delta^{y^T} \mathbf{h}_\delta \leq \mathbf{j}_\delta \\ &\mathbf{h}_\delta(\text{ind}) = 0, \ \text{ind is for 0 in particular structure } \mathbf{H} \end{aligned} \tag{4.17}$$

where $\mathbf{h}_\delta \in \mathbb{R}^{n_u n_y \times 1}, \mathbf{j}_\delta \in \mathbb{R}^{n_u n_u \times 1}, \mathbf{G}_\delta^{y^T} \in \mathbb{R}^{n_u n_u \times n_y n_u}, \mathbf{F}_\delta \in \mathbb{R}^{n_u n_y \times n_u n_y}$.

Solving (4.17) results in controlled variables $\mathbf{c}'s$ as combinations of measurements with particular structure in $\mathbf{H}$.

4.3.3 Convex approximation method 3: imposing constraint on $\mathbf{J}_{uu}^{1/2}(\mathbf{H}\mathbf{G}^y)^{-1}$ to have structure of D

In this method, we try to make the matrix $\mathbf{J}_{uu}^{1/2}(\mathbf{H}\mathbf{G}^y)^{-1}$ to have a structure of $\mathbf{D}$ that preserves the structure in $\mathbf{D}\mathbf{H}$. Then the constraint becomes $\mathbf{H}\mathbf{G}^y - \mathbf{D}^{-1}\mathbf{J}_{uu}^{1/2} = 0$. We introduce a new matrix $\mathbf{D}_i = \mathbf{D}^{-1}$ to make a convex approximation as

$$\begin{aligned} &\min_{\mathbf{H},\mathbf{D}_i} \|\mathbf{H}\mathbf{Y}\|_F \\ &\text{s.t. } \mathbf{H}\mathbf{G}^y - \mathbf{D}_i\mathbf{J}_{uu}^{1/2} = 0 \\ &\quad \mathbf{H} = [\text{particular structure}] \end{aligned} \tag{4.18}$$

4.4 MIQP formulations

We consider Problem 4.2, where there are some zero columns in $\mathbf{H}$ and Problem 4.4, structured $\mathbf{H}$ with measurement subsets, where there are specified zero elements and some zero columns in $\mathbf{H}$. In Problems 4.2 and 4.4, we do not want to use all measurements and the mixed integer constraints are formulated using the standard big-m approach used in MIQP formulations (Hooker and Osorio, 1999). The m value should be chosen suitably in these big-m approaches.

4.4.1 Optimal measurement selection (Problem 4.2)

Let us first recall the results from (4.6). The idea is to use quadratic programming formulation in Theorem 7 and add to them additional mixed

integer constraints to deal with the measurement selection. Each measurement is complemented with a binary variable to describe the mixed integer constraints suitably. Let $\boldsymbol{\sigma}_\delta = \begin{bmatrix}\sigma_1 & \sigma_2 & \dots & \sigma_{n_y}\end{bmatrix}^T$, $\sigma_j \in \{0,1\}$, be the n_y binary variables vector. σ_j is used to represent the presence or not of the j^{th} candidate measurement (j^{th} column in $\mathbf{H}$ matrix) of a process plant. $\sigma_j = 0$ implies $h_{ij} = 0$; $\forall i = 1, 2, \dots, n_u$ in $\mathbf{H}$. The chosen measurements j will take $\sigma_j = 1$. The corresponding decision variables $h_{1j}, h_{2j}, \dots, h_{n_u j}$ (i.e. the j^{th} column in combination matrix $\mathbf{H}$) are chosen to have a value between $-m$ to m, these bounds are formulated as big-m constraints. The constraints on the binary variables can be written in the form

$$\mathbf{P}\boldsymbol{\sigma}_\delta = \mathbf{s}$$

and the resulting generalized MIQP problem in the decision variables $\mathbf{h}_\delta$ and $\boldsymbol{\sigma}_\delta$ is

$$\begin{aligned} \min_{\mathbf{h}_\delta, \boldsymbol{\sigma}_\delta} \quad & \mathbf{h}_\delta^T \mathbf{F}_\delta \mathbf{h}_\delta \\ \text{s.t.} \quad & \mathbf{G}_\delta^{\mathrm{y}^{\mathrm{T}}} \mathbf{h}_\delta = \mathbf{j}_\delta \end{aligned} \tag{4.19a}$$

$$\mathbf{P}\boldsymbol{\sigma}_\delta = \mathbf{s}$$

$$\begin{bmatrix} -m \\ -m \\ \vdots \\ -m \end{bmatrix} \sigma_j \leq \begin{bmatrix} h_{1j} \\ h_{2j} \\ \vdots \\ h_{n_u j} \end{bmatrix} \leq \begin{bmatrix} m \\ m \\ \vdots \\ m \end{bmatrix} \sigma_j, \quad \forall j \in 1, 2, \cdots, n_y \tag{4.19b}$$

where $\mathbf{h}_\delta = \begin{bmatrix} h_{11} & \dots & h_{1n_y} & h_{21} & \dots & h_{2n_y} & \dots h_{n_u 1} & \dots & h_{n_u n_y} \end{bmatrix}^T \in \mathbb{R}^{n_u n_y \times 1}$; $\boldsymbol{\sigma}_\delta = \begin{bmatrix}\sigma_1 & \sigma_2 & \dots & \sigma_{n_y}\end{bmatrix}^T$; $\sigma_j \in \{0,1\}$ and $\mathbf{s}$ is the vector with numbers of measurements. The m value should be chosen small to reduce the computational time, but it should be sufficiently large to avoid that it becomes an active constraint. Selecting an appropriate m is an iterative method for a problem and can increase the computational intensiveness of the big-m based MIQP formulations. In such cases, one can use indicator constraints in MIQP problem to set the columns in $\mathbf{H}$ directly to zero, when $\sigma_j = 0$. This can be done by replacing the constraints in (4.19b) with indicator constraints as

$$\text{indicator constraints} : \sigma_j = 0 \implies \begin{bmatrix} h_{1j} \\ h_{2j} \\ \vdots \\ h_{n_u j} \end{bmatrix} = \underline{0}_{n_u \times 1} \quad \forall j \in 1, 2, \cdots, n_y \tag{4.20}$$

where $\underline{0}$ is a column vector of zeros. For MIQP, theoretically, indicator constraint approach (3.28) would be faster than using big-m approach (3.27c). This is because in MIQP, indicator constraint approach (3.28) solves an equality constrained QP at each node, whereas big-m approach (3.27c) solves an inequality constrained QP.
We provide examples on how to formulate $\mathbf{P}\boldsymbol{\sigma}_\delta = \mathbf{s}$. For

$$\mathbf{H} = \begin{bmatrix} 0 & h_{12} & 0 & h_{14} & h_{15} \\ 0 & h_{22} & 0 & h_{24} & h_{25} \end{bmatrix}$$

The resulting constraints can be written with

$$\mathbf{P} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \ \mathbf{s} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

4.4.2 CV as combinations of a fewer measurement subsets with the particular structure (Problem 4.4)

This is the case where we have a structured $\mathbf{H}$ and do not want to use all measurements. This is an extension of Problem 4.3, so here only convex approximation based formulations are studied. The idea is to use quadratic programming with convex approximations (Problem 4.3) and add to it additional mixed integer constraints to deal the measurement selection. To describe these mixed integer constraints suitably, we complement each measurement with a binary variable. Let $\boldsymbol{\sigma}_\delta = \begin{bmatrix}\sigma_1 & \sigma_2 & \dots & \sigma_{n_y}\end{bmatrix}^T$,$\sigma_j \in \{0,1\}$, be the n_y binary variables vector. σ_j is used to represent the presence or not of the j^{th} candidate measurement (j^{th} column in $\mathbf{H}$ matrix) of a process plant. $\sigma_j = 0$ implies $h_{ij} = 0$; $\forall i = 1, 2, \dots, n_u$ in $\mathbf{H}$. This is the case where we do not want to use all measurements and the mixed integer constraints are formulated using the standard big-m approach (Hooker and Osorio, 1999). The m value should be chosen suitably in these big-m approaches.

Convex approximation method 1: Matching the elements in $\mathbf{HG}^y$ to $\mathbf{J}_{uu}^{1/2}$ with measurement subsets

It is easy to extend the problem formulation in (4.9) to find CV as best combinations of a fewer measurements with particular structured $\mathbf{H}$ by adding big-m constraints (4.19b) to (4.14). A few more constraints such as selecting n_k measurements from a block k, where n_{u_k} and n_{y_k} are the number of inputs and measurements in the block k, (i.e. $\sum_k n_{u_k} = n_u$;$\sum_k n_{y_k} = n_y$;$\sum_k n_k = n$), can be formulated by appropriate modification of $\mathbf{P}\boldsymbol{\sigma}_\delta = \mathbf{s}$.

Convex approximation method 2: Relaxing the equality constraint to $\mathbf{HG}^y \leq \mathbf{J}_{uu}^{1/2}$ with measurement subsets

It is easy to extend the problem formulation (4.17) to find CV as best combinations of a fewer measurements with particular structured $\mathbf{H}$ by adding big-m constraints (4.19b) to (4.16). A few more constraints such as selecting n_k measurements from a block k, where n_{u_k} and n_{y_k} are the number of inputs and measurements in the block k, (i.e. $\sum_k n_{u_k} = n_u$; $\sum_k n_{y_k} = n_y$;$\sum_k n_k = n$), can be formulated by appropriate modification of $\mathbf{P}\boldsymbol{\sigma}_\delta = \mathbf{s}$.

4.5 Case studies

4.5.1 Random tests

The main purpose of the random tests is to see how well the proposed methods are performing in finding a local minimum for the non-convex optimization (4.9) (Problem 4.3). We consider a process with 2 inputs, 6 measurements and 3 disturbances to find a block diagonal $\mathbf{H}$.

$$\mathbf{H} = \begin{bmatrix} h_{11} & h_{12} & h_{13} & 0 & 0 & 0 \\ 0 & 0 & 0 & h_{24} & h_{25} & h_{26} \end{bmatrix}$$

For illustration, out of 1000 random cases, we present a typical case with

$$\mathbf{G}^y = \begin{bmatrix} 1.5815 & 0.7408 \\ 0.2926 & -0.8407 \\ -1.1876 & -0.3495 \\ 1.0759 & 0.0296 \\ -1.2974 & 1.9524 \\ -0.1218 & 0.4590 \end{bmatrix}, \mathbf{G}_d^y = \begin{bmatrix} -0.3993 & 0.2406 & 0.6326 \\ -0.2254 & -0.0946 & 1.9033 \\ -0.2803 & 0.7932 & -1.1600 \\ 1.3067 & 0.9594 & -0.3473 \\ -0.2844 & 1.0871 & -1.6951 \\ -0.7917 & 0.6472 & 0.9194 \end{bmatrix},$$

,

$$\mathbf{J}_{uu} = \begin{bmatrix} 7.2120 & -0.9842 \\ -0.9842 & 0.9595 \end{bmatrix}, \mathbf{J}_{ud} = \begin{bmatrix} 1.3803 & 0.7609 & -0.2084 \\ -0.9415 & 0.2379 & 0.0247 \end{bmatrix}$$

$$\mathbf{W}_d = \begin{bmatrix} 0.5074 & 0 & 0 \\ 0 & 0.3662 & 0 \\ 0 & 0 & 0.2266 \end{bmatrix}, \mathbf{W}_n = \begin{bmatrix} 0.0535 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.0290 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.0068 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.0085 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.0068 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.0410 \end{bmatrix}$$

The results for the convex approximation methods 1, 2 and 3 with block diagonal $\mathbf{H}$ are denoted by L_1, L_2 and L_3. The minimum loss with 10 random initial guesses is denoted by L_4. The solutions of convex approximation methods are given as initial guesses to NLP to find the local optimums L_1^*, L_2^* and L_3^*. The best solution of non-convex problem using NLP solver (fmincon in Matlab R2009a) with 10 random initial guesses is denoted by L_4^*. In addition, the best local minimum is denoted by L_{local}^*, which is the minimum of L_1^*, L_2^*, L_3^* and L_4^*. For the typical case all the three methods

Table 4.1: Performance of proposed convex approximation methods on a illustrative random case

Random case	Convex approximation methods			Original non-convex problem
	1	2	3	4 (best of 10 initial guesses)
Original (L_i)	0.1287	0.1313	0.1328	0.8274
After re-optimization (L_i^*)	0.1136	0.1136	0.1136	0.1136

Table 4.2: Performance (% of locating local minimum) of proposed three convex approximation methods on 1000 random cases

Random cases (1000)	Convex approximation methods			Original non-convex problem
	1	2	3	4 (best of 10 initial guesses)
Original (L_i)	54% (5.9215†)	5% (17.3463)	41% (6.5061)	0% (19.5423)
*After re-optimization (L_i^*)	82% (0.1800††)	75% (0.2276)	77% (0.1926)	12 % (0.0172)

*Sum greater than 100% because methods are converging to same local optimum after reoptimization in many cases
$L^*_{local} = min(L_1^*, L_2^*, L_3^*, L_4^*)$
Average absolute deviations from best local minimum $\sum_{i=1}^{N}\left(\frac{L_i - L^*_{local}}{N}\right)$ is shown in the brackets
† 410 random cases are 0.1 magnitude away from best local optimum
†† 900 random cases are 0.1 magnitude away from best local optimum

converge to same local solution (Table 4.1). From Table 4.1, the convex approximation method 1 performs better before re-optimization and gives a solution close to the best local solution.

The analysis is repeated for $N = 1000$ random cases and the results are tabulated (Table 4.2). Later, NLP is solved with the convex approximation methods solution as initial guess (4.9) and the percentages of the absolute deviation from best local minimum L^*_{local} within 0.001 tolerance are reported. The numbers in the brackets are the average absolute deviations, $\sum_{i=1}^{N}\left(\frac{L_i - L^*_{local}}{N}\right)$, of the methods from the best local optimum. From Table 4.2 and based on the average relative deviation the convex approximation method 1 is the best and when not best it is still not "poor". Even though convex approximation method 1 is better, we cannot discard the other two methods as the other two can also locate a local optimum in few cases. Overall, the proposed methods can be used to find reasonable initial guess for the NLP (Problem 4.3) to arrive at better solutions even if the absolute deviation is significantly high.

4.5.2 Evaporator case study

The main purpose of case study is to evaluate the convex approximation based MIQP methods in Section 4.4.2 for particular structured $\mathbf{H}$ (Problem 4.4). We consider the evaporator case study (Newell and Lee, 1989) (Figure 4.3) as modified by (Kariwala et al., 2008). The process has 2 inputs and 10 candidate measurements and 3 disturbances. Candidate measurements $\mathbf{y}$ and inputs $\mathbf{u}$ are

$$\begin{aligned}\mathbf{y} &= [P_2 \quad T_2 \quad T_3 \quad F_2 \quad F_{100} \quad T_{201} \quad F_3 \quad F_5 \quad F_{200} \quad F_1]^T \\ \mathbf{u} &= [F_{200} \quad F_1]^T \\ \mathbf{d} &= [X_1 \quad T_1 \quad T_{200}]^T\end{aligned}$$

Note that inputs $\mathbf{u}$ are also included in measurements $\mathbf{y}$. The economic objective is to maximize the operating profit [\$/h], formulated as minimization of the negative profit (Kariwala et al., 2008).

$$J = 600F_{100} + 0.6F_{200} + 1.009(F_2 + F_3) + 0.2F_1 - 4800F_2 \tag{4.21}$$

The objective in self-optimizing control is to find optimal CV that minimize the loss, $L = J(\mathbf{u}, \mathbf{d}) - J_{opt}(\mathbf{d})$, in the presence of disturbances and implementation errors. The measurements associated to evaporator are $\{T_2, F_2, F_{100}, F_3, F_1\}$ and the measurements associated to the condenser and separator units are $\{P_2, T_3, T_{201}, F_5, F_{200}\}$. For the case studies $\mathbf{M} = \mathbf{J}_{uu}^{1/2}(\mathbf{H}\mathbf{G}^y)^{-1}\mathbf{H}\mathbf{Y}$ and loss is evaluated as $L = \frac{1}{2}\|\mathbf{M}\|_F^2$. The matrices required for (4.6) are (Kariwala et al., 2008)

$$\mathbf{G}^y = \begin{bmatrix} -0.0930 & 11.6780 \\ -0.0520 & 6.5590 \\ -0.0470 & 5.9210 \\ 0 & 0.1410 \\ -0.0010 & 1.1150 \\ -0.0940 & 2.1700 \\ -0.0320 & 6.5940 \\ 0 & 0.8590 \\ 1.0000 & 0 \\ 0 & 1.0000 \end{bmatrix}, \mathbf{G}_d^y = \begin{bmatrix} -3.6260 & 0 & 1.9720 \\ -2.0360 & 0 & 1.1080 \\ -1.8380 & 0 & 1.0000 \\ 0.2670 & 0 & 0 \\ -0.3170 & -0.0180 & 0.0200 \\ -0.6740 & 0 & 1.0000 \\ -2.2530 & -0.0660 & 0.6730 \\ -0.2670 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

,

$$\mathbf{J}_{uu} = \begin{bmatrix} 0.0060 & -0.1330 \\ -0.1330 & 16.7370 \end{bmatrix}, \mathbf{J}_{ud} = \begin{bmatrix} 0.0230 & 0 & -0.0010 \\ -158.3730 & -1.1610 & 1.4840 \end{bmatrix}, \mathbf{W}_d = \begin{bmatrix} 0.25 & 0 & 0 \\ 0 & 8 & 0 \\ 0 & 0 & 5 \end{bmatrix}$$

$$\mathbf{W}_n = \begin{bmatrix} 1.285 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.0270 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.1890 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.4940 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.1630 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4.3550 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.1890 \end{bmatrix}$$

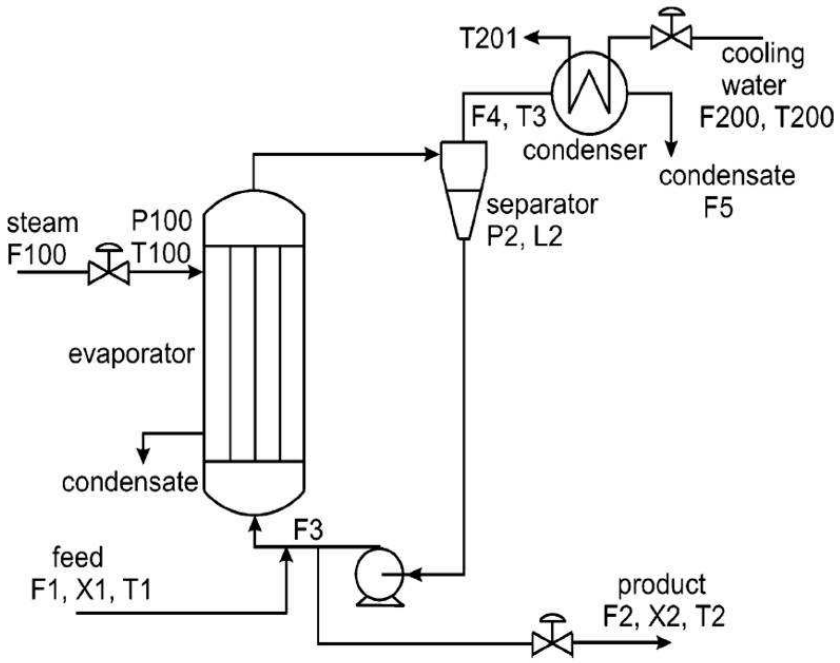

Figure 4.3: The evaporator system

Table 4.3: Comparison of proposed methods with the methods of Heldt (2010)

No. Meas	Disjoint meas. sets	Structure			
		$\mathbf{c}'s$ from Convex approximation methods			$\mathbf{c}'s$ from (Heldt, 2010)
		1	2	3	
4	$\{F_2 \quad F_{100}\}, \{F_{200} \; F_1\}$	$c_1 = -6.259F_2 + F100$ $c_2 = F_{200} - 21.723F_1$	$c_1 = -6.259F_2 + F100$ $c_2 = F_{200} - 21.723F_1$	$c_1 = -7.904F_2 + F100$ $c_2 = F_{200} - 128.004F_1$	$c_1 = -6.27F_2 + F100$ $c_2 = F_{200} - 23.3F_1$
	Loss $\frac{1}{2}\|\mathbf{M}\|_F^2$	11.864	11.864	1458.176	11.907
4	$\{F_3\}, \{T_2 \quad T_3 \quad T_{201}\}$	$c_1 = F_3$ $c_2 = T_2 + 0.894T_3 - 1.313T_{201}$	$c_1 = F_3$ $c_2 = T_2 + 0.894T_3 - 1.313T_{201}$	$c_1 = NaN$ $c_2 = NaN$	$c_1 = F_3$ $c_2 = 0.36T_2 + 0.33T_3 + 0.87T_{201}$
	Loss $\frac{1}{2}\|\mathbf{M}\|_F^2$	60.367	60.367	NaN	62.378

NaN - not a number;

We benchmark/compare the performance of the proposed convex approximation methods with the results reported in (Heldt, 2010) for the reported block diagonal $\mathbf{H}$ structures for this evaporator case study (Table 4.3). From Table 4.3, it can be seen the proposed convex approximation methods 1 and 2 are comparable to the methods reported (Heldt, 2010). For the solution of method 3, the $\mathbf{HG}^y$ matrix does not have a full rank and results in NaN (Not a Number).

We study Problems 4.2 and 4.4 to find $\mathbf{c}'s$ as combinations of

(i) Best subset of measurements (Problem 4.2): An MIQP is set up for Problem 4.2 for this evaporator case study (4.19) with structural constraints to select measurements from different process units. The structural constraints are to select n measurements, $\lfloor n/2 \rfloor$ number of measurements should be selected from the evaporator measurements and the rest of the measurements should be selected from the condenser and separator units measurements. This is the full $\mathbf{H}$ case with the following structural constraints. For illustration

   (a) to select 2 measurements, $\lfloor n/2 \rfloor = 1$ measurement is from the evaporator measurement set and other measurement is from the condenser and separator measurement set.

   (b) to select 5 measurements, $\lfloor n/2 \rfloor = 2$ measurements are from the evaporator measurement set and other 3 measurements are from the condenser and separator measurement set.

   The IBM ILOG Optimizer CPLEX solver is used to solve the MIQP problem (4.19) to find the CV with $m = 200$. The minimized loss as a function of number of measurements used between 2 and 10 is plotted in Figure 4.4.

(ii) Disjoint measurement sets with a fewer measurements (Problem 4.4): For this evaporator case study, two disjoint measurement subsets are

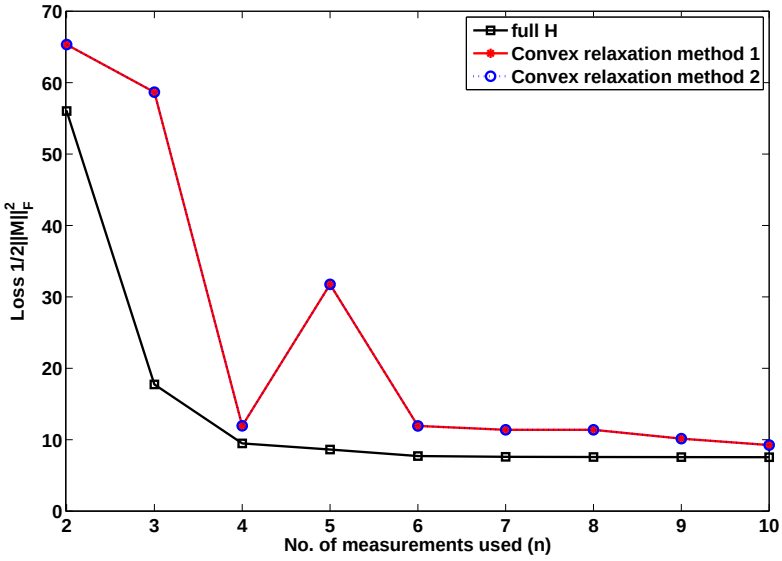

Figure 4.4: Evaporator case study: loss vs the number of included measurements (n) for (i) full **H**, (ii) block diagonal **H** with convex approximation method 1, (iii) block diagonal **H** with convex approximation method 2

evaporator measurements $\{T_2, F_2, F_{100}, F_3, F_1\}$, condenser and separator units measurements $\{P_2, T_3, T_{201}, F_5, F_{200}\}$. This is block diagonal $\mathbf{H}$ (4.4) with c_1 as combination of measurements in the evaporator unit and c_2 as combination of measurements in the condenser and separator units and is desirable mainly for dynamic reasons. The block diagonal $\mathbf{H}$ for this case is

$$\mathbf{H} = \begin{bmatrix} 0 & h_{12} & 0 & h_{14} & h_{15} & 0 & h_{17} & 0 & 0 & h_{110} \\ h_{21} & 0 & h_{23} & 0 & 0 & h_{26} & 0 & h_{28} & h_{29} & 0 \end{bmatrix}$$

In addition to the disjoint measurement sets constraints, the following structural constraints are also incorporated. To select n number of measurements, $\lfloor n/2 \rfloor$ number of measurements should be selected from the evaporator measurements and the rest of the measurements should be selected from the condenser and separator units measurements; for illustration

(a) to select 2 measurements, $\lfloor n/2 \rfloor = 1$ measurement is from evaporator measurement set and other 1 measurement is from condenser and separator measurement set.

(b) to select 5 measurements, $\lfloor n/2 \rfloor = 2$ measurements are from the evaporator measurement set and other 3 measurements are from the condenser and separator measurement set.

The convex approximation methods 1 and 2 are formulated for Problem 4.4 with block diagonal $\mathbf{H}$ and the above structural constraints with $m = 200, b = 100$ in big-m constraints as described in Section 4.4.2. IBM ILOG Optimizer CPLEX solver is used for MIQP solution. The minimized loss with the number of measurements used between 2 and 10 are plotted in Figure 4.4. From the Figure 4.4, it can be seen that the loss with the convex approximation methods 1 and 2 for block diagonal $\mathbf{H}$ for subset size 6 and above are closer to full $\mathbf{H}$ than for the subset size from 2 to 5. Note that the convex approximation methods 1 and 2 give exactly the same results for this evaporator case study, but this may not be true for all the problems. From the Figure 4.4, the loss $\|\mathbf{J}_{uu}^{1/2}(\mathbf{H}\mathbf{G}^y)^{-1}(\mathbf{H}\mathbf{Y})||_F$ behaves irregularly, that is for $n = 5$ loss is higher than for $n = 4$. This is because we are minimizing the convex formulation in (4.16) and the $\|\mathbf{H}\mathbf{Y}\|_F$ is smaller for $n = 5$ than $n = 4$ but the loss is higher. The optimal controlled variables for full $\mathbf{H}$ and block diagonal $\mathbf{H}$ with convex approximation methods 1 and 2 with their associated loss and computational times to solve MIQP using Windows XP SP2 notebook with Intel ®Core$^{\text{TM}}$ Duo Processor T7250 (2.00

Table 4.4: Evaporator case study: the optimal measurements $\mathbf{c}'s$ with their associated losses and computational times

Meas		Structure		
		Full $\mathbf{H}$	Block diagonal $\mathbf{H}$	
			Convex approximation method 1	Convex approximation method 2
2	CV	$c_1 = F_3$ $c_2 = F_{200}$	$c_1 = T_2$ $c_2 = T_{201}$	$c_1 = T_2$ $c_2 = T_{201}$
	Loss $\frac{1}{2}\|\mathbf{M}\|_F^2$	56.026	65.324^*	65.324^*
	CPU time	0.015	0.013	0.009
3	CV	$c_1 = F_2 - 0.007F_{200}$ $c_2 = F_5 - 0.037F_{200}$	$c_1 = T_2$ $c_2 = F_5 - 0.038F_{200}$	$c_1 = T_2$ $c_2 = F_5 - 0.038F_{200}$
	Loss $\frac{1}{2}\|\mathbf{M}\|_F^2$	17.737	58.655^{**}	58.655^{**}
	CPU time	0.014	0.018	0.014
4	CV	$c_1 = F_2 - 0.001F_3 - 0.007F_{200}$ $c_2 = T_{201} - 1.8F_3 + 0.457F_{200}$	$c_1 = -6.259F_2 + F_{100}$ $c_2 = F_5 - 0.039F_{200}$	$c_1 = -6.259F_2 + F_{100}$ $c_2 = F_5 - 0.039F_{200}$
	Loss $\frac{1}{2}\|\mathbf{M}\|_F^2$	9.481	11.935^{**}	11.935^{**}
	CPU time	0.086	0.096	0.062
5	CV	$c_1 = F_2 + 0.0005F_3 + 0.105F_5 - 0.012F_{200}$ $c_2 = T_{201} - 2.046F_3 - 13.275F_5 + 1.028F_{200}$	$c_1 = P_2 + 117.795F_5 - 4.945F_{200}$ $c_2 = F_2 - 0.032F_3$	$c_1 = P_2 + 117.795F_5 - 4.945F_{200}$ $c_2 = F_2 - 0.032F_3$
	Loss $\frac{1}{2}\|\mathbf{M}\|_F^2$	8.615	31.748^{**}	31.748^{**}
	CPU time	0.028	0.068	0.036
10	CV	$c_1 = f(\mathbf{y})$ $c_2 = f(\mathbf{y})$	$c_1 = f(\mathbf{y})$ $c_2 = f(\mathbf{y})$	$c_1 = f(\mathbf{y})$ $c_2 = f(\mathbf{y})$
	Loss $\frac{1}{2}\|\mathbf{M}\|_F^2$	7.550	9.245^{**}	9.245^{**}
	CPU time	0.001	0.008	0.001

$*$ clearly not optimal because with n_u measurements, all structures of $\mathbf{H}$ must give same solution

$**$ are the convex approximations solutions to structured $\mathbf{H}$

GHz, 2M Cache, 800 MHz FSB) using MATLAB ®R2009a are tabulated in Table 4.4. In conclusion, for the evaporator case study, the proposed convex approximation based MIQP methods give reasonably good upper bounds for CV with block diagonal $\mathbf{H}$ structure.

4.5.3 Distillation case study

This case study is included to apply the methods of finding structured $\mathbf{H}$ with fewer measurements (Section 4.4.2) on a case with large number of measurements. We considered particular structures as block diagonal $\mathbf{H}$ (4.4) and triangular $\mathbf{H}$ (4.5). We consider indirect composition control of a binary distillation column case study with 41 stages (Skogestad, 1997; Hori and Skogestad, 2008) and reflux (L) and boil up (V) as the remaining unconstrained steady state degrees of freedom ($\mathbf{u}$). Stage numbers are counted from bottom to top. The main disturbances are in feed flow rate (F), feed composition (z_F) and vapor fraction (q_F), which can vary between $1 \pm 0.2, 0.5 \pm 0.1$ and 1 ± 0.1, respectively. As online composition measurements are assumed unavailable, we use stage temperatures inside the column to control the compositions indirectly (Hori and Skogestad, 2008). The boiling points difference between light key component (L) and heavy key component (H) is 10 ^oC. Then temperature T_i (^oC) on each stage i is

calculated as a simple linear function of the liquid composition x_i on each stage (Skogestad, 1997).

$$T_i = 0x_i + 10(1 - x_i) \tag{4.22}$$

The candidate measurements are the 41 stage temperatures that are measured with an accuracy of $\pm 0.5^oC$. Note that we do *not* include the inputs (flows L and V) in the candidate measurements for this case study. The cost function J for the indirect composition control problem is

$$J = \left(\frac{x^H_{top} - x^H_{top,s}}{x^H_{top,s}} \right)^2 + \left(\frac{x^L_{btm} - x^L_{btm,s}}{x^L_{btm,s}} \right)^2 \tag{4.23}$$

where J is the relative steady state composition deviation and x^H_{top}, x^L_{btm} denote the heavy key component (H) composition in top product, light key component (L) composition in bottom product. The specification or set point value is denoted with subscript 's'.

MIQP problems for Problem 4.2 (4.19) and convex approximations methods (Section 4.4.2) for Problem 4.4 for block diagonal $\mathbf{H}$ and triangular $\mathbf{H}$ as particular structures are formulated as described in Section 4.4. For this case study, $m = 2,\ b = 100$ are used for the big-m constraints.

Measurements selection problems (Problem 4.2)

The optimal measurements selection (4.19) problem is formulated with additional structural constraints. The additional constraints are to select n number of measurements, $\lfloor n/2 \rfloor$ number of measurements from top part {21 to 41} and rest of the measurements from any stages {1 to 20}; for illustration

(i) to select 2 measurements, $\lfloor n/2 \rfloor = 1$ should be selected from top part and the other from bottom part of the column

(ii) to select 9 measurements, $\lfloor n/2 \rfloor = 4$ should be selected from top part and the rest from bottom part of the column

The formulated MIQP problem is solved on Windows XP SP2 notebook with Intel ®Core^{TM} Duo Processor T7250 (2.00 GHz, 2M Cache, 800 MHz FSB) using MATLAB ®R2009a using IBM ILOG Optimizer CPLEX solver to find 2 CV as the optimal subset combinations of 2 to 41 stage temperatures. The minimized loss as a function of the number of used measurements (n) is shown in both Figure 4.6 and Figure 4.8.

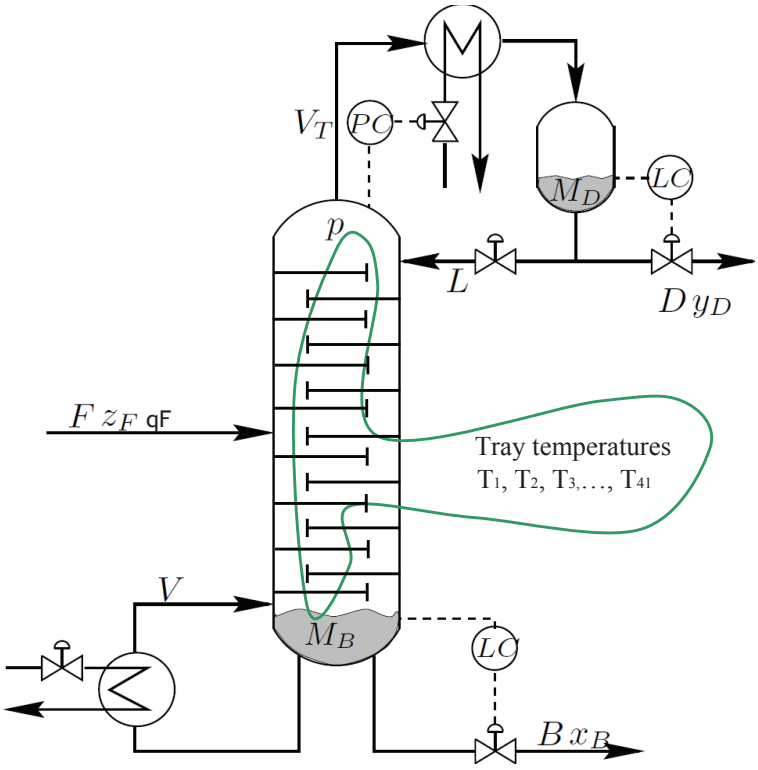

Figure 4.5: Distillation column using LV-configuration

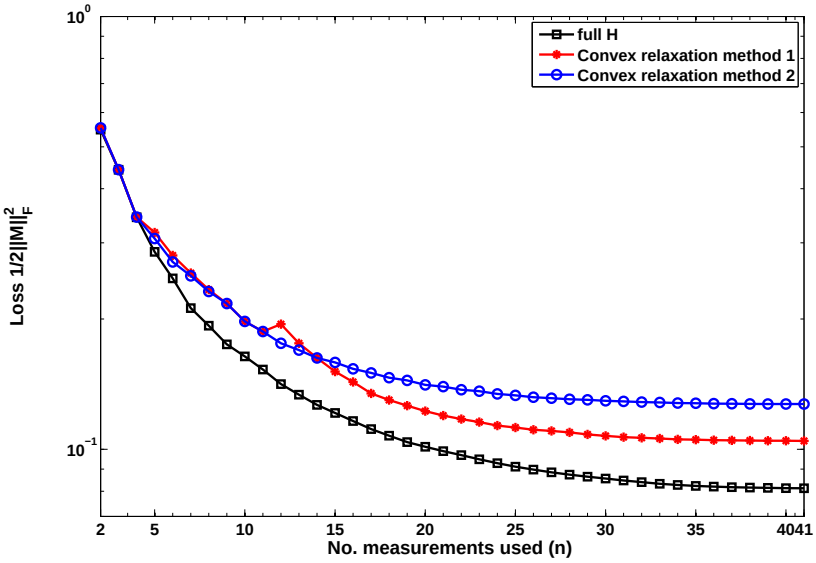

Figure 4.6: The loss vs. the number of included measurements (n) for (i) full **H**, (ii) block diagonal **H** with convex approximation method 1, (iii) block diagonal **H** with convex approximation method 2

.

The optimal controlled variables (measurement combination matrix **H**) for full **H** with 2, 3, 4 and 41 measurements are shown in Table 4.5. For the case with 2 measurements, we just give the measurements, and not the combination, because we can always choose the **D** matrix to make $\mathbf{H} = \mathbf{I}$ (identity). For the case with 3 and 4 measurements, we use the degrees of freedom in **D** to make selected elements in **H** equal to 1.

Block diagonal H

The block diagonal **H** (4.4) structure is desirable mainly for dynamic reasons. In this structure one combined measurement c_1 is selected from the top section (stages 21 to 41) and one combined measurement c_2 is selected from the bottom section (stages 1 to 20). In addition structural constraints such as, to select n number of measurements, $\lfloor n/2 \rfloor$ number of measurements from top stages {21 to 41} and rest of the measurements from bottom stages {1 to 20} are included; for illustration

(i) to select 2 measurements, $\lfloor n/2 \rfloor = 1$ should be selected from top part

Table 4.5: Distillation case study: the self optimizing variables **c** as (i) full **H** (ii) triangular **H** (iii) block diagonal **H** with their associated losses

Meas		Structure				
		Full **H**	Triangular **H**		Block diagonal **H**	
			Convex approximation method 1	Convex approximation method 2	Convex approximation method 1	Convex approximation method 2
2	CV	$c_1 = T_{12}$ $c_2 = T_{26}$	$c_1 = T_{12}$ $c_2 = T_{26}$	$c_1 = T_{12}$ $c_2 = T_{26}$	$c_1 = T_{12}$ $c_2 = T_{26}$	$c_1 = T_{12}$ $c_2 = T_{26}$
	Loss $\blacktriangleright$[M]$\square$	0.548	0.548	0.548	0.553*	0.553*
3	CV	$c_1 = -0.0397T_{12} + 0.6449T_{26} + 0.6572T_{31}$ $c_2 = -1.2508T_{12} + 0.2051T_{26} + 0.1537T_{31}$	$c_1 = T_{26} + 0.9898T_{31}$ $c_2 = T_{11} + 0.7365T_{26} + 0.7812T_{31}$	$c_1 = T_{26} + 0.9887T_{31}$ $c_2 = T_{11} + 0.7365T_{26} + 0.7812T_{31}$	$c_1 = 0.637_{26} + 0.6229T_{31}$ $c_2 = 0.9675T_{12}$	$c_1 = 0.637_{26} + 0.6229T_{31}$ $c_2 = 0.9675T_{12}$
	Loss $\blacktriangleright$[M]$\square$	0.443	0.464**	0.464**	0.443*	0.443*
4	CV	$c_1 = 0.017T_{11} - 0.4607T_{12} + 0.6450T_{26} + 0.6574T_{31}$ $c_2 = -0.6576T_{11} - 0.6548T_{12} + 0.2011T_{26} + 0.1413T_{31}$	$c_1 = 0.6301T_{26} + 0.6237T_{31}$ $c_2 = -0.3463T_{10} - 0.3484T_{11} - 0.2390T_{26} - 0.2680T_{31}$	$c_1 = 0.6306T_{26} + 0.6229T_{31}$ $c_2 = -0.3463T_{26} - 0.3484T_{11} - 0.2390T_{26} - 0.2680T_{31}$	$c_1 = 0.637_{26} + 0.6229T_{31}$ $c_2 = -0.5151T_{11} - 0.5110T_{12}$	$c_1 = 0.637_{26} + 0.6229T_{31}$ $c_2 = -0.5151T_{11} - 0.5110T_{12}$
	Loss $\blacktriangleright$[M]$\square$	0.344	0.353*†	0.353*†	0.344†	0.344†
41	CV	$c_1 = f(T_1, T_2, \ldots, T_{31})$ $c_2 = f(T_1, T_2, \ldots, T_{31})$	$c_1 = f(T_{31}, T_2, \ldots, T_{31})$ $c_2 = f(T_1, T_2, \ldots, T_{31})$	$c_1 = f(T_{31}, T_{26}, \ldots, T_{31})$ $c_2 = f(T_1, T_2, \ldots, T_{31})$	$c_1 = f(T_{31}, T_{26}, \ldots, T_{31})$ $c_2 = f(T_1, T_2, \ldots, T_{39})$	$c_1 = f(T_{31}, T_{26}, \ldots, T_{31})$ $c_2 = f(T_1, T_2, \ldots, T_{39})$
	Loss $\blacktriangleright$[M]$\square$	0.081	0.0941	0.1411	0.105†	0.127†

$*$ clearly not optimal because with n_u measurements all structures of **H** must give same solution

$**$ clearly not optimal because optimal solution with triangular **H** is at least as good as block diagonal **H**

† Small differences in the optimal solution in convex approximation methods 1 and 2 for triangular **H** and block diagonal **H**

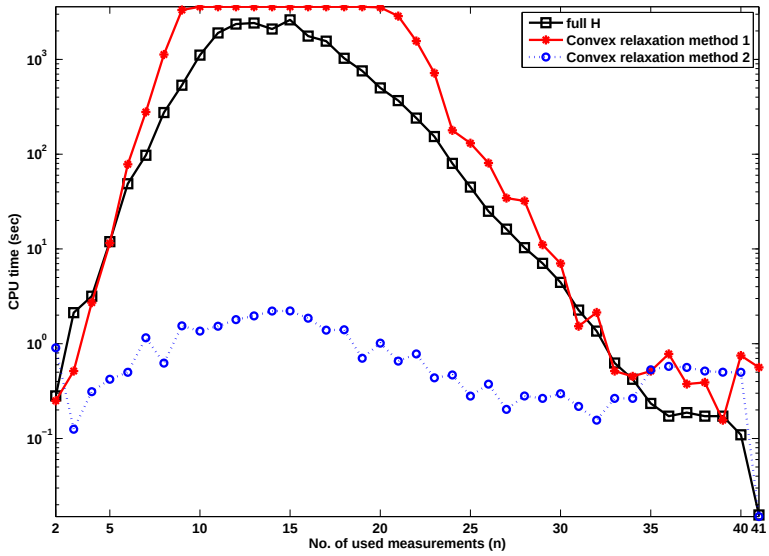

Figure 4.7: Distillation column case study: CPU time requirement for computations for (i) full **H**, (ii) block diagonal **H** with convex approximation method 1, (iii) block diagonal **H** with convex approximation method 2 in Figure 4.6

.

and the other from bottom part of the column

(ii) to select 9 measurements, $\lfloor n/2 \rfloor = 4$ should be selected from top part and the rest from bottom part of the column

The minimized loss associated to disjoint $\mathbf{H}$ (4.4) and structural constraints with the number of included measurements (n) is shown in Figure 4.6. To highlight the small differences in the solutions obtained in convex approximation methods 1 and 2, semi log plot is used. The loss in terms of the relative composition deviation (4.23), decreases as the number of included measurements increases from 2 to 41. From Figure 4.6, we see that the losses with the particular structures are very close to the loss with $\mathbf{c}'s$ as combinations of all the included measurements. For each number of measurements, the actual measurements set is obtained as part of the MIQP solution.

The optimal controlled variables for $n = 2, 3, 4$ and 41 measurements are shown in Table 4.5. For the case with 2 measurements, we just give the measurements, and not the combination, because we can always choose the $\mathbf{D}$ matrix to make $\mathbf{H} = \mathbf{I}$ (identity). For the case with 3 and 4 measurements, we use the degrees of freedom in $\mathbf{D}$ to make selected elements in $\mathbf{H}$ equal to 1.

The computational time required to solve the MIQP using a Windows XP SP2 notebook with Intel ®Core^{TM} Duo Processor T7250 (2.00 GHz, 2M Cache, 800 MHz FSB) using MATLAB ®R2009a to find the optimal $\mathbf{H}$ with full, decentralized (4.4) in convex approximation methods 1 and 2 for each subset size are plotted in in Figure 4.7. The computational time taken for block diagonal $\mathbf{H}$ (4.4) with convex approximation method 2 is 2.5 and 2.6 orders of magnitude faster than full $\mathbf{H}$ and convex approximation method 1, respectively.

Triangular H

The triangular $\mathbf{H}$ (4.5) is to obtain CV, where c_1 is selected from top stages temperatures and c_2 is selected from all stages temperatures. Triangular $\mathbf{H}$ is dynamically desirable to avoid the large time delays between c_1 and L that can arise by including the bottom tray temperatures in c_1. In addition to the triangular $\mathbf{H}$ structure, the following structural constraints are also incorporated. To select n number of measurements, $\lfloor n/2 \rfloor$ number of measurements from top stages {21 to 41} and rest of the measurements from any stages {1 to 41}; for illustration

(i) to select 2 measurements, $\lfloor n/2 \rfloor = 1$ should be selected from top part and the other from any part of the column

(ii) to select 9 measurements, $\lfloor n/2 \rfloor = 4$ should be selected from top part and the rest from any part of the column

The minimized loss associated to triangular **H** (4.5) by including the structural constraints with number of measurements (n) included is shown in Figure 4.8. Figure 4.8 show that the minimized loss in terms of the relative composition deviation (4.23) decreases as the number of included measurements increases from 2 to 41. For each number of measurements, the actual measurements set is determined as part of the MIQP solution. Semi log plot is used to highlight the small differences in the solutions obtained in convex approximation methods 1 and 2. The loss decreases as the number of measurements increases from 2 to 41. The loss with triangular **H** for $n = 5$ is higher than for $n = 4$. The reason is that we are only minimizing the convex formulation (4.16) for the triangular **H** structure and at the optimal solution, $\|\mathbf{HY}\|_F^2$ is smaller for triangular **H** for $n = 5$ than $n = 4$ but the original loss $\|\mathbf{J}_{uu}^{1/2}(\mathbf{HG}^y)^{-1}\mathbf{HY}\|_F^2$ is higher for $n = 5$ than $n = 4$. From Figure 4.8, we see that the losses with the triangular **H** in both convex approximation methods 1 and 2 are very close to the loss with full **H**.

The actual optimal controlled variables (measurement combination **H**) for the cases with 2, 3, 4 and 41 measurements for both convex approximation methods 1 and 2 for triangular **H** are also reported (Table 4.5). For the case with 2 measurements, we just give the measurement, and not the combination, because we can always choose the **D** matrix to make $\mathbf{H} = \mathbf{I}$ (identity). For the case with 3 and 4 measurements, we use the degrees of freedom in **D** to make selected elements in **H** equal to 1.

The computational time required to solve MIQP using Windows XP SP2 notebook with Intel ®Core$^{\text{TM}}$ Duo Processor T7250 (2.00 GHz, 2M Cache, 800 MHz FSB) using MATLAB ®R2009a in finding full **H**, triangular **H** (4.5) with convex approximation methods 1 and 2 are shown in Figure 4.9. The computational times are almost equivalent for full **H**, triangular **H** in convex approximation methods 1 and 2.

For the case with best n_u independent measurements all the structures should give same optimal set. The proposed methods for full **H** and triangular **H** in (4.16) gave optimal measurement set $\{T_{12}, T_{30}\}$, but for block diagonal **H** (4.4) the optimal measurement set $\{T_{12}, T_{29}\}$ found is not optimal. The reason for this is the sub optimality of the proposed convex approximation methods. The loss with particular structure as triangular **H** should at least be as good as block diagonal **H**, but in Table 4.5 the loss with

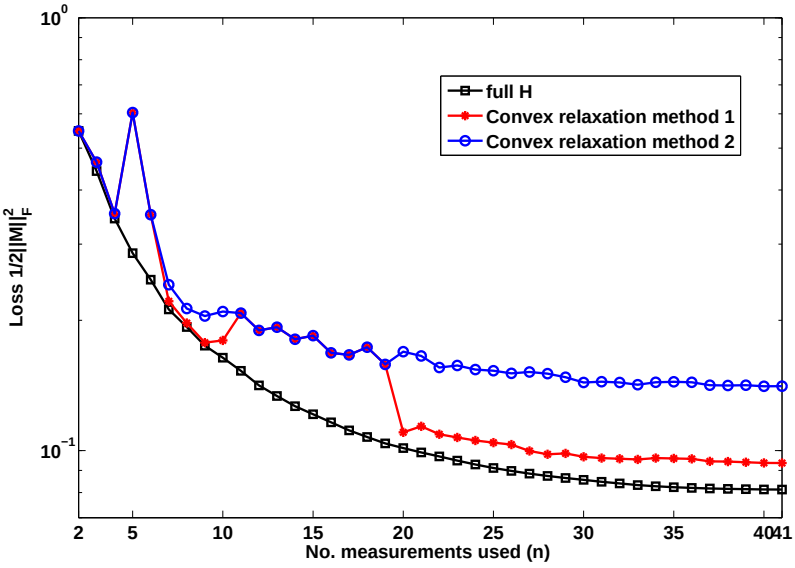

Figure 4.8: The loss vs. the number of included measurements (n) for (i) full **H**, (ii) triangular **H** with convex approximation method 1, (iii) triangular **H** with convex approximation method 2

.

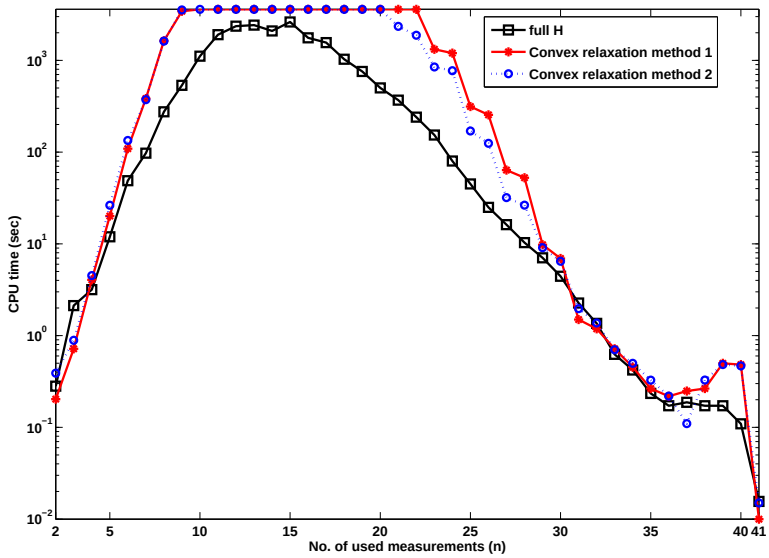

Figure 4.9: Distillation column case study: CPU time requirement for computations for (i) full **H**, (ii) triangular **H** with convex approximation method 1, (iii) triangular **H** with convex approximation method 2 in Figure 4.8

.

triangular **H** is higher than block diagonal **H** case. The reason is that we are only minimizing the convex formulation (4.16) for the given **H** structure and at the optimal solution, $\|\mathbf{HY}\|_F^2$ is smaller for triangular **H** than block diagonal **H**, but when we evaluate the original loss $\|\mathbf{J}_{uu}^{1/2}(\mathbf{HG}^y)^{-1}\mathbf{HY}\|_F^2$ the block diagonal **H** has smaller loss.

Interestingly, for the measurement subset size 3 and 4, the optimal measurement sets are same for both full **H** and block diagonal **H** cases in both convex approximation methods 1 and 2 (Table 4.5). However, since we are restricted in how we can combine measurements in the decentralized case, there is a small difference in the associated losses. In conclusion convex approximation methods for structured **H** problems are observed to give practically acceptable upper bounds for distillation column case study.

We include open loop transient response for a step change to highlight the advantages of controllability and dynamics for decentralized **H** over full **H**. The response with controlled variables as combination of 3 temperature measurements for a step change of +5% in V for full **H** ($c_1 = -0.0369T_{12} + 0.6449T_{30} + 0.6572T_{31}$, $c_2 = -1.2500T_{12} + 0.2051T_{30} + 0.1537T_{31}$) and decentralized **H** ($c_1 = 0.63T_{30} + 0.6229T_{31}$, $c_2 = 0.9675T_{12}$) are shown in Figure 4.10 and 4.11. For full **H**, the transient response may have lead-lag behavior as seen for c_2 in Figure 4.10, which may be difficult to control. For a change in V, the lead-lag behavior in c_2 occur as the measurements of bottom section with faster dynamics are combined with measurements of top section with slower dynamics. For decentralized **H**, the lead-lag behavior may be eliminated as seen in Figure 4.11 as we combine measurements from only one section and the decentralized **H** may inherit better controllability and dynamic properties.

4.6 Conclusions

The optimal CV selection in self-optimizing control, $\mathbf{c} = \mathbf{Hy}$, as measurement combinations that minimize the loss from the optimal operation is given. For ease of implementation and better dynamic controllability, we included particular structures in **H** in self-optimizing control and these form non-convex problems. We presented a few new ideas and two convex approximation methods for structured **H** problems in self-optimizing control to find practically significant upper bounds. The proposed convex approximation methods are extended to find optimal fewer measurements with MIQP formulations. Both of the proposed convex approximation methods are observed to provide reasonably good upper bounds for the true optimal solution in the considered block diagonal **H** and triangular **H** structures for

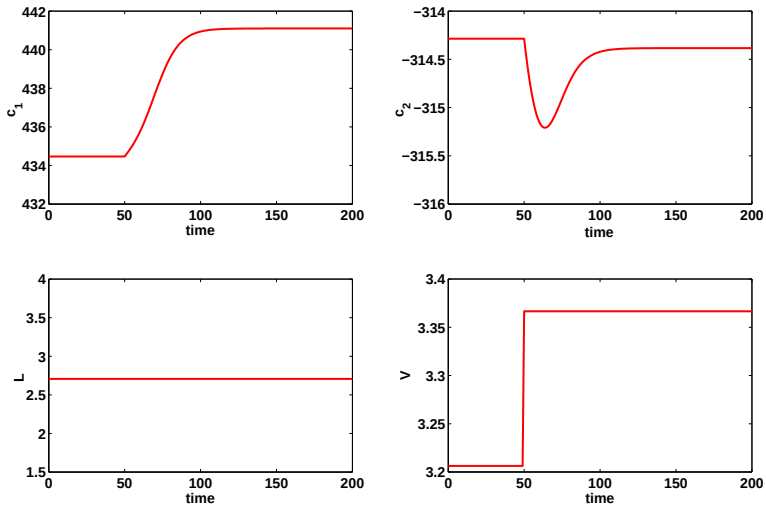

Figure 4.10: Transient response with +5% step change in V for $c_1 = -0.0369T_{12}+0.6449T_{30}+0.6572T_{31}$, $c_2 = -1.2500T_{12}+0.2051T_{30}+0.1537T_{31}$ as combination of 3 temperature measurements with full **H**

.

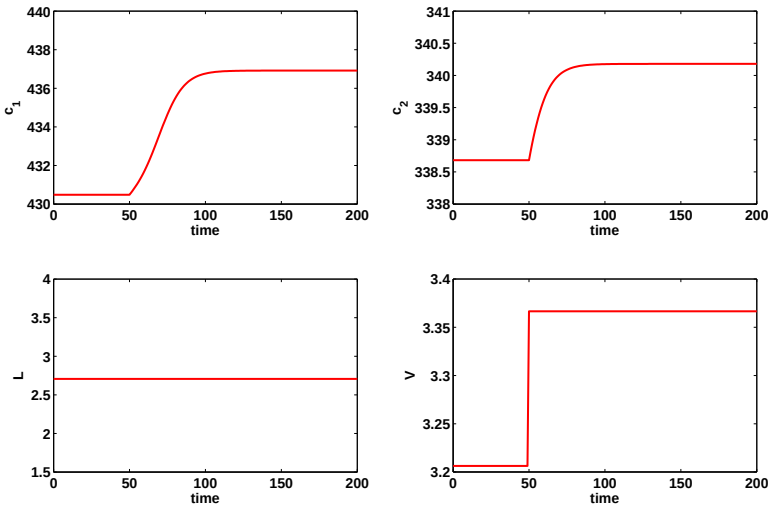

Figure 4.11: Transient response with +5% step change in V for $c_1 = 0.63T_{30} + 0.6229T_{31}$, $c_2 = 0.9675T_{12}$ as combination of 3 temperature measurements with decentralized **H**

.

evaporator and distillation column case studies.

Bibliography

Alstad, V., Skogestad, S., Hori, E., 2009. Optimal measurement combinations as controlled variables. Journal of Process Control 19 (1), 138–148.

Ariyur, K. B., Krstic, M., 2003. Real-Time Optimization by Extremum-Seeking Control. Wiley-Interscience.

Engell, S., 2007. Feedback control for optimal process operation. Journal of Process Control 17 (3), 203 – 219, special Issue ADCHEM 2006 Symposium.

Forbes, J. F., Marlin, T. E., 1996. Design cost: A systematic approach to technology selection for model-based real-time optimization systems. Computers & Chemical Engineering 20 (6-7), 717 – 734, fifth International Symposium on Process Systems Engineering.

Foss, A., 1973. Critique of chemical process control theory. AIChE Journal 19, 209–214.

Guay, M., Zhang, T., 2003. Adaptive extremum seeking control of nonlinear dynamic systems with parametric uncertainties. Automatica 39 (7), 1283 – 1293.

Halvorsen, I. J., Skogestad, S., Morud, J. C., Alstad, V., 2003. Optimal selection of controlled variables. Ind. Eng. Chem. Res. 42.

Heldt, S., 2010. Dealing with structural constraints in self-optimizing control engineering. Journal of Process Control 20 (9), 1049 – 1058.

Hooker, J. N., Osorio, M. A., October 1999. Mixed logical-linear programming. Discrete Appl. Math. 96-97, 395–442.

Hori, E. S., Skogestad, S., 2008. Selection of controlled variables: Maximum gain rule and combination of measurements. Industrial & Engineering Chemistry Research 47 (23), 9465–9471.

Kadam, J. V., Marquardt, W., Srinivasan, B., Bonvin, D., 2007. Optimal grade transition in industrial polymerization processes via NCO tracking. AIChE Journal 53 (3), 627–639.

Kariwala, V., Cao, Y., 2009. Bidirectional branch and bound for controlled vaiable selection. Part II: Exact local method for self-optimizing control. Computers and Chemical Engineering 33, 1402–1414.

Kariwala, V., Cao, Y., 2010. Bidirectional branch and bound for controlled vaiable selection. Part III: Local average loss minimization. IEEE Transactions on Industrial Informatics 6, 54–61.

Kariwala, V., Cao, Y., Janardhanan, S., 2008. Local self-optimizing control with average loss minimization. Ind. Eng. Chem. Res. 47, 1150–1158.

Kassidas, A., Patry, J., Marlin, T., 2000. Integrating process and controller models for the design of self-optimizing control. Computers & Chemical Engineering 24 (12), 2589 – 2602.

Larsson, T., Skogestad, S., 2000. Plantwide control - A review and a new design procedure. Modeling, Identification and Control 21 (4), 209–240.

Morari, M., Stephanopoulos, G., Arkun, Y., 1980. Studies in the synthesis of control structures for chemical processes. Part I: formulation of the problem. process decomposition and the classification of the control task. analysis of the optimizing control structures. AIChE Journal 26 (2), 220–232.

Newell, R. B., Lee, P., 1989. Applied process control : A case study. Prentice-Hall of Australia, New York ; Sydney.

Skogestad, S., 1997. Dynamics and control of distillation columns: A tutorial introduction. Chemical Engineering Research and Design 75 (6), 539 – 562, distillation.

Skogestad, S., 2000. Plantwide control: The search for the self-optimizing control structure. Journal of Process Control 10, 487–507.

Srinivasan, B., Bonvin, D., Visser, E., Palanki, S., 2003. Dynamic optimization of batch processes: II. Role of measurements in handling uncertainty. Computers & Chemical Engineering 27 (1), 27 – 44.

van de Wal, M., de Jager, A., 2001. A review of methods for input/output selection. Automatica 37 (4), 487–510.

Yelchuru, R., Skogestad, S., 2011. Optimal controlled variable selection for individual process units in self optimizing control with MIQP formulations. American Control Conference, June 29 - July 1,San Francisco, 342 –347.

Yelchuru, R., Skogestad, S., Manum, H., 2010. MIQP formulation for controlled variable selection in self optimizing control. DYCOPS, July 7-9, Brussels, 61–66.

Chapter 5

Quantitative methods for Regulatory control layer selection

Based on the paper submitted for publication in Journal of Process Control

In this paper, we extend the self-optimizing control ideas to find optimal controlled variables in the regulatory layer. The regulatory layer is designed to facilitate stable operation, to regulate and to keep the operation in the linear operating range and its performance is here quantified using the state drift criterion. Quantitative method for the regulatory layer selection with one, two or more closed loops is proposed to minimize the drift in states. The proposed quantitative methods are evaluated on two distillation column case studies.

5.1 Introduction

The plantwide control system for the overall plant is in most cases organized in a hierarchical structure (Figure 5.1), based on time scale separation between the layers. As shown in Figure 5.1, the control layer is usually divided in two parts. The main task of the upper slower "supervisory" layer is to keep the "economic" or primary controlled variables CV_1 close to their economic optimal set points.

$$J_1 = \|CV_1 - CV_{1s}\|^2 \tag{5.1}$$

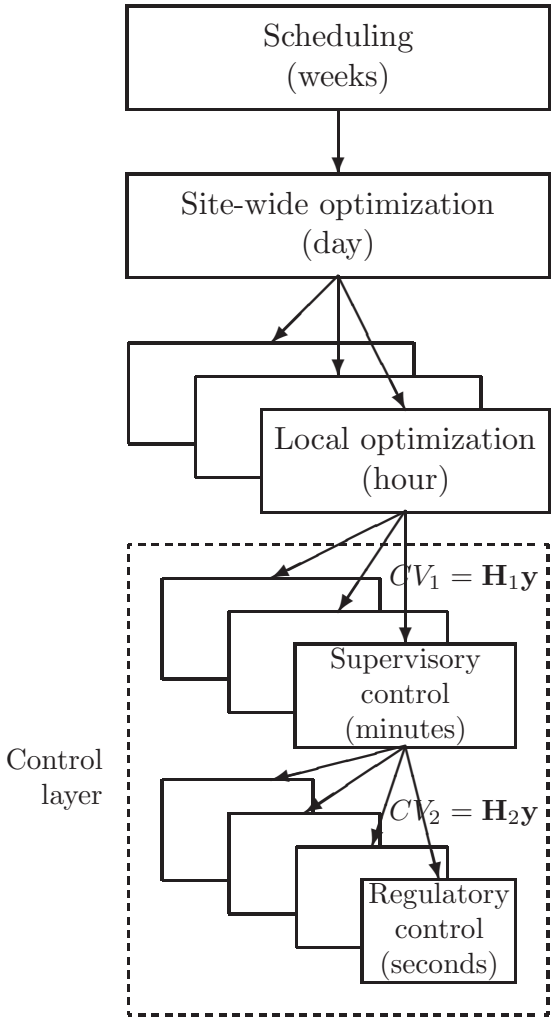

Figure 5.1: Control system hierarchy for plantwide control in chemical plants (Skogestad and Postlethwaite, 2005)

Here, the controlled variables are a subset or combination of the measurements $\mathbf{y}$, and usually we can write $CV_1 = \mathbf{H}_1\mathbf{y}$, where $\mathbf{H}_1$ is a real-valued matrix, which generally is selected based on economics.

On the other hand, the task of the lower faster "regulatory" layer is to avoid that the process drifts too far away from its desired steady state. More specifically, it should stabilize any unstable modes, provide for local (fast) disturbance rejection and keep the operation in the linear operating range. The controlled variables in the regulatory layer are $CV_2 = \mathbf{H}_2\mathbf{y}$, where $\mathbf{H}_2$ is a real-valued matrix, and the selection of $\mathbf{H}_2$ is based on the arguments related to "stabilization" and disturbance rejection.

Ideally, we would like to have a tool that based on a process model, automatically selects the optimal structure of the regulatory control layer, including the controlled variables (CV_2) and the pairing with manipulated variables (usually valves). However, this requires a detailed dynamic model and a carefully defined problem that also includes economics. Perkins and co-workers (Narraway and Perkins, 1993, 1994; Heath et al., 2000; Kookos, 2011) and others (Hamid et al., 2010) suggested to formulate a mixed-integer nonlinear programming (MINLP) problem which involves also finding the optimal controller for the selected structure. Because of the combinatorial nature this is very time consuming and generally global optimality cannot be guaranteed.

In this paper, we focus on the selection of controlled variables CV_2 for the regulatory control layer, and we will quantify the regulatory objectives in terms of a scalar function J_2, which is the weighted state drift away from the desired nominal point,

$$J_2 = \|\mathbf{W}\mathbf{x}\|_2^2 \tag{5.2}$$

Here, $\mathbf{W}$ is a weighting matrix and $\mathbf{x}$ are the states. More precisely, we should write $\Delta\mathbf{x}$, because $\mathbf{x}$ denotes the deviation from the nominal value of the state, but we usually drop the Δ to simplify notation. $\mathbf{W}\mathbf{x}$ is a vector, which generally is a function of time or frequency. Many norms may be used, but we will consider the 2-norm where $\mathbf{x}(j\omega)$ is evaluated at a selected frequency ω. We will in the application consider steady-state, $\omega = 0$.

Another objective is that the regulatory layer should be "simple", and we will quantify this by the number of loops that need to be closed, that is, by the number of physical degrees of freedom (usually valves) that are used by the regulatory layer. This can be related to the partial control idea, where we control the process reasonably well with only a subset of process variables (Shinnar, 1981; Kothare et al., 2000).

One may question the division of the control layer into a supervisory

(economic) and regulatory (stabilizing) layer, but this paradigm is widely used and is the basis for this paper. The main justification is that the two tasks of stabilization and optimal operation are fundamentally different and also that trying to do both at the same time is much more complex as has limited benefit.

This paper focuses on selecting controlled variables (CV_2) in the regulatory layer. Another important decision in the regulatory layer is the pairing of selected outputs (CV_2) with available inputs (valves). However, this issue is not treated in this paper because we make the simplifying assumption of perfect control of the selected controlled variables (CV_2), that is, we do not consider how this is done. This is obviously a limitation, but on the other hand it greatly simplifies the selection problem (CV_2).

Traditionally, the regulatory layer decisions are based on heuristic methods using process insight (e.g., (Luyben, 1996) and references therein). Typical variables that are selected for control (CV_2) are inventories such as liquid levels, and other "sensitive" variables such as selected pressures and temperatures. All of these variables are related to drift in the process and thus to the state drift criterion in (5.2). For example, any accumulating trace component will also be detected by the state drift criterion, as will any unstable mode which gives an infinite state drift. The minimization of weighted steady-state state drift from nominal point at steady state was considered in the absence of measurement noise (Skogestad and Postlethwaite, 2005; Hori et al., 2005). In this paper, we provide a justification for looking at the steady state drift and using self-optimizing control ideas (Skogestad, 2000; Halvorsen et al., 2003), we extend the results to the more realistic case with measurement noise.

The rest of the paper is organized as follows: Section 5.2 provides the justification to use state drift at steady state as a criterion for regulatory layer. Section 5.3 describes the problem for optimal regulatory layer selection. Section 5.4 extends the self-optimizing control concepts to state drift and various cases to find optimal $\mathbf{H}_2$ are described. Section 5.5 presents evaluation on a distillation column case study with 41 stages to find regulatory layer with optimal CV_2 as individual/combinations of measurements. Section 5.6 is included to describe the ease of implementing the controlled variables in dynamic simulations in practice. Section 5.7 presents evaluation on a Kaibel column case study with 71 stages to find regulatory layer with optimal CV_2 as individual/combinations of measurements. The conclusions are given in Section 5.8.

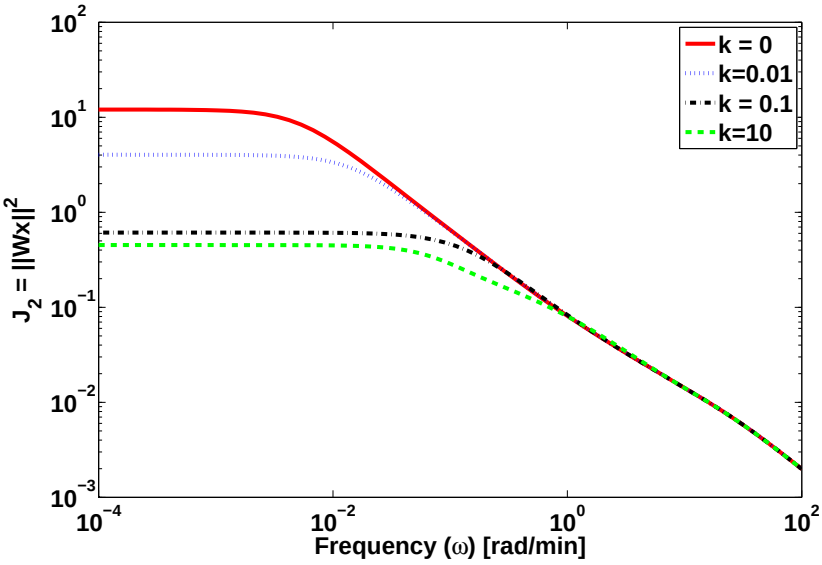

Figure 5.2: State drift J_2 for distillation column as a function of temperature controller gain k

5.2 Justification for considering steady-state state drift

To illustrate how $J_2(j\omega) = \|\mathbf{W}\mathbf{x}(j\omega)\|_2^2$ typically depends on frequency in process control application, we consider a distillation column where the liquid levels are controlled using the product flows, D and B. This is known as LV-configuration, but as noted later the choice of configuration ($\mathbf{u}$) does not actually matter for the results in this paper. In Figure 5.2, the solid red curve ($k = 0$) gives the expected state drift J_2 as a function of frequency with no composition or temperature control (L and V constant) for combined disturbances in feed rate (F), feed composition (z_F) and feed liquid fraction (q_F). The other curves show the effect when boil-up V is used for temperature control

$$V = V_0 + k(y - y_0) \tag{5.3}$$

for increasing value of the controller gain k. L remains constant. As k increases, we get tight control of y temperature on stage 12, and the value of $k = 10$ gives close to "perfect control", where $y(j\omega) = 0$.

From Figure 5.2, it is clear that for a given controller gain k, the state drift is almost constant over the frequency band from 0.0001 to 0.02

rad/min. Also note that the state drift is reduced by a factor 27 (from 12 to 0.45) by closing the temperature loop. We conclude that for this example, a steady state analysis for state drift alone would be sufficient.

More generally, in process control $J_2 = \|\mathbf{W}\mathbf{x}(j\omega)\|_2^2$ as a function of frequency is often flat at lower frequencies and drops at higher frequencies similar to Figure 5.2, which means that we often get very good results by considering steady state ($\omega = 0$). If J_2 has a higher peak at a different frequency, then the methods of this paper can be used to find optimal CV_2 to minimize the state drift by considering the frequency corresponding to the peak.

5.3 Minimization of state drift (Problem definition)

5.3.1 Classification of variables

- $\mathbf{x}$: States (usually deviation variables)
- $\mathbf{Wx}$: Weighted states, which characterizes the drift of the system away from its steady state.
- $\mathbf{u}$: Set of n_u independent variables (inputs).

  Note 1: In our approach, it does not really matter what these variables are as long as they form an independent set, e.g. one may close loops and instead introduce the new set points as the variables $\mathbf{u}$. The reason is that we assume perfect control of the selected controlled variables and closing lower-level loops will not change the problem.

- $\mathbf{u}_0$: Set of n_{u_0} physical degrees of freedom (inputs) which may or may not be constant in the regulatory layer. For example, for a distillation columns with given feed and given pressure, the physical degrees of freedom are the two product flows (D, B) plus the reflux (L) and boilup (V), that is $\mathbf{u}_0 = \{L, V, D, B\}$.

  Note 2: One may select $\mathbf{u} = \mathbf{u}_0$, but this is not required. In particular, at steady state there may be degrees of freedom with no steady-state effect and these may be eliminated (i.e., $n_u < n_{u_0}$) to simplify the problem.

- $\mathbf{y}_m$: Set of measurements (in addition to measured or known values of $\mathbf{u}_0$).

- **d**: Set of disturbances
- $\mathbf{y} = [\mathbf{y}_m \quad \mathbf{u}_0]$: Combined set of measurements and physical inputs that we consider as candidates for including in CV_2, $\mathbf{c} = \mathbf{H}_2\mathbf{y}$.
- $\mathbf{c} = CV_2 = \mathbf{H}_2\mathbf{y}$: Selected set of $n_c = n_u$ independent controlled variables in the regulatory layer. The selection or combination matrix $\mathbf{H}_2$ is here assumed to be a constant real-valued matrix.

  Note 3: Since $n_c = n_u$ the specification of $\mathbf{c}$ will uniquely determine $\mathbf{u}$.

  Note 4: Since $\mathbf{u}_0$ is included in the set $\mathbf{y}$, controlling $\mathbf{c} = \mathbf{H}_2\mathbf{y}$ also includes open-loop and partially controlled systems.

5.3.2 Assumptions

- A linear model is used at the nominal operating point, this model may at each frequency ω be written

$$\mathbf{x} = \mathbf{G}^x(j\omega)\mathbf{u} + \mathbf{G}_d^x(j\omega)\mathbf{d} \tag{5.4a}$$

$$\mathbf{y} = \mathbf{G}^y(j\omega)\mathbf{u} + \mathbf{G}_d^y(j\omega)\mathbf{d} + \mathbf{n}^y \tag{5.4b}$$

  where $\mathbf{G}^x(j\omega)$,$\mathbf{G}_d^x(j\omega)$ and $\mathbf{G}^y(j\omega)$,$\mathbf{G}_d^y(j\omega)$ are frequency-dependent gain matrices.

- To avoid the need to explicitly design the controller, we assume that the selected variables in $\mathbf{c}$ are perfectly controlled at the frequency ω, i.e. $\mathbf{c}(j\omega) = 0$. At steady state ($\omega = 0$) this is not a limitation since perfect control can always be achieved by using integral action, provided the system is operable in the first place. At other frequencies, we may assume perfect control, but the feasibility of this (including closed-loop stability) then needs to be addressed separately.

5.3.3 Problem formulation

The objective is to find what to control in the stabilizing layer,

$$\mathbf{c} = \mathbf{H}_2\mathbf{y} \tag{5.5}$$

given that we want to minimize the state drift (5.2) for the expected disturbances ($\mathbf{d}$) and implementation error (measurement noise, $\mathbf{n}^y$), and that we want to close k loops, $\forall k = 1, 2, \ldots, n_u$. This is explored in more detail next.

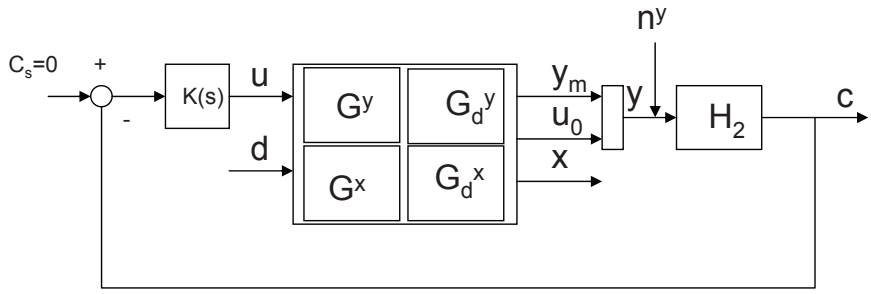

Figure 5.3: Regulatory control layer with control of variables $\mathbf{c} = \mathbf{H}_2\mathbf{y}$

In the frequency domain, the problem can be stated as follows (Figure 5.3): Assuming perfect control of the selected $\mathbf{c}$ (5.5), i.e. $\mathbf{c}(j\omega) = 0$, we want to find the optimal $\mathbf{H}_2$ that minimizes the state drift $J_2(\mathbf{x}(j\omega))$ for a given frequency range $\omega \in [\omega_{B_1}, \omega_{B_2}]$, when there are disturbances. In the rest of this paper, we consider steady state only ($\omega_{B_1} = \omega_{B_2} = 0$), but more generally it will be the frequency range over which we need regulatory control.

We use the self-optimizing control concepts (Skogestad, 2000; Halvorsen et al., 2003) and we consider minimization of the loss rather than the cost, because loss minimization can be formulated as a convex optimization problem in $\mathbf{H}_2$ (Alstad et al., 2009). The loss is $L = J_2 - J_{2,opt}(\mathbf{d})$, where $J_{2,opt}(\mathbf{d})$ is the minimum state drift achievable with the given degrees of freedom. In our case, this gives the same optimal $\mathbf{H}_2$ as minimizing the cost J_2, because minimizing the state drift loss L on an average basis, e.g. using the Frobenius norm, is exactly the same as minimizing the cost J_2. In Figure 5.3, $K(s)$ is the regulatory controller, but since we make the assumption of perfect control ($\mathbf{c}(j\omega) = 0$), it does not actually matter what $K(s)$ is. Our task is to select what to control, $\mathbf{c} = \mathbf{H}_2\mathbf{y}$, where $\mathbf{H}_2$ is a constant real matrix.

We want to close as few loops as possible, that is we want to select in $\mathbf{c} = \mathbf{H}_2\mathbf{y}$ as many variables as possible from the set $\mathbf{u}_0$ physical degrees of freedom (valves). Let

$$\begin{aligned} \mathbf{H}_2 &= [\mathbf{H}_y \quad \mathbf{H}_u] \\ \mathbf{c} = \mathbf{H}_2\mathbf{y} &= \mathbf{H}_y\mathbf{y}_m + \mathbf{H}_u\mathbf{u}_0 \end{aligned} \tag{5.6}$$

and we want to find the best controlled variables for various possibilities for

closing loops

- Close 0 loops: In the set $\mathbf{c}$, select n_c variables from the set $\mathbf{u}_0$ ($\mathbf{H}_y = 0$, n_c columns in $\mathbf{H}_u$ are nonzero)
- Close 1 loop (Partial control): In the set $\mathbf{c}$, select $n_c - 1$ variables from the set $\mathbf{u}_0$ (one column in $\mathbf{H}_y$ is nonzero, the rest are zero)
- Close 2 loops (Partial control): In the set $\mathbf{c}$, select $n_c - 2$ variables from the set $\mathbf{u}_0$ (two columns in $\mathbf{H}_y$ are nonzero, the rest are zero)
- Close k loops (Partial control): In the set $\mathbf{c}$, select $n_u - k$ variables from the set $\mathbf{u}_0$
- Close all n_c loops: In the set $\mathbf{c}$, select 0 variables from the set $\mathbf{u}_0$

In addition, we can have restrictions on the set $\mathbf{c}$ such as selecting only single measurements (each column in $\mathbf{H}_2$ containing one 1 and the rest 0's).

We can make use of mixed integer quadratic programming methods (Yelchuru et al., 2010) or partial branch and bound methods (Kariwala and Cao, 2010) to find optimal $\mathbf{H}_2$ to arrive at optimal regulatory layer with $1, 2$ and more closed loops.

5.3.4 Selection of the variables u

We have mentioned that it does not really matter what the "base" variables $\mathbf{u}$ are as long as they form an independent set. Mathematically, the requirement of an independent set is that we can make $\text{rank}(\mathbf{H}_2\mathbf{G}^y) = n_c$, so that $\mathbf{H}_2\mathbf{G}^y$ is invertible. It may seem surprising that it does not matter what the variables are, and it is because we consider the frequency domain and assume perfect control at a given frequency ω, $\mathbf{c}(j\omega) = 0$. With given $\mathbf{c}(j\omega)$ and given $\mathbf{d}$, all other variables are then uniquely determined, including $\mathbf{u}(j\omega)$.

To show this, let the linear model for the effect of $\mathbf{u}$ and $\mathbf{d}$ on the selected states $\mathbf{x}$ and $\mathbf{y}$ be

$$\mathbf{y} = \mathbf{G}^y\mathbf{u} + \mathbf{G}_d^y\mathbf{d} \tag{5.7a}$$

$$\mathbf{x} = \mathbf{G}^x\mathbf{u} + \mathbf{G}_d^x\mathbf{d} \tag{5.7b}$$

$$\mathbf{c} = \mathbf{H}_2\mathbf{y} \tag{5.7c}$$

with the $\mathbf{c} = 0$ we find $\mathbf{u} = -(\mathbf{H}_2\mathbf{G}^y)^{-1}(\mathbf{H}_2\mathbf{G}_d^y)\mathbf{d}$ and with this input the states are

$$\mathbf{x} = \mathbf{P}_d\mathbf{d} \tag{5.7d}$$

where $\mathbf{P}_d = (\mathbf{G}_d^x - \mathbf{G}^x(\mathbf{H}_2\mathbf{G}^y)^{-1}\mathbf{H}_2\mathbf{G}_d^y)$. With $\mathbf{d}$ given and $\mathbf{c} = 0$, $\mathbf{u}$ and $\mathbf{x}$ are uniquely determined, so $\mathbf{P}_d$ is independent of the choice for $\mathbf{u}$. However, we note that we must select $\mathbf{u}$ so that $\mathbf{H}_2\mathbf{G}^y$ is invertible.

5.3.5 Shifting of integrators

We just stated it does not matter what the base variables $\mathbf{u}$ are. Therefore, to avoid numerical problems with poles on the $j\omega$-axis in $\mathbf{G}^y$ (including integrators), one may introduce proportional controllers to shift (stabilize) these modes. For example, one may use $u = k(y - y_s)$, where y is integrating mode and k is proportional controller gain, and the set points y_s (e.g, level set points) are then chosen as new independent variable in the set $\mathbf{u}$.

At steady state the set point $\mathbf{y}_s$ may have no effect, for example for liquid levels, and we may reduce the number of independent variables in $\mathbf{u}$, such that the number in $\mathbf{u}_0$ with this reduced base set $\mathbf{u}$ (e.g. $\mathbf{u} = \{L, V\}$ for distillation). One may use the steady-state model to obtain the linearized effect of $\mathbf{u}$ and the $\mathbf{d}$ on the original degrees of freedom in $\mathbf{u}_0$. For example, a distillation column with the LV-configuration has $\mathbf{u}_0 = \{L, V, D, B\}$ and $\mathbf{u} = \{L, V\}$. This is explained in more detail in the distillation column case study.

5.4 Minimizing the state drift (optimal $\mathbf{H}_2$)

Assume we want to find the matrix $\mathbf{H}_2$ that minimizes at a given frequency the state drift, $J_2 = \|\mathbf{W}\mathbf{x}\|_2^2$, where $\mathbf{x}$ is the deviation of states from the desired operating point and $\mathbf{W}$ is the square diagonal state weighting matrix. The selection of appropriate square weighting matrix $\mathbf{W}$ allows the user to easily study the state drift in certain states only.

For a disturbance $\mathbf{d}$, the input that gives minimum state drift is denoted $\mathbf{u}_{opt}(\mathbf{d})$. Any input $\mathbf{u}$ that is different from $\mathbf{u}_{opt}(\mathbf{d})$ will result in the loss in state drift (i.e. the deviation from the optimum state drift), which can be defined as

$$L = J_2(\mathbf{u}, \mathbf{d}) - J_{2,opt}(\mathbf{u}_{opt}(\mathbf{d}), \mathbf{d}) \tag{5.8}$$

A second order accurate Taylor expansion of the state drift gives (noting that $\mathbf{J}_u = 0$)

$$L = (\mathbf{u} - \mathbf{u}_{opt}(\mathbf{d}))^T \mathbf{J}_{2_{uu}} (\mathbf{u} - \mathbf{u}_{opt}(\mathbf{d})) \tag{5.9}$$

with the linear model in (5.7),

$$\mathbf{J}_{2_{uu}} \triangleq \frac{\partial^2 J_2}{\partial \mathbf{u}^2} = 2\mathbf{G}^{xT}\mathbf{W}^T\mathbf{W}\mathbf{G}^x \tag{5.10}$$

5.4.1 Finding optimal $\mathbf{H}_2$ for case with no noise (Previous work)(Skogestad and Postlethwaite, 2005; Hori et al., 2005)

In the absence of measurement noise ($\mathbf{n}^y$), the optimal choice for $\mathbf{H}_2$ when the number of measurements $n_y \geq n_u + n_d$ (Skogestad and Postlethwaite, 2005; Hori et al., 2005).

$$\mathbf{H}_2 = (\mathbf{W}\mathbf{G}^x)^T \left[\mathbf{W}\mathbf{G}^x \quad \mathbf{W}\mathbf{G}^x_d\right] \left[\mathbf{G}^y \quad \mathbf{G}^y_d\right]^\dagger \tag{5.11}$$

where $\mathbf{W}$ is state weighting matrix, † represents the pseudo inverse of the matrix, .

In the following, we use newer results from self-optimizing control (Alstad et al., 2009; Yelchuru et al., 2010; Kariwala and Cao, 2010; Kariwala et al., 2008) to generalize this by allowing for measurement noise, eliminating the requirement $n_y \geq n_u + n_d$ and allowing for CV_2 as individual measurements and not only combination as given in (5.11).

5.4.2 Loss as a function of d, $\mathbf{n}^y$ and control policy $\mathbf{H}_2$

To include measurement noise, we need to quantify its expected magnitude. Let the linear model be

$$\mathbf{y} = \mathbf{G}^y\mathbf{u} + \mathbf{G}^y_d\mathbf{W}_d\mathbf{d}' + \mathbf{W}_n\mathbf{n}^{y'} \tag{5.12a}$$

$$\mathbf{x} = \mathbf{G}^x\mathbf{u} + \mathbf{G}^x_d\mathbf{W}_d\mathbf{d}' \tag{5.12b}$$

$$\mathbf{c} = \mathbf{H}_2\mathbf{y} \tag{5.12c}$$

where the usually diagonal matrices $\mathbf{W}_d$ and $\mathbf{W}_n$ represent the magnitudes of disturbances and measurement noises, and $\mathbf{d}'$, $\mathbf{n}^{y'}$ denote normalized disturbances and noise.

The average or expected loss resulting from keeping (5.5) at constant set point, for a normal distributed set $\begin{bmatrix} \mathbf{d}' \\ \mathbf{n}^{y'} \end{bmatrix} \in \mathcal{N}(0,1)$ is given by (Kariwala et al., 2008; Alstad et al., 2009)

$$L_{avg} = \mathbb{E}(L) = \frac{1}{2}\|\mathbf{M}_2\|_F^2 \tag{5.13}$$

where

$$\mathbf{M}_2(\mathbf{H}_2) = \mathbf{J}_{2_{uu}}^{1/2}(\mathbf{H}_2\mathbf{G}^y)^{-1}\mathbf{H}_2\mathbf{Y}_2 \tag{5.14}$$

$$\mathbf{Y}_2 = [\mathbf{F}_2\mathbf{W}_d \quad \mathbf{W}_n]\,; \quad \mathbf{F}_2 = \frac{\partial \mathbf{y}_{opt}}{\partial \mathbf{d}} = \mathbf{G}^y\mathbf{J}_{2_{uu}}^{-1}\mathbf{J}_{2_{ud}} - \mathbf{G}^y_d \tag{5.15}$$

where $\mathbf{J}_{2_{ud}} \triangleq \frac{\partial^2 J_2}{\partial \mathbf{u}\partial \mathbf{d}} = 2\mathbf{G}^{x^T}\mathbf{W}^T\mathbf{W}\mathbf{G}^x_d$, $\|\mathbf{M}_2\|_F = \sqrt{\sum_{i,j}\mathbf{M}_{2_{ij}}^2}$ denotes the Frobenius norm of the matrix $\mathbf{M}_2$.

5.4.3 Optimal full $\mathbf{H}_2$

Finding the optimal $\mathbf{H}_2$ in (5.13) is a convex optimization problem for the case where $\mathbf{H}_2$ is a full matrix (Alstad et al., 2009; Yelchuru et al., 2010). For the case when $\mathbf{Y}_2\mathbf{Y}_2^T$ is full rank matrix, an analytical solution for $\mathbf{H}_2$ is (Alstad et al., 2009)

$$\mathbf{H}_2{}^T = \left(\mathbf{Y}_2\mathbf{Y}_2{}^T\right)^{-1}\mathbf{G}^y\left(\mathbf{G}^{y^T}\left(\mathbf{Y}_2\mathbf{Y}_2{}^T\right)^{-1}\mathbf{G}^y\right)^{-1}\mathbf{J}_{2_{uu}}^{1/2} \tag{5.16}$$

However, when $\mathbf{H}_2$ has a particular structure, the loss minimization (5.13) for $\mathbf{H}_2$ is a non-convex optimization problem (Heldt, 2010).

5.4.4 Optimal $\mathbf{H}_2$ with CV_2 as individual measurements

The optimal $\mathbf{H}_2$ with CV_2 as individual measurements, e.g. $\mathbf{H}_2 = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$, gives an MIQP that require us to solve a convex QP at each node. This is because we may use a "trick" where $\mathbf{H}_2$ is full in the selected measurements (Yelchuru et al., 2010).

For a system where $n_u < n_{u_0}$ (like the distillation example with $n_u = n_c = 2$ and $n_{u_0} = 4$), the regulatory layer with 0 loops closed is such a problem and with n_{u_0} inputs and n_u steady state degrees of freedom, we need to explore $\binom{n_{u_0}}{n_c}$ possibilities. The partial control problem with 1 closed loop is to find (5.6) with one column in $\mathbf{H}_y$ nonzero and $n_c - 1$ columns in $\mathbf{H}_u$ nonzero, and we need to explore $\binom{n_{u_0}}{n_c-1}\binom{n_y}{1}$ possibilities. The partial control problem with 2 closed loops is to find (5.6) with two columns in $\mathbf{H}_y$ nonzero and n_c-2 columns in $\mathbf{H}_u$ nonzero, and we need to explore $\binom{n_{u_0}}{n_c-2}\binom{n_y}{2}$ possibilities. The regulatory layer with k closed loops is to find (5.6) with k columns in $\mathbf{H}_y$ nonzero and $n_c - k$ columns in $\mathbf{H}_u$ nonzero, and we need to explore $\binom{n_{u_0}}{n_c-k}\binom{n_y}{k}$ possibilities. The regulatory layer with n_c closed loops is to find (5.6) with n_c columns in $\mathbf{H}_y$ nonzero, and we need to explore $\binom{n_y}{n_u}$ possibilities. The total possibilities are $\binom{n_{u_0}}{n_c} + \binom{n_{u_0}}{n_c-1}\binom{n_y}{1} + \binom{n_{u_0}}{n_c-2}\binom{n_y}{2} + \cdots + \binom{n_{u_0}}{n_c-k}\binom{n_y}{k} + \cdots + \binom{n_y}{n_c}$. For a case with $n_{u_0} = 4$, $n_u = n_c = 2$, and $n_y = 41$, the total possibilities are 990.

In the regulatory layer with i loops closed require us solve (5.13) to find the best CV using mixed integer quadratic programming (MIQP) (Yelchuru et al., 2010). Hence, the regulatory layer with $0, 1, 2$ and more closed loops can be obtained by solving $(n_u + 1)$ mixed integer quadratic programming problems. For example, for a case with $n_{u_0} = 4$, $n_u = 2$, and $n_y = 45$, the total MIQP problems that need to be solved are 3. Even though the number of MIQP problems need to be solved increase with n_u, the regulatory layer

selection problem is tractable as it is an offline method. Later, depending on the allowable state drift threshold set by the user, the minimum regulatory layer is obtained. Generally, in the regulatory layer, CV_2 are individual measurements, if the state drift loss is very large then CV_2 can be selected as measurement combination.

5.4.5 Optimal $\mathbf{H}_2$ for partial control with CV_2 as measurement combinations

We now consider the partial regulatory control problem where we allow for measurement combination for the controlled variables in CV_2. This can be viewed as solving (5.13) with a particular structure in $\mathbf{H}_2$, which is generally a non-convex problem. For example, a partially controlled system with 3 process measurements and 2 inputs, resulting in 5 candidate measurements in $\mathbf{y}$, is

$$\mathbf{H}_2 = \begin{bmatrix} h_{11} & h_{12} & h_{13} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \text{ or } \mathbf{H}_2 = \begin{bmatrix} h_{11} & h_{12} & h_{13} & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix} \quad (5.17)$$

To solve (5.13) with this particular structure, we propose a two step approach which may not be optimal but which is convex. The first step is to partition the system inputs into two sets $\mathbf{u}_1$ and $\mathbf{u}_2$ ($\mathbf{u} = \{\mathbf{u}_1 \cup \mathbf{u}_2\}$) where we keep the inputs in the set $\mathbf{u}_2 \in \mathbf{u}_0$ constant. The matrix for such a partial control system $\mathbf{G}^{y,partial} \in \mathbb{R}^{n_y \times n_{u_1}}$ is obtained by picking the columns associated to input set $\mathbf{u}_1$ and $\mathbf{J}_{uu,x}^{partial} \in \mathbb{R}^{n_{u_1} \times n_{u_1}}$, $\mathbf{J}_{ud,x}^{partial} \in \mathbb{R}^{n_{u_1} \times n_d}$ has elements associated to the inputs in the input set $\mathbf{u}_1$. The disturbance gain matrix $\mathbf{G}_d^y \in \mathbb{R}^{n_y \times n_d}$, disturbance magnitude matrix $\mathbf{W}_d \in \mathbb{R}^{n_d \times n_d}$ and measurement noise magnitude matrix $\mathbf{W}_n \in \mathbb{R}^{n_y \times n_y}$ will remain the same. The second step is to solve (5.13) with the matrices obtained in the first step as a convex optimization problem (Yelchuru et al., 2010) to obtain $\mathbf{H}_2^{partial}$ as a full matrix for the partially controlled system. For a case with n_u inputs, there are totally $2^{n_u} - 2$ partially controlled systems.

As $\mathbf{u}_2 \in \mathbf{u}_0$ varies in each partial controlled system, we cannot directly compare the losses obtained from different partial control systems. Hence, in order to compare the losses on an equivalent basis, the loss value is calculated for the full system with the optimal controlled variables $CV_2^{partial}$ obtained for the partially controlled system and the constant inputs in $\mathbf{u}_2$ as the other CV_2.

5.4.6 Summary

Step 1 Define states $\mathbf{x}$ as the deviations from the nominal value of states and define the weighted state drift (5.2).

Step 2 Obtain the linear gain matrices from $\mathbf{u}$ to $\mathbf{y}$, $\mathbf{G}^y$, and $\mathbf{d}$ to $\mathbf{y}$, $\mathbf{G}_d^y$ (5.7), and define the magnitudes for disturbances $\mathbf{d}$ and implementation errors $\mathbf{n}^y$ as $\mathbf{W}_d$ and $\mathbf{W}_n$. The second derivatives of the weighted state drift with respect to $\mathbf{u}$, and $\mathbf{u}$ and $\mathbf{d}$ as $\mathbf{J}_{uu}$ and $\mathbf{J}_{ud}$.

Step 3 Define the state drift loss (5.13) using the matrices in Steps 1 and 2 using self-optimizing control concepts (Skogestad, 2000; Halvorsen et al., 2003).

Step 4 Use the new results of self-optimizing control (Alstad et al., 2009; Yelchuru et al., 2010; Kariwala and Cao, 2010; Kariwala et al., 2008) to find an optimal $\mathbf{H}_2$ that minimizes (5.13) to find the optimal controlled variables as individual measurements in the partial regulatory control problem with one, two and more closed loops (Section 5.4.4).

Step 5 If the state drift is higher than what is acceptable, then find the regulatory layer CV_2 as combination of measurements (Section 5.4.5).

5.5 Distillation column case study

The main purpose of this case study is to illustrate the proposed methods on a binary distillation column with 41 stages where we want to choose best temperature loop(s) to avoid state drift. The analysis is based on the LV-configuration (Skogestad, 1997; Hori and Skogestad, 2008), where distillate flow (D) and bottoms flow (B) are used to control the integrating levels (M_D, M_B) and reflux (L) and boilup (V) are the remaining steady-state degrees of freedom ($\mathbf{u}$) (Figure 5.4). However, note that we would obtain identical results if we started with another configuration, e.g. the DV-configuration.

The considered disturbances are in feed flow rate (F), feed composition (z_F) and feed liquid fraction (q_F), which can vary between $1 \pm 0.2, 0.5 \pm 0.1$ and 1 ± 0.1, respectively. In summary, we have

$$\mathbf{u}_0 = \begin{pmatrix} L \\ V \\ D \\ B \end{pmatrix}, \ \mathbf{u} = \begin{pmatrix} L \\ V \end{pmatrix}, \ \mathbf{d} = \begin{pmatrix} F \\ z_F \\ q_F \end{pmatrix}, \ \mathbf{y}_m = \begin{pmatrix} T_1 \\ T_2 \\ \vdots \\ T_{41} \end{pmatrix}$$

We assume a binary mixture with constant relative volatility α between the components, constant pressure, no vapour hold up, equilibrium on each stage and constant molar flows. The column has 41 stages and the feed on stage 21. At the steady state operating point, $L = 2.706\ mol/min$, $V = 3.206\ mol/min$, $F = 1\ mol/min$, $z_F = 0.5$, $q_F = 1$, $\alpha = 1.5$, $x_D = 0.99$, $x_B = 0.01$. The linearized relationship between the two base degrees of freedom $\mathbf{u}$ and the four physical degrees of freedom $\mathbf{u}_0$ can be obtained based on steady state mass balances (see Appendix D)

$$\mathbf{u}_0 = \mathbf{G}^u \mathbf{u} + \mathbf{G}_d^u \mathbf{d} \tag{5.18}$$

where

$$\mathbf{G}^u = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -1 & 1 \\ 1 & -1 \end{bmatrix}, \quad \mathbf{G}_d^u = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 1 \end{bmatrix}$$

The boiling points difference between the light key component (L) and heavy key component (H) is 13.5 ^oC. For simplicity, the temperature $T_i(^oC)$ on each stage i is calculated as a linear function of the liquid composition x_i (Skogestad, 1997)

$$T_i = 0x_i + 13.5(1 - x_i) \tag{5.19}$$

The 41 stage temperatures ($\mathbf{y}_m$) and the manipulated input flows $\mathbf{u}_0 = \{L, V, D, B\}$ are taken as candidate measurements. The measurement error for temperatures is $\pm 0.5^oC$ and it is $\pm 10\%$ for the flows. The state drift J_2 in the compositions on all 41 stages is

$$J_2 = \|\mathbf{W}\mathbf{x}\|_2^2 \tag{5.20}$$

where we select $\mathbf{W} = \mathbb{I}^{41\times 41}$ (identity matrix) to have equal weights on the mole fraction $\mathbf{x}$.

The distillation column case study has $n_{u_0} = 4$ physical inputs, $n_u = 2$ steady state degrees of freedom and $n_y = 45$ candidate measurements. For each i closed loops we need to solve an MIQP. With single measurements in CV_2 with $0, 1$ and 2 closed loops, there are $n_u + 1 = 3$ MIQP problems. The MIQP problems are solved using IBM ILOG CPLEX solver in Matlab ®R2009a on a Windows XP SP2 notebook with Intel ®Core$^{\text{TM}}$ Duo Processor T7250 (2.00 GHz, 2M Cache, 800 MHz FSB). The QP that needs to be solved at each node in MIQP is convex and the initial conditions do not play any role.

The presence of integrating modes requires that we first close two loops for integrating levels (M_D, M_B). Next, in addition to these, we want to

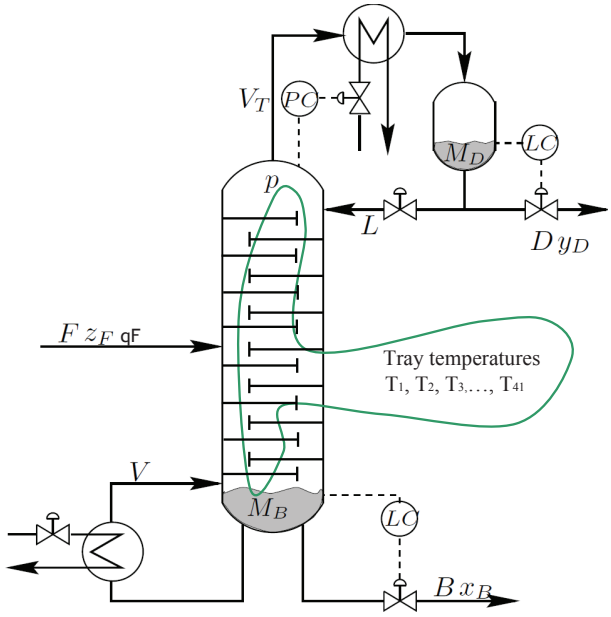

Figure 5.4: Distillation column using LV-configuration

close loops to minimize the state drift. In general, the loss decreases as we close more loops, but for simplicity we want to close as few loops as possible in the regulatory layer, that is we want to select in $\mathbf{y}$ as many variables as possible from the set $\mathbf{u}_0$. This is a multi-objective problem involving a trade-off between the loss (magnitude of the state drift) and the number of loops closed. There is no simple mathematical solution to such problems, so the best is to provide the results and let the engineer make the decision. The loss with 0 loops closed (2 flows from $\mathbf{u}_0$ are constant), 1 loop closed (one flow from $\mathbf{u}_0$ is constant), 2 loops closed (no flows from $\mathbf{u}_0$ are constant) are tabulated in Table 5.1 (upper part with 2 measurements used). From Table 5.1, the best system with zero temperature loops closed (that is with only liquid level loops closed) is to keep $\{V, B\}$ constant, with a loss 109.669. The best single temperature loop policy is to keep L constant and control tray temperature T_{18} with a much lower loss of 0.188. The best policy with two temperature loops is to control tray temperatures T_{15} and T_{27} with a loss of 0.026. This should be compared with the minimal achievable state drift of 0.0204 obtained when allowing for measurement combinations. The loss reduction by closing one loop is very large (from 109.7 to 0.188), but the further reduction by closing two loops (from 0.188 to 0.026) is probably not significant from a state drift J_2 (regulatory) point of view. This is

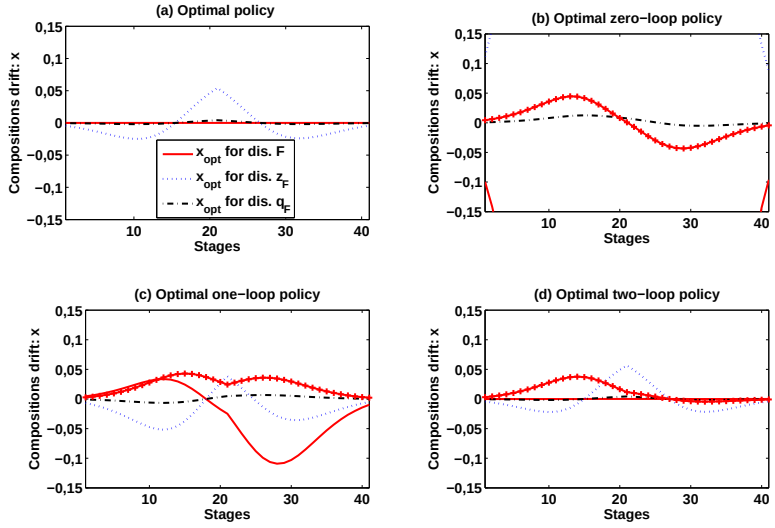

Figure 5.5: Distillation column state drift in the presence of disturbances F,z_F, q_F: (a) optimal policy (minimum achievable state drift), (b) optimal zero-loop policy, (c) optimal one-loop policy, (d) optimal two-loop policy. Effect of a measurement noise on state drift is shown with + in subplots (b),(c) and (d)

further illustrated by comparing the composition state drift profiles with an optimal, zero-loop, one-loop and two-loop policies are shown in Figure 5.5 (a), (b), (c) and (d) in the presence of disturbances F, z_F, q_F, respectively. Note that the contribution of one measurement noise is also included in Figure 5.5 (b),(c) and (d).

We next study the effect of using temperature measurement combinations. For the distillation case study, we have $n_u = 2$ and the number of partial control systems are $2^{n_u} - 2 = 2$ for each additional measurement and require us to solve $2^{n_u} - 2 = 2$ more MIQP problems. The optimal CV_2 for the partial control systems with CV_2 as combination of $3, 4, 5$ and 41 measurements while closing $1, 2$ loops are also tabulated in Table 5.1. The reduction in loss with the number of measurements, when one loop, two loops are closed is shown as a bar chart in Figure 5.6. From Table 5.1, the best single loop control CV_2 with 3 measurements is to control $1.072T_{15} + T_{26}$ while keeping L constant. In conclusion, based on the acceptable steady state drift loss defined by the user, minimum regulatory layer can be obtained by finding CV_2 as individual measurements or mea-

Table 5.1: Distillation column case study: the self optimizing variables $\mathbf{c}'s$ as combinations of $2, 3, 4, 5, 41$ measurements with their associated losses in state drift

No. of loops closed †	No. of meas. used	Optimal meas.	$\mathbf{c}'s$	Loss $(J - J_{opt}(\mathbf{d}))$ $(\frac{1}{2}\|\mathbf{M_2}\|_F^2)$	$J = \|\mathbf{Wx}\|_2^2$
0	2	$[V \quad B]$	$c_1 = V$ $c_2 = B$	109.669††	109.690
1	2	$[T_{18} \quad L]$	$c_1 = L$ $c_2 = T_{17}$	0.188	0.209
2	2	$[T_{15} \quad T_{27}]$	$c_1 = T_{15}$ $c_2 = T_{27}$	0.026	0.047
1	3	$[T_{15} \quad T_{26} \quad L]$	$c_1 = L$ $c_2 = 1.072T_{15} + T_{26}$	0.129*	0.150
2	3	$[T_{15} \quad T_{26} \quad T_{28}]$	$c_1 = T_{15} - 0.1352T_{28}$ $c_2 = T_{26} + 1.0008T_{28}$	0.020	0.040
1	4	$[T_{15} \quad T_{16} \quad T_{27} \quad L]$	$c_1 = L$ $c_2 = 0.6441T_{15} + 0.6803T_{16} + T_{27}$	0.126*	0.146
2	4	$[T_{14} \quad T_{16} \quad T_{26} \quad T_{28}]$	$c_1 = T_{14} - 6.1395T_{26} - 6.3356T_{28}$ $c_2 = T_{16} + 6.2462T_{26} + 6.2744T_{28}$	0.014	0.034
1	5	$[T_{15} \quad T_{16} \quad T_{26} \quad T_{27} \quad L]$	$c_1 = L$ $c_2 = 1.1926T_{15} + 1.1522T_{16} + 0.9836T_{26} + T_{27}$	0.123*	0.144
2	5	$[T_{14} \quad T_{16} \quad T_{26} \quad T_{27} \quad T_{28}]$	$c_1 = T_{14} - 4.9975T_{26} - 5.0717T_{27} - 4.9813T_{28}$ $c_2 = T_{16} + 5.1013T_{26} + 5.0847T_{27} + 4.9166T_{28}$	0.011	0.032
1	41	$[T_1, T_2, \ldots, T_{41} \quad L, V, D, B]$	$c_1 = L$ $c_2 = f(T_1, T_2, \ldots, T_{41}, L, V, D, B)$	0.118*	0.138
2	41	$[T_1, T_2, \ldots, T_{41}]$	$c_1 = f(T_1, T_2, \ldots, T_{41})$ $c_2 = f(T_1, T_2, \ldots, T_{41})$	0.003	0.023

† In addition to two closed level loops
The loss is minimized to obtain $\mathbf{H}_2$
The optimal state drift $J_{opt}(\mathbf{d}) = 0.0204$
1 loop closed : 1 $\mathbf{c}$ from $\mathbf{y}_m$, 1 $\mathbf{c}$ from $\mathbf{u}_0$
2 loops closed: 2 $\mathbf{c}$ from $\mathbf{y}_m$
The loss is minimized to obtain $\mathbf{H}_2$
†† Such a high value is not physical, but it follows because our linear analysis is not appropriate when we close 0 loops
* used partial control idea to find optimal $\mathbf{H}_2$ in two step approach

surement combinations.

5.6 Dynamic simulations

The dynamic simulations for this distillation column alone are included to show the ease of implementing the regulatory layer controlled variables obtained using the methods of this paper in practice. The open loop gain and time constants with controlled variables $c_1 = T_{27}, c_2 = T_{15}$ are obtained based on transient responses of $+5\%$ steps in L and V. A Proportional Integral (PI) controller between L and c_1 with tuning parameters $k_{c_1} = -0.5191, \tau_{I_1} = 8\ min$ and an another PI controller between V and c_2 with tuning parameters $k_{c_2} = 0.6307, \tau_{I_2} = 8\ min$ are obtained using SIMC tunings (Skogestad, 2003) with $\tau_c = 2\ min$.

Dynamic simulations are performed with these settings to evaluate the

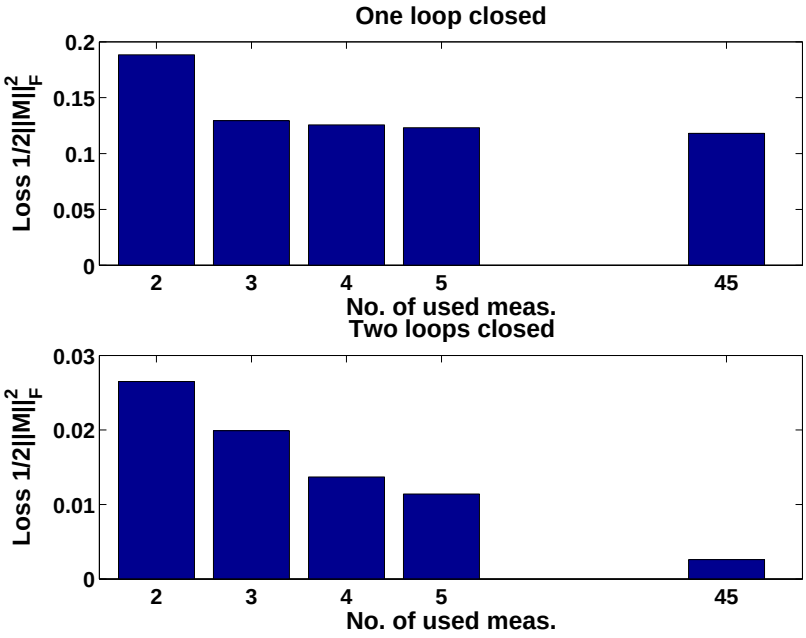

Figure 5.6: Distillation case study: The reduction in loss in state drift vs number of used measurements, top: loss with one loop closed, bottom : loss with two loops closed

.

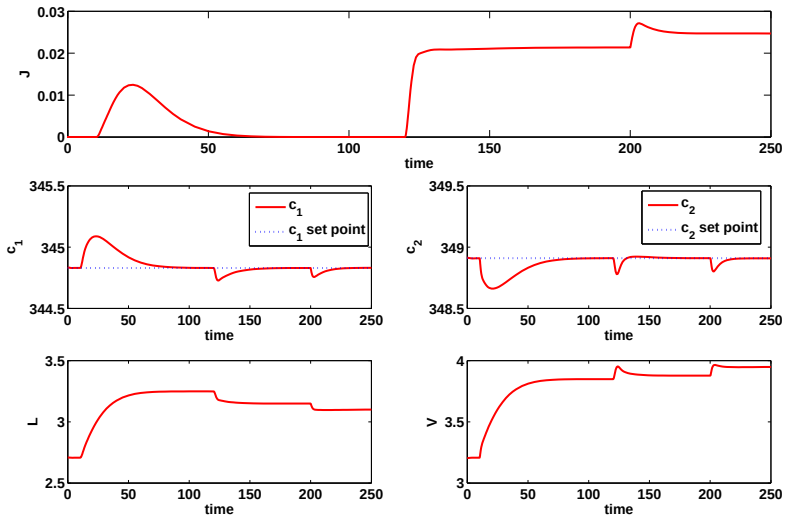

Figure 5.7: Distillation case study: transient responses of state drift, J with two temperature loops closed ($c_1 = T_{27}$, $c_2 = T_{15}$) with inputs L, V for +20% disturbance in F at time 10 min, +20% disturbance in z_F at time 120 min and +10% disturbance in q_F at time 200 min

disturbance rejection performance with the controlled variables $c_1 = T_{27}$ and $c_2 = T_{15}$. The disturbances are +20% disturbance in feed rate F at time 10 min, +20% disturbance in feed composition z_F at time 120 min, and +10% disturbance in feed liquid fraction q_F at time 200 min are shown in Figure 5.7. The transient responses of the state drift, J, selected controlled variables, $c_1 = T_{27}, c_2 = T_{15}$, with their set points, manipulated variables, L, V, are shown in Figure 5.7 in the presence of disturbances **d**.

5.7 Kaibel column

The main purpose of the Kaibel column case study is to evaluate the proposed methods on a case with more inputs and states. The Kaibel column can separate four components into four products in a single column shell with a single reboiler (Kaibel, 1987). The Kaibel column is an extension of the Petlyuk column (Petlyuk et al., 1965). The capital savings in the separation of four products with Kaibel column compared to conventional three columns in series makes it an attractive alternative (Halvorsen and Skogestad, 2003; Adrian et al., 2004).

The given 4-product Kaibel column arrangement separates a mixture of methanol (A), ethanol (B), propanol (C), butanol (D) into almost pure components. The Kaibel column is modeled using a stage-by-stage model with the following simplifying assumptions: Constant pressure, equilibrium stages and constant molar flows. The vapor-liquid equilibrium is modeled using the Wilson equation. The Kaibel column is modeled with 7 sections and we indicate the temperature measurements of each section in Figure 5.8. Sections 1 and 2 make up the prefractionator, while the main column consists of sections 3 - 7. Each section has 10 stages and the reboiler is counted as an additional stage, which gives Kaibel column with 71 stages in total. Each stage has 3 compositions, 1 holdup and 1 temperature state resulting in a total of 355 states. The economic objective function J_1 is to minimize the sum of impurities in the products.

$$J_1 = D(1 - x_{A,D}) + S_1(1 - x_{B,S_1}) + S_2(1 - x_{C,S_2}) + B(1 - x_{D,B}) \quad (5.21)$$

where D, S_1, S_2 and B are the distillate, side product 1, side product 2 and bottom flow rates (mol/min) respectively. $x_{i,j}$ is mole fraction of component i in product j.

The objective of the regulatory layer is to minimize the state drift in the 225 mole fractions of A, B and C components of the process streams (213 mole fractions for 71 trays plus 12 mole fraction states for streams L, D, S_1 and S_2)

$$J_2 = \|\mathbf{W}\mathbf{x}\|^2 \quad (5.22)$$

where $\mathbf{W} = \mathbb{I}^{225\times225}$ (identity matrix) to have equal weights on mole fractions of A,B and C components in process streams.

The considered Kaibel column then has 6 inputs, $\mathbf{u}_0 = \{L, S_1, S_2, R_L, D, B\}$ with 4 steady state degrees of freedom ($\mathbf{u} = \{L, S_1, S_2, R_L\}$) and 71 temperature measurements (7 sections with each section having 10 tray temperatures plus 1 temperature for reboiler). We included the 71 temperature measurements and the 6 inputs as candidate measurements ($\mathbf{y}$) and $n_y = 77$. We

assume that the temperatures are measured with an accuracy of $\pm 1^oC$ and flows are measured with an accuracy of $\pm 10\%$. The considered disturbances are in vapor boil up (V), vapor split (R_V), feed flow rate (F), mole fraction of A in feed stream (z_A), mole fraction of B in feed stream (z_B), mole fraction of C in feed stream (z_C), liquid fraction in feed stream (q_F), which vary between $3\pm 0.25, 0.4\pm 0.1, 1\pm 0.25, 0.25\pm 0.05, 0.25\pm 0.05, 0.25\pm 0.05, 0.9\pm 0.05$, respectively. The reader is referred to Strandberg (2006) for further details. We optimize the system for the products impurity (5.21) and we operate the plant around that optimal operating point.

The Kaibel column has $n_{u_0} = 6$ physical inputs, $n_u = 4$ steady state degrees of freedom and $n_y = 77$ candidate measurements. An MIQP needs to be solved for each i closed loops. To obtain CV_2 as individual measurements with $0, 1, 2, 3$ and 4 closed loops, we need to solve $n_u + 1 = 5$ MIQP problems. These five MIQP problems are solved using IBM ILOG CPLEX solver in Matlab ®R2009a on a Windows XP SP2 notebook with Intel ®Core$^{\text{TM}}$ Duo Processor T7250 (2.00 GHz, 2M Cache, 800 MHz FSB). The QP that needs to be solved at each node in MIQP is convex and initial conditions do not play any role.

The presence of integrating modes result in infinite state drift, so first we close 2 loops for integrating levels (M_D, M_B). Next, we want to close additional loops to minimize the state drift. The loss with 0 loops closed (4 flows in $\mathbf{u}_0$ constant), 1 loop closed (3 flows in $\mathbf{u}_0$ constant), 2 loops closed (2 flows in $\mathbf{u}_0$ constant), 3 loops closed (1 flow in $\mathbf{u}_0$ constant), 4 loops closed (no flows in $\mathbf{u}_0$ constant) are tabulated in Table 5.2. The best measurements for $0, 1, 2, 3$ and 4 loops closed are shown in Table 5.2 (upper part with 4 measurements). From Table 5.2, the "best" system with zero loops closed is to keep $\{S_1, R_L, D, B\}$ constant with a loss 8018.243. The best single-loop policy is to keep $\{S_1, S_2, R_L\}$ constant and control T_{56} with a loss of 1628.773. The best two-loop policy is to keep $\{S_1, S_2\}$ constant and control $\{T_{13}, T_{42}\}$ with a loss of 469.941. The best three-loop policy is to keep S_1 constant and control $\{T_7, T_{39}, T_{51}\}$ with a loss of 33.150. Finally, the best four-loop policy is to control $\{T_9, T_{31}, T_{51}, T_{66}\}$ with a loss of 0.089. This should be compared with the minimal achievable state drift of 0.347 obtained when allowing for measurement combinations. The loss reduces by every additional closed loop and the reduction ratio is very high when we close the final (4th) loop. This is further illustrated by the composition state drift profiles for the optimal, two-loop, three-loop and four-loop policies are shown in Figures 5.9 (a), (b), (c) and (d).

We next study the effect of using temperature measurement combinations. For Kaibel column case study, we have $n_u = 4$ and to find CV_2 as

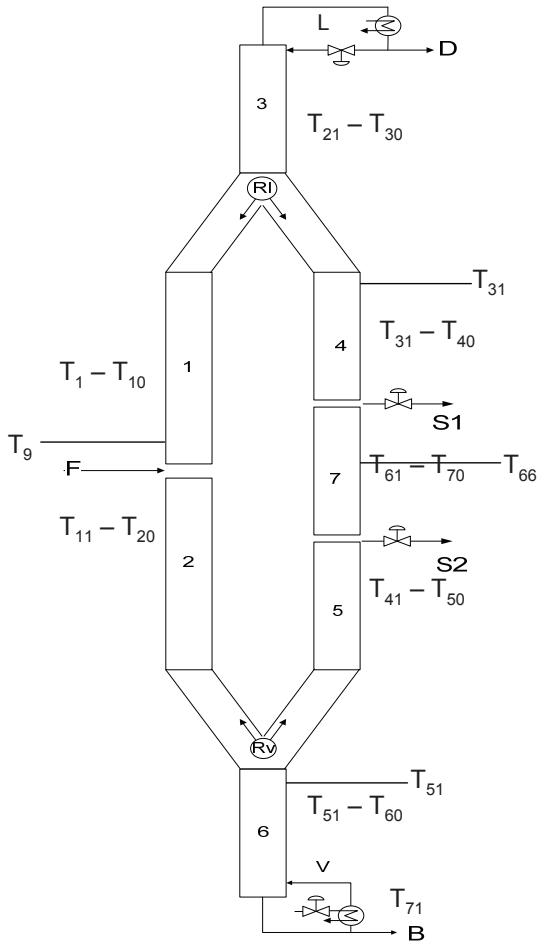

Figure 5.8: Kaibel column with 7 sections

.

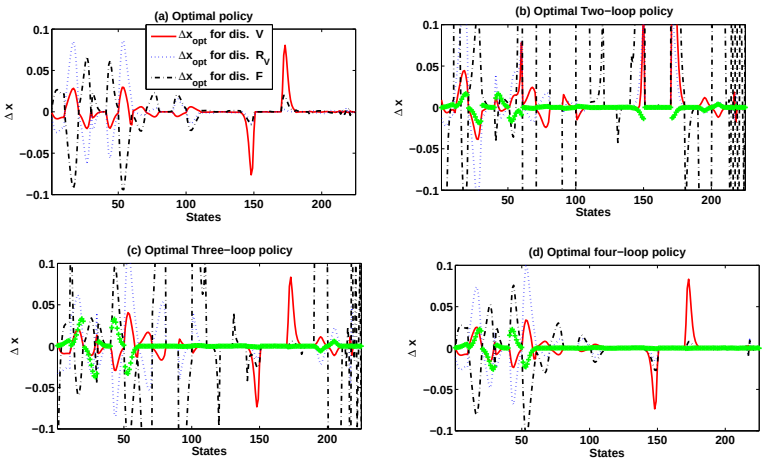

Figure 5.9: Kaibel column state drift in the presence of disturbances in V, R_V and F, (a) optimal policy (minimum achievable state drift), (b) optimal two-loop policy, (c) optimal three-loop policy, (d) optimal four-loop policy. Effect of one measurement noise on state drift is shown with + in subplots (b), (c) and (d)

measurement combinations, the number of partial control systems (number of MIQP problems) further increase by $2^{n_u} - 2 = 14$ for every additional measurement included to obtain CV_2 as a combination. The optimal measurements to find CV_2 as combinations of 5, 6 and 77 measurements for 1, 2, 3 and 4 loops closed are also tabulated in Table 5.2. The reduction of loss with number of measurements, when one loop, two loops, three loops and four loops closed is shown as bar charts in Figures 5.10 and 5.11. From the Table 5.2 and the acceptable steady state drift loss defined by the user, the minimum regulatory layer can be obtained.

5.8 Conclusions

The self optimizing control concepts are extended to select optimal controlled variables that minimize the state drift in the presence of disturbances. In process control, $\|\mathbf{W}\mathbf{x}(j\omega)\|_2^2$ is often flat at lower frequencies and drops at higher frequencies, so minimizing the state drift for steady-state ($\omega = 0$) yields good results. We presented a framework on how to use self-optimizing control minimum loss method to minimize the state drift to arrive at optimal regulatory layer with $1, 2$ and more closed loops. The

Table 5.2: Kaibel column: the regulatory CV_2 as combinations of $4, 5, 6$ and 77 measurements with their associated losses

No. of loops closed †	No. of meas. used	Optimal meas.	Loss $\frac{1}{2}\|\mathbf{M}_2\|_F^2$	Cost $J = \|\mathbf{Wx}\|_2^2$
0	4	$[S_1 \quad R_L \quad D \quad B]$	8018.243††	8018.590
1	4	$[T_{56} \quad S_1 \quad S_2 \quad R_L]$	1628.773	1629.121
2	4	$[T_{15} \quad T_{43} \quad S_1 \quad S_2]$	469.037	469.385
3	4	$[T_7 \quad T_{39} \quad T_{51} \quad S_1]$	33.150	33.497
4	4	$[T_9 \quad T_{31} \quad T_{51} \quad T_{66}]$	0.089	0.437
1	5	$[T_{54} \quad T_{61} \quad S_1 \quad S_2 \quad R_L]$	1605.107*	1605.455
2	5	$[T_8 \quad T_{39} \quad T_{51} \quad S_1 \quad S_2]$	454.122*	454.470
3	5	$[T_9 \quad T_{29} \quad T_{51} \quad T_{65} \quad S_1]$	31.379*	31.727
4	5	$[T_9 \quad T_{29} \quad T_{31} \quad T_{51} \quad T_{66}]$	0.075	0.422
1	6	$[T_{15} \quad T_{39} \quad T_{51} \quad S_1 \quad S_2 \quad R_L]$	1603.225*	1603.572
2	6	$[T_9 \quad T_{29} \quad T_{51}T_{65} \quad S_1 \quad S_2]$	454.017*	454.364
3	6	$[T_9 \quad T_{31} \quad T_{51} \quad T_{66} \quad S_1 \quad D]$	31.368*	31.715
4	6	$[T_{10} \quad T_{31} \quad T_{51} \quad T_{66} \quad D \quad B]$	0.052	0.400
1	77	$f(T_1, T_2, \ldots, T_{71}, L, S_1, S_2, R_L, D, B)$	1603.161*	1603.508
2	77	$f(T_1, T_2, \ldots, T_{71}, L, S_1, S_2, R_L, D, B)$	453.975*	454.322
3	77	$f(T_1, T_2, \ldots, T_{71}, L, S_1, S_2, R_L, D, B)$	31.319*	31.666
4	77	$f(T_1, T_2, \ldots, T_{71}, L, S_1, S_2, R_L, D, B)$	0.009	0.357

† In addition to two closed level loops
The loss is minimized to obtain $\mathbf{H}_2$
The optimal state drift $J_{opt}(d) = 0.347$
1 loop closed : 1 $\mathbf{c}$ from $\mathbf{y}_m$, 3 $\mathbf{c}$ from $\mathbf{u}_0$
2 loops closed: 2 $\mathbf{c}$ from $\mathbf{y}_m$, 2 $\mathbf{c}$ from $\mathbf{u}_0$
3 loop closed : 3 $\mathbf{c}$ from $\mathbf{y}_m$, 1 $\mathbf{c}$ from $\mathbf{u}_0$
4 loops closed: 4 $\mathbf{c}$ from $\mathbf{y}_m$
The optimal state drift $J_{opt}(d) = 0.347$
†† Such a high value is not physical, but it follows because our linear analysis is not appropriate when we close 0 loops
$*$ used partial control system idea to find optimal $\mathbf{H}_2$ in to step approach

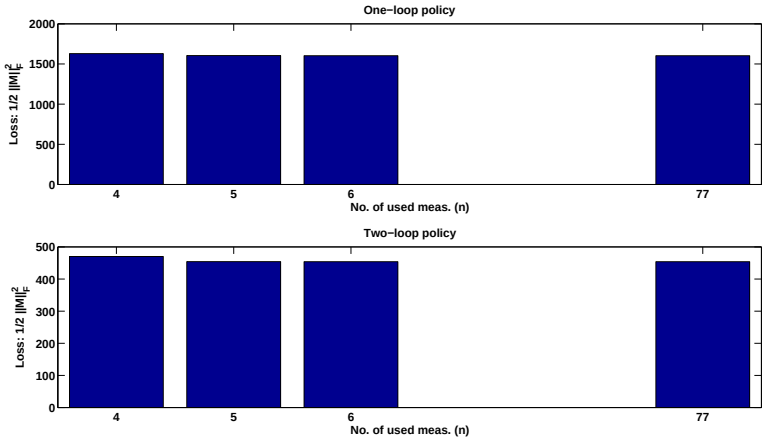

Figure 5.10: The reduction in loss vs number of used measurements, top: loss with one loop closed, bottom : loss with two loops closed

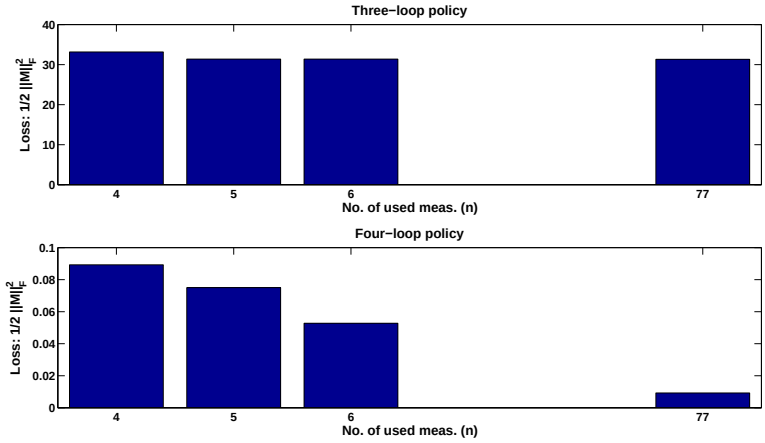

Figure 5.11: The reduction in loss vs number of used measurements, top : loss with three loop closed, bottom: loss with four loops closed

proposed method to find both optimal individual and combination of measurements as controlled variables was evaluated on a distillation column case study with 41 stages and Kaibel column case study with 71 stages to arrive at optimal regulatory layer with $1, 2$ and more closed loops. We included the dynamic simulations for the distillation column to show the ease of using these methods in practice.

Bibliography

Adrian, T., Schoenmakers, H., Boll, M., 2004. Model predictive control of integrated unit operations: Control of a divided wall column. Chemical Engineering and Processing 43 (3), 347–355.

Alstad, V., Skogestad, S., Hori, E., 2009. Optimal measurement combinations as controlled variables. Journal of Process Control 19 (1), 138–148.

Halvorsen, I. J., Skogestad, S., 2003. Minimum energy consumption in multicomponent distillation. 3. more than three products and generalized petlyuk arrangements. Industrial & Engineering Chemistry Research 42 (3), 616–629.

Halvorsen, I. J., Skogestad, S., Morud, J. C., Alstad, V., 2003. Optimal selection of controlled variables. Ind. Eng. Chem. Res. 42.

Hamid, M. K. A., Sin, G., Gani, R., 2010. Integration of process design and controller design for chemical processes using model-based methodology. Computers & Chemical Engineering 34 (5), 683 – 699, selected Paper of Symposium ESCAPE 19, June 14-17, 2009, Krakow, Poland.

Heath, J. A., Kookos, I. K., Perkins, J. D., 2000. Process control structure selection based on economics. AIChE Journal 46 (10), 1998–2016.

Heldt, S., 2010. Dealing with structural constraints in self-optimizing control engineering. Journal of Process Control 20 (9), 1049 – 1058.

Hori, E. S., Skogestad, S., 2008. Selection of controlled variables: Maximum gain rule and combination of measurements. Industrial & Engineering Chemistry Research 47 (23), 9465–9471.

Hori, E. S., Skogestad, S., Kwong, W., 2005. Use of perfect indirect control to minimize steady-state deviations. Proc. European Symposium on Computer Aided Process Engineering (ESCAPE-15), 29 May - 1 June, Barcelona, Spain, 1021–1026.

Kaibel, G., 1987. Distillation columns with vertical partitions. Chemical Engineering & Technology 10 (1), 92–98.

Kariwala, V., Cao, Y., 2010. Bidirectional branch and bound for controlled vaiable selection. Part III: Local average loss minimization. IEEE Transactions on Industrial Informatics 6, 54–61.

Kariwala, V., Cao, Y., Janardhanan, S., 2008. Local self-optimizing control with average loss minimization. Ind. Eng. Chem. Res. 47, 1150–1158.

Kookos, I. K., 2011. Control structure selection of an ideal reactive distillation column. Industrial & Engineering Chemistry Research 50 (19), 11193–11200.
URL http://pubs.acs.org/doi/abs/10.1021/ie201404j

Kothare, M. V., Shinnar, R., Rinard, I., Morari, M., 2000. On defining the partial control problem: Concepts and examples. AIChE Journal 46 (12), 2456–2474.

Luyben, W. L., 1996. Simple regulatory control of the eastman process. Industrial & Engineering Chemistry Research 35 (10), 3280–3289.

Narraway, L., Perkins, J., 1994. Selection of process control structure based on economics. Computers & Chemical Engineering 18, Supplement 1 (0), S511 – S515.

Narraway, L. T., Perkins, J. D., 1993. Selection of process control structure based on linear dynamic economics. Industrial & Engineering Chemistry Research 32 (11), 2681–2692.

Petlyuk, F., Platonov, V., Slavinskii, D., 1965. Thermodynamically optimal method for separating multicomponent mixtures. International Chemical Engineering 5 (3), 555–561.

Shinnar, R., 1981. Chemical reactor modelling for purposes of controller design. Chemical Engineering Communications 9 (1-6), 73–99.

Skogestad, S., 1997. Dynamics and control of distillation columns: A tutorial introduction. Chemical Engineering Research and Design 75 (6), 539 – 562, distillation.

Skogestad, S., 2000. Plantwide control: The search for the self-optimizing control structure. Journal of Process Control 10, 487–507.

Skogestad, S., 2003. Simple analytic rules for model reduction and pid controller tuning. Journal of Process Control 13 (4), 291 – 309.

Skogestad, S., Postlethwaite, I., 2005. Multivariable Feedback Control, 2. Edition. Wiley.

Strandberg, Jens; Skogestad, S., 2006. Stabilizing operation of a 4-product integrated kaibel column. Institution of Chemical Engineers Symposium Series 152, 636–647.

Yelchuru, R., Skogestad, S., Manum, H., 2010. MIQP formulation for controlled variable selection in self optimizing control. DYCOPS, July 7-9, Brussels, 61–66.

Chapter 6

Dynamic simulations with self optimizing controlled variables

The purpose of this chapter is to show the ease of using measurement combinations $\mathbf{c} = \mathbf{H}\mathbf{y}$ as controlled variables in dynamic simulations and same analysis is also reported in Alstad (2005). In addition, the dynamic performance in rejecting the process disturbances with these controlled variables is evaluated. The dynamic simulations with individual measurements and measurement combinations as controlled variables are also performed for a binary distillation column case study with 41 stages.

6.1 Distillation column

The distillation column (Figure 6.1) is included to show the ease of implementing measurement combinations as controlled variables in dynamic simulations. For this distillation column case study, we consider indirect composition control of a binary distillation column with 41 stages (Skogestad, 1997; Hori and Skogestad, 2008) and reflux (L) and boil-up (V) as the remaining unconstrained steady state degrees of freedom ($\mathbf{u}$). The considered disturbances are in feed flow rate (F), feed composition (z_F) and liquid fraction (q_F), which can vary between $1 \pm 0.2, 0.5 \pm 0.1$ and 1 ± 0.1, respectively. As online composition measurements are assumed unavailable, we use stage temperatures inside the column to control the compositions indirectly. The boiling points difference between light key component (L) and heavy key component (H) is 10 ^oC. We assume constant relative volatility

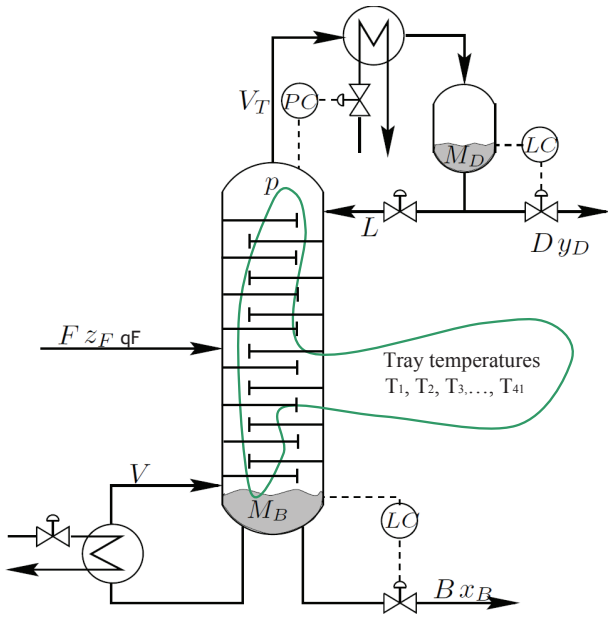

Figure 6.1: Distillation column using LV-configuration

of the components, constant pressure, no vapor hold up, equilibrium on each stage and constant molar flow rate. Under these assumptions only mass and component balances are included in this binary distillation column model and temperatures are approximated as linear functions of mole fractions. The temperature T_i (^oC) on stage i is calculated as a simple linear function of the liquid composition x_i on each stage (Skogestad, 1997).

$$T_i = 0x_i + 10(1 - x_i) \tag{6.1}$$

The candidate measurements are the 41 stage temperatures which are measured with an accuracy of $\pm 0.5^oC$. Note that we do *not* include the inputs (flows L and V) in the candidate measurements for this example because we would like to use only temperature combinations for control. The cost function J for the indirect composition control problem is the relative steady-state composition deviation,

$$J = \left(\frac{x^H_{top} - x^H_{top,s}}{x^H_{top,s}} \right)^2 + \left(\frac{x^L_{btm} - x^L_{btm,s}}{x^L_{btm,s}} \right)^2 \tag{6.2}$$

where x^H_{top} and x^L_{btm} denote the heavy key component (H) composition in top product and light key component (L) composition in bottom product.

Table 6.1: Distillation column: optimal measurements and optimal controlled variables with loss

No. Meas n	$\mathbf{c}'s$ as combinations of measurements	Loss $\frac{1}{2}\|\mathbf{M}\|_F^2$
2	$c_1 = T_{12}$ $c_2 = T_{30}$	0.5477
3	$c_1 = -0.0369T_{12} + 0.6449T_{30} + 0.6572T_{31}$ $c_2 = -1.2500T_{12} + 0.2051T_{30} + 0.1537T_{31}$	0.4425
4	$c_1 = 0.0100T_{11} - 0.0459T_{12} + 0.6450T_{30} + 0.6574T_{31}$ $c_2 = -0.6576T_{11} - 0.6548T_{12} + 0.2010T_{30} + 0.1413T_{31}$	0.3436
41	$c_1 = f(T_1, T_2, \ldots, T_{41})$ $c_2 = f(T_1, T_2, \ldots, T_{41})$	0.0813

The specification or set point value is denoted with subscript 's' (Hori and Skogestad, 2008). The optimal controlled variables (measurement combination matrix **H**) for the cases with 2, 3, 4 and 41 measurements using the methods of Chapter 3 are given in Table 6.1. Note that the controlled variables given here are directly the solutions from MIQP whereas the controlled variables are scaled to make the selected elements in **H** as 1 in Table 3.2.

6.2 Open loop simulations

To find the open loop dynamics of the distillation column in LV-configuration from reflux L, boil-up V to different controlled variables sets, the transient responses for a +5% step change in L and V at time 50 units, with controlled variables (i.e. $c_1 = T_{30}$, $c_2 = T_{12}$) are shown in Figures 6.2 and 6.3, respectively. The transient responses for a +5% step change in L and V with controlled variables as combinations of 3 temperature measurements (i.e. $c_1 = -0.0369T_{12} + 0.6449T_{30} + 0.6572T_{31}$, $c_2 = -1.2500T_{12} + 0.2051T_{30} + 0.1537T_{31}$) are also shown in Figures 6.4 and 6.5. The open loop transient responses (Figures 6.2 - 6.5) are used to find process gain, time constant from L to c_1 and V to c_2 approximately.

6.3 Dynamic simulations

Controlled variables as individual measurements

From the open loop transient responses of controlled variables (i.e. $c_1 = T_{30}$, $c_2 = T_{12}$) in Figures 6.2 and 6.3, a Proportional Integral (PI) con-

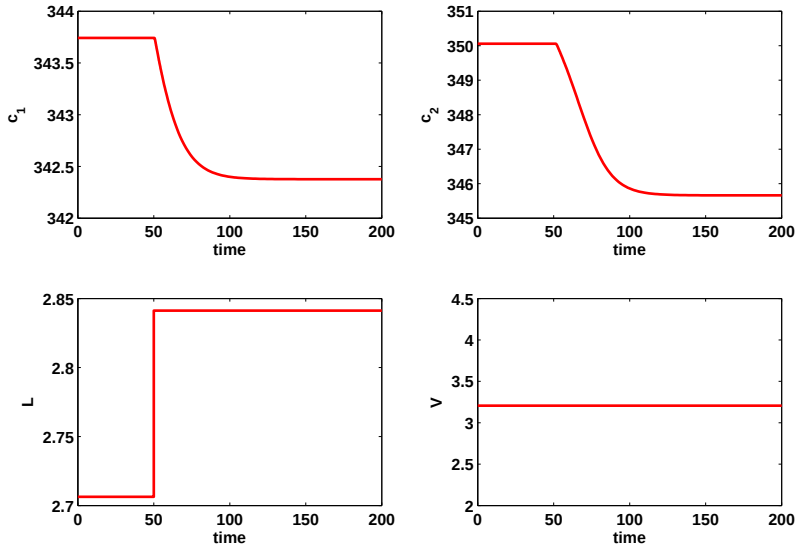

Figure 6.2: Controlled variables as individual temperature measurements (T_{30}, T_{12}): step change +5% in L

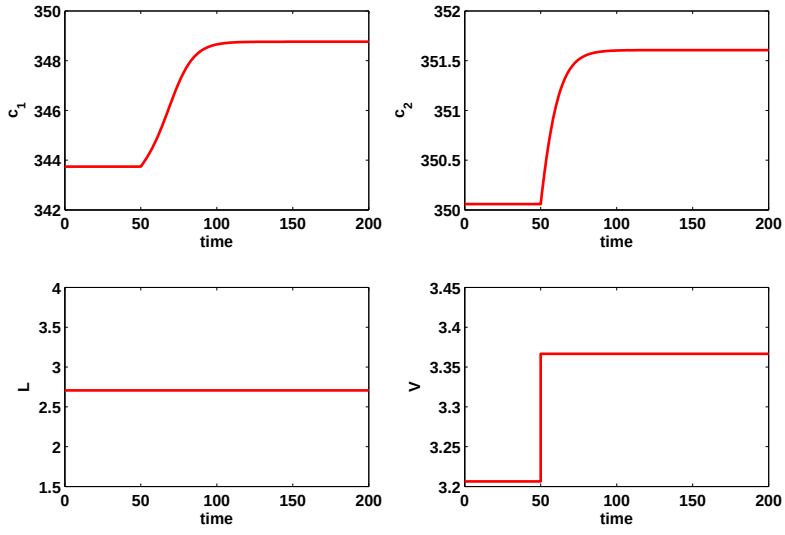

Figure 6.3: Controlled variables as individual temperature measurements (T_{30}, T_{12}): step change +5% in V

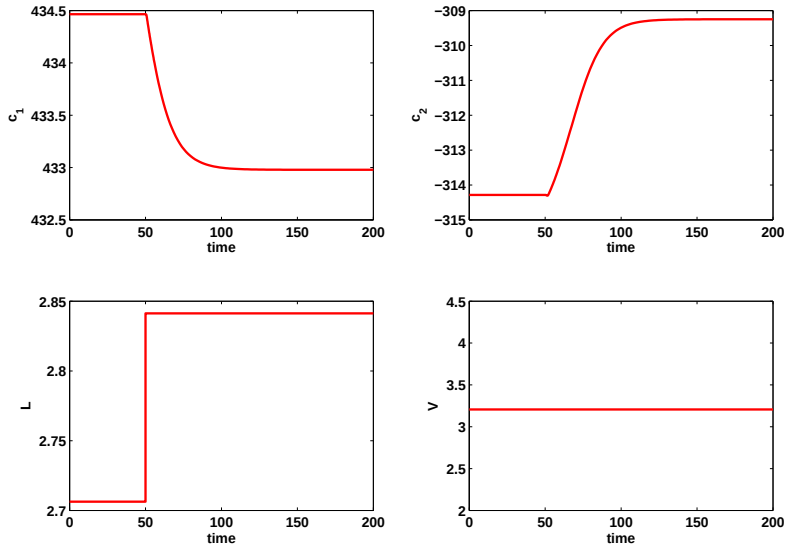

Figure 6.4: Controlled variables as combinations of 3 temperature measurements: step change +5% in L

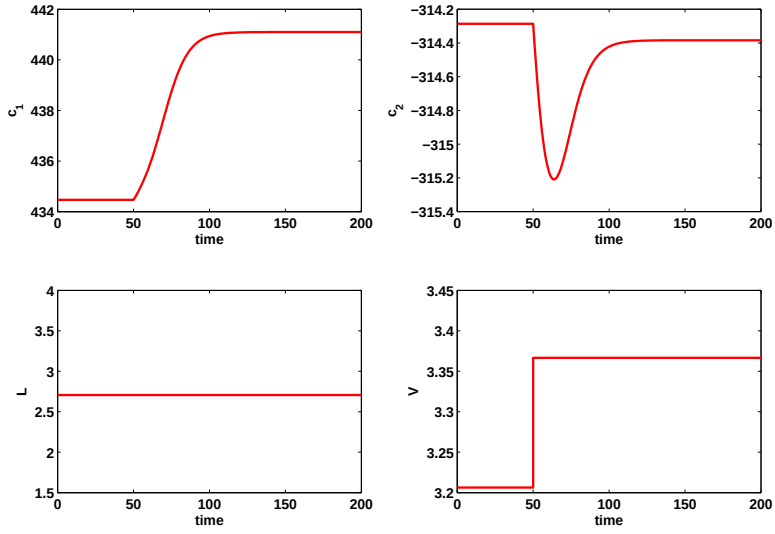

Figure 6.5: Controlled variables as combinations of 3 temperature measurements: step change +5% in V

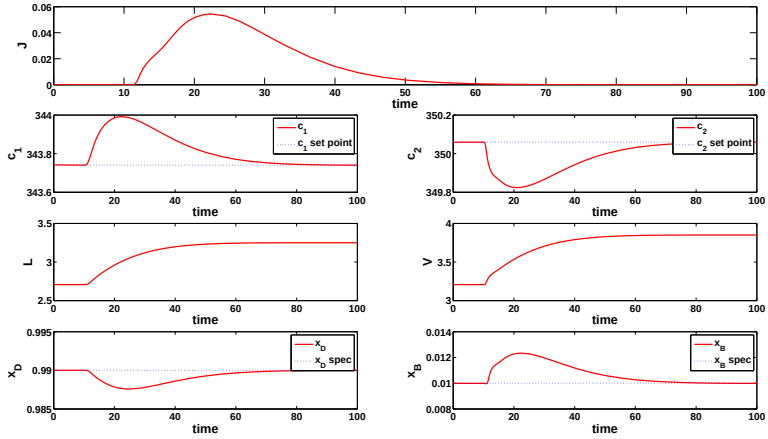

Figure 6.6: Transient responses of cost (J), c_1, c_2 as individual measurements, L, V, x_D, x_B for a step disturbance of +20% magnitude in feed rate F

troller between L and c_1 with tuning parameters $k_{c_1} = -0.5449, \tau_{I_1} = 8$ and an another PI controller between V and c_2 with tuning parameters $k_{c_2} = -11.5129, \tau_{I_2} = 8$ are obtained using SIMC tunings (Skogestad, 2003) with $\tau_c = 2$. The set points for the controlled variables c_1 and c_2 are based on the temperatures at nominal optimal point, i.e. $c_{1,s} = 343.74$ and $c_{2,s} = 350.06$. The performance of decentralized PI controllers in rejecting disturbances in feed rate F, feed composition z_F and feed liquid fraction q_F are shown in Figures 6.6, 6.7, and 6.8, respectively.

The transient responses of the cost (J), selected controlled variables (c_1, c_2) with their set points, manipulated variables (L, V) and the product compositions (x_D, x_B) with their specifications are shown in each of the Figures 6.6, 6.7, and 6.8 in the presence of disturbances **d**.

Controlled variables as combinations of 3 temperature measurements

From the open loop transient responses of controlled variables (i.e. $c_1 = -0.0369T_{12} + 0.6449T_{30} + 0.6572T_{31}$, $c_2 = -1.2500T_{12} + 0.2051T_{30} + 0.1537T_{31}$) in Figures 6.4 and 6.5, a PI controller between L and c_1 with tuning parameters $k_{c_1} = -0.5933, \tau_{I_1} = 8$ and an another PI controller between V and c_2 with tuning parameters $k_{c_2} = -0.7249, \tau_{I_2} = 8$ are obtained using SIMC tunings (Skogestad, 2003) with $\tau_c = 2$. The set points for these controlled

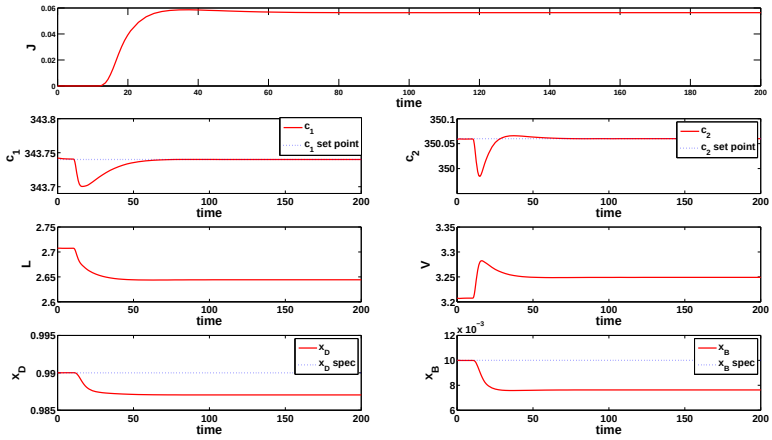

Figure 6.7: Transient responses of cost (J), c_1, c_2 as individual measurements, L, V, x_D, x_B for a step disturbance of +20% magnitude in feed composition z_F

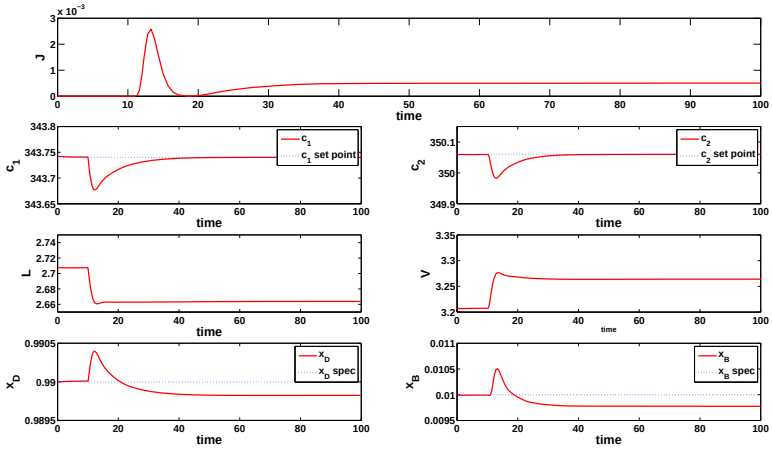

Figure 6.8: Transient responses of cost (J), c_1, c_2 as individual measurements, L, V, x_D, x_B for a step disturbance of +10% magnitude in feed liquid fraction q_F

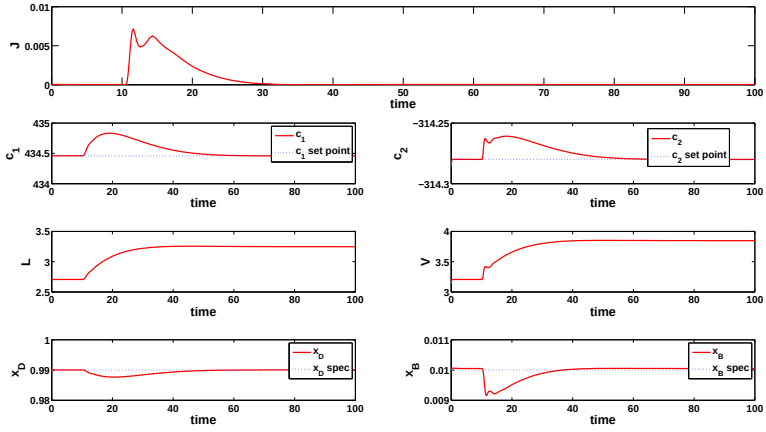

Figure 6.9: Transient responses of cost (J), c_1, c_2 as combinations of 3 temperatures, L, V, x_D, x_B for a step disturbance of +20% magnitude in feed rate F

variables c_1 and c_2 are based on the temperatures at nominal optimal point, $c_{1,s} = 434.46$ and $c_{2,s} = -314.28$. The performance of the decentralized PI controllers in rejecting disturbances in feed rate F, feed composition z_F and feed liquid fraction q_F are shown in Figures 6.9, 6.10, and 6.11, respectively.

The transient responses of the cost (J), selected controlled variables (c_1, c_2) with their set points, manipulated variables (L, V) and the product compositions (x_D, x_B) with their specifications are shown in each of the Figures 6.9, 6.10, and 6.11 in the presence of disturbances **d**. The dynamic performance analysis is also repeated for controlled variables as combinations of 4 measurements (the transient responses are not shown). From the Figures 6.6 - 6.11, it can be seen that using more measurements in controlled variable combinations inherit better self optimizing properties in rejecting the same magnitudes of disturbances **d**.

6.4 Conclusions

We showed the ease of implementing measurement combinations as controlled variables in dynamic simulations. The performance in rejecting the main disturbances is studied using dynamic simulations. The better self optimizing abilities with controlled variables as combination of measurements is demonstrated.

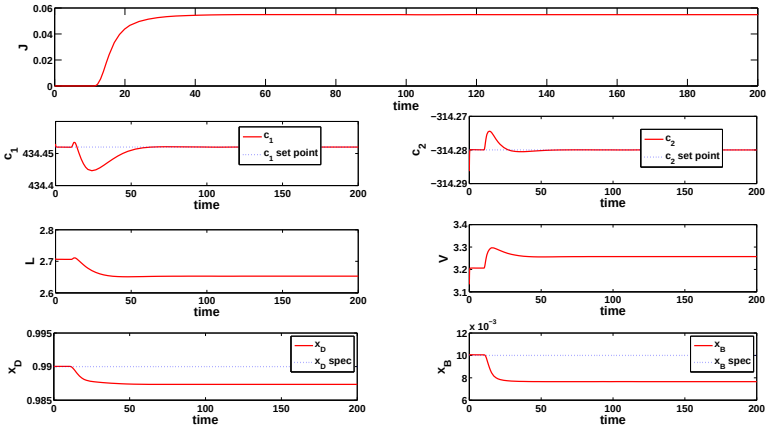

Figure 6.10: Transient responses of cost (J), c_1, c_2 as combinations of 3 temperatures, L, V, x_D, x_B for a step disturbance of +20% magnitude in feed composition z_F

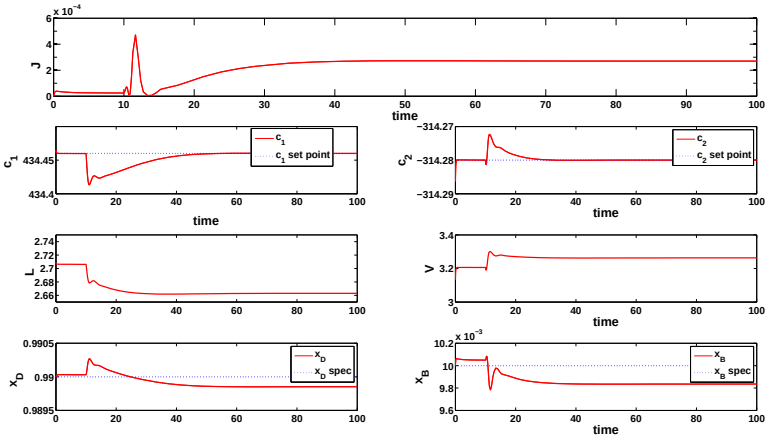

Figure 6.11: Transient responses of cost (J), c_1, c_2 as combinations of 3 temperatures, L, V, x_D, x_B for a step disturbance of +10% magnitude in feed liquid fraction q_F

Bibliography

Alstad, V., 2005. Studies on selection of controlled variables. Ph.D. thesis, Norwegian University of Science and Technology, Department of Chemical Engineering.

Hori, E. S., Skogestad, S., 2008. Selection of controlled variables: Maximum gain rule and combination of measurements. Industrial & Engineering Chemistry Research 47 (23), 9465–9471.

Skogestad, S., 1997. Dynamics and control of distillation columns: A tutorial introduction. Chemical Engineering Research and Design 75 (6), 539 – 562, distillation.

Skogestad, S., 2003. Simple analytic rules for model reduction and pid controller tuning. Journal of Process Control 13 (4), 291 – 309.

Chapter 7

Conclusions and future work

7.1 Concluding remarks

Optimal operation of process plants is the main focus of this thesis and we precisely address the optimal controlled variables selection problem in self-optimizing control. The self-optimizing control is a simple feedback strategy with appropriate controlled variables selection and controlling them at constant set point to result in an acceptable steady state loss from optimality. The mathematical formulation of controlled variables selection as linear measurement combinations, $\mathbf{c} = \mathbf{H}\mathbf{y}$, (Halvorsen et al., 2003) that minimize the steady state loss from optimality for a combined disturbance and implementation error space is the precursor for our research. Solving for an optimal $\mathbf{H}$ is main focus of this thesis.

The formulations with controlled variables, $\mathbf{c} = \mathbf{H}\mathbf{y}$, for acceptable steady state loss are originally believed to be non-convex and are assumed to be difficult to solve numerically (Halvorsen et al., 2003). Hence, previously few qualitative requirements, minimum singular value rule (Halvorsen et al., 2003), minimum loss method (Halvorsen et al., 2003) and null space method (Alstad and Skogestad, 2007) are proposed to find the controlled variables that minimize the steady state deviation from optimal operation. Later, the problem of finding optimal $\mathbf{H}$ was reformulated as a convex quadratic optimization problem (Alstad et al., 2009) .

7.1.1 Optimal selection of controlled variables and measurement subsets with full H

The problem of finding an optimal CV as measurement combinations that minimize the loss from optimal operation is solved. The optimal CV selection problem from self optimizing control framework is reformulated as a QP and the measurement subset selection is formulated as an MIQP problem. The developed MIQP based method allows for additional structural constraints compared to the bidirectional branch and bound methods reported in literature. The MIQP based method was found to use about 10 times more CPU time than the bidirectional branch and bound methods, but this is acceptable as the optimal CV selection problem is done offline. In addition, the MIQP method can be used on some problems where the branch and bound methods do not apply, as shown for the Kaibel column example.

7.1.2 Optimal selection of controlled variables and measurements with structured H

For ease of implementation and better dynamic controllability, we included particular structures in $\mathbf{H}$ in self-optimizing control and these form non-convex problems. We presented a few new ideas and two convex approximation methods for structured $\mathbf{H}$ problems in self-optimizing control to find practically significant upper bounds. The proposed convex approximation methods are extended to find optimal fewer measurements with MIQP formulations. The proposed convex approximation methods are observed to provide reasonably good upper bounds for the true optimal solution in the considered (decentralized) block diagonal $\mathbf{H}$ and triangular $\mathbf{H}$ structures for evaporator and distillation column case studies.

7.1.3 Regulatory layer selection

The self optimizing control concepts are extended to select optimal controlled variables that minimize the state drift in the presence of disturbances. In process control, $\|\mathbf{W}\mathbf{x}(j\omega)\|_2^2$ is often flat at lower frequencies and drops at higher frequencies, so minimizing the state drift for steady-state ($\omega = 0$) yields good results. We presented a framework on how to use self-optimizing control minimum loss method that minimize the state drift to arrive at optimal regulatory layer with $1, 2$ or more closed loops. The proposed method to find both optimal individual and combination of measurements as controlled variables was evaluated on a distillation column

case study with 41 stages and on a Kaibel column case study with 71 stages to arrive at optimal regulatory layer with $1, 2$ or more closed loops.

7.1.4 Dynamic simulations with measurement combinations as CV

We showed the ease of implementing measurement combinations as controlled variables in dynamic simulations. The disturbance rejection ability is assessed for main disturbances. We demonstrated the better self optimizing abilities with controlled variables as combination of measurements.

7.2 Directions for future work

7.2.1 Integrated process design and operation

Arriving at an optimal operating point for a integrated process plant with recycles is difficult due to the recycles, nonlinear behavior and multiple local minimums with in the range of process operation. Performing an integrated process design without accounting for the ease in optimal operation can make the gains of integrated process design only partially realizable. Hence efficient process models should be developed that result in a single local minimum and new methods that account for integrated design and ease in operation should be developed.

7.2.2 Robust optimal controlled variable selection methods

Uncertainties in process modeling are inevitable. To account for these uncertainties, robust controlled variables selection methods based on economics should be developed. These uncertainties can be either structured or unstructured uncertainties. To address these, we can introduce part of structured uncertainties that cannot be represented as linear combinations of the considered disturbances as new disturbances and part of unstructured uncertainties that cannot be represented as linear combinations of the considered implementation errors as new implementation errors. The open research area here is the characterization of the new disturbances and new implementation errors due to the uncertainties.

7.2.3 Fixed CV for all active constraint regions

The self-optimizing control provides systematic and good methods to find optimal controlled variables for a chosen active constraints set. But it should

be repeated for all the possible different active constraints sets over the disturbance space. The resulting controlled variables in different active constraint regions may require reconfiguration of control loops that are difficult to implement in practice. To obviate this, new methods need to be developed to arrive at fixed controlled variables for all active constraint regions with minimal loss in all regions from true optimal solutions. For these new methods, the controlled variables and the losses obtained for each active constraint region with the methods of this thesis can serve as the best achievable lower bounds.

7.2.4 Experimental validation of proposed methods

The proposed methods in this thesis arrive at optimal controlled variables as individual /combinations of measurements that minimize the steady state loss from optimality. The performance of these controlled variables should be verified by experiments in the presence of disturbances.

7.2.5 Economic optimal CV selection based on dynamics

The thesis assumes that process economics are governed by steady/pseudo steady state and we obtain optimal controlled variables in self-optimizing control. Extending these self-optimizing control concepts to arrive at quantitative methods that result in economic optimal controlled variables based on dynamics is an open area of research.

Bibliography

Alstad, V., Skogestad, S., 2007. Null space method for selecting optimal measurement combinations as controlled variables. Ind. Eng. Chem. Res. 46, 846–853.

Alstad, V., Skogestad, S., Hori, E., 2009. Optimal measurement combinations as controlled variables. Journal of Process Control 19 (1), 138–148.

Halvorsen, I. J., Skogestad, S., Morud, J. C., Alstad, V., 2003. Optimal selection of controlled variables. Ind. Eng. Chem. Res. 42.

Appendix A

Vectorization procedure

The vectorization procedure of convex optimization problem in decision matrix $\mathbf{H}$

$$\begin{aligned} &\min_{\mathbf{H}} \|\mathbf{HY}\|_F \\ &\text{s.t. } \mathbf{HG}^y = \mathbf{J}_{uu}^{1/2} \end{aligned} \tag{A.1}$$

to convex optimization problem in $\mathbf{h}_\delta$ is described (Alstad, 2005; Alstad et al., 2009). We write

$$\mathbf{H} = \begin{bmatrix} h_{11} & h_{12} & \dots & h_{1n_y} \\ h_{21} & h_{22} & \dots & h_{2n_y} \\ \vdots & \vdots & \ddots & \vdots \\ h_{n_u1} & h_{n_u2} & \dots & h_{n_un_y} \end{bmatrix} = \begin{bmatrix} \mathbf{h}_1 & \mathbf{h}_2 & \dots & \mathbf{h}_{n_y} \end{bmatrix} = \begin{bmatrix} \tilde{\mathbf{h}}_1^T \\ \tilde{\mathbf{h}}_2^T \\ \vdots \\ \tilde{\mathbf{h}}_{n_u}^T \end{bmatrix}$$

where

$$\begin{aligned} \mathbf{h}_j &= j^{th}\text{column of } \mathbf{H},\ \mathbf{h}_j \in \mathbb{R}^{n_u \times 1} \\ \tilde{\mathbf{h}}_j &= j^{th}\text{row of } \mathbf{H},\ \tilde{\mathbf{h}}_j \in \mathbb{R}^{n_y \times 1} \end{aligned}$$

The transpose must be included because all vectors including $\tilde{\mathbf{h}}_i$ are column vectors. Similarly, let $\mathbf{J}_{uu}^{1/2} = [\mathbf{j}_1 \quad \mathbf{j}_2 \quad \dots \quad \mathbf{j}_{n_u}]$. We further introduce the

long vectors $\mathbf{h}_\delta$ and $\mathbf{j}_\delta$,

$$\mathbf{h}_\delta = \begin{bmatrix} \tilde{\mathbf{h}}_1 \\ \tilde{\mathbf{h}}_2 \\ \dots \\ \tilde{\mathbf{h}}_{n_u} \end{bmatrix} = \begin{bmatrix} h_{11} \\ h_{12} \\ \vdots \\ h_{1n_y} \\ h_{21} \\ h_{22} \\ \vdots \\ h_{2n_y} \\ h_{n_u 1} \\ h_{n_u 2} \\ \vdots \\ h_{n_u n_y} \end{bmatrix} \in \mathbb{R}^{n_u n_y \times 1}$$

$\mathbf{j}_\delta^T = \begin{bmatrix} \mathbf{j}_1^T & \mathbf{j}_2^T & \dots & \mathbf{j}_{n_u}^T \end{bmatrix} \in \mathbb{R}^{n_u n_u \times 1}$ and the large matrices

$$\mathbf{G}_\delta^T = \begin{bmatrix} \mathbf{G}^{y^T} & 0 & 0 & \cdots \\ 0 & \mathbf{G}^{y^T} & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \\ 0 & 0 & \dots & \mathbf{G}^{y^T} \end{bmatrix}; \ \mathbf{Y}_\delta = \begin{bmatrix} \mathbf{Y} & 0 & 0 & \cdots \\ 0 & \mathbf{Y} & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \\ 0 & 0 & \dots & \mathbf{Y} \end{bmatrix}$$

Then, $\mathbf{HY} = \begin{bmatrix} \tilde{\mathbf{h}}_1^T \mathbf{Y} \\ \tilde{\mathbf{h}}_2^T \mathbf{Y} \\ \dots \\ \tilde{\mathbf{h}}_{n_u}^T \mathbf{Y} \end{bmatrix}$ and for the Frobenius norm the following equalities apply.

$$\|\mathbf{HY}\|_F^2 = \left\| \begin{bmatrix} \tilde{\mathbf{h}}_1^T \mathbf{Y} \\ \tilde{\mathbf{h}}_2^T \mathbf{Y} \\ \vdots \\ \tilde{\mathbf{h}}_{n_u}^T \mathbf{Y} \end{bmatrix} \right\|_F = \| \begin{array}{cccc} \tilde{\mathbf{h}}_1^T \mathbf{Y} & \tilde{\mathbf{h}}_2^T \mathbf{Y} & \dots & \tilde{\mathbf{h}}_{n_u}^T \mathbf{Y} \end{array} \|_F$$
$$= \|\mathbf{h}_\delta^T \mathbf{Y}_\delta\|_F = \|\mathbf{h}_\delta \mathbf{Y}_\delta^T\|_F = \mathbf{h}_\delta^T \underbrace{\mathbf{Y}_\delta \mathbf{Y}_\delta^T}_{\mathbf{F}_\delta} \mathbf{h}_\delta = \mathbf{h}_\delta^T \mathbf{F}_\delta \mathbf{h}_\delta$$

Because $\mathbf{HG}^y = \mathbf{J}_{uu}^{1/2}$ where $\mathbf{J}_{uu}^{1/2}$ is symmetric matrix, we have $\mathbf{HG}^y = \mathbf{G}^{y^T}\mathbf{H}^T = \mathbf{J}_{uu}^{1/2}$ and

$$\begin{bmatrix} \mathbf{G}^{y^T} \tilde{\mathbf{h}}_1 & \mathbf{G}^{y^T} \tilde{\mathbf{h}}_2 & \dots & \mathbf{G}^{y^T} \tilde{\mathbf{h}}_{n_u} \end{bmatrix} = [\mathbf{j}_1 \quad \mathbf{j}_2 \dots \mathbf{j}_{n_u}] \implies \mathbf{G}_\delta^T \mathbf{h}_\delta = \mathbf{j}_\delta$$

.

The resulting vectorized convex QP is

$$\begin{aligned} &\min_{\mathbf{h}_\delta} \ \mathbf{h}_\delta^T \mathbf{F}_\delta \mathbf{h}_\delta \\ &\text{s.t. } \mathbf{G}_\delta^{y^T} \mathbf{h}_\delta = \mathbf{j}_\delta \end{aligned} \tag{A.2}$$

Bibliography

Alstad, V., 2005. Studies on selection of controlled variables. Ph.D. thesis, Norwegian University of Science and Technology, Department of Chemical Engineering.

Alstad, V., Skogestad, S., Hori, E., 2009. Optimal measurement combinations as controlled variables. Journal of Process Control 19 (1), 138–148.

Appendix B

Evaporator model equations

The evaporator case study is a simple but a realistic process to evaluate the quantitative methods developed in this thesis. The evaporator is a "forced-circulation" evaporator and is used to increase the concentration of dilute liquor by evaporating solvent from the feed stream through a vertical heat exchanger with circulated liquor. The evaporator process Figure B.1 is taken from Newell and Lee (1989) and is modified as described in Kariwala et al. (2008).

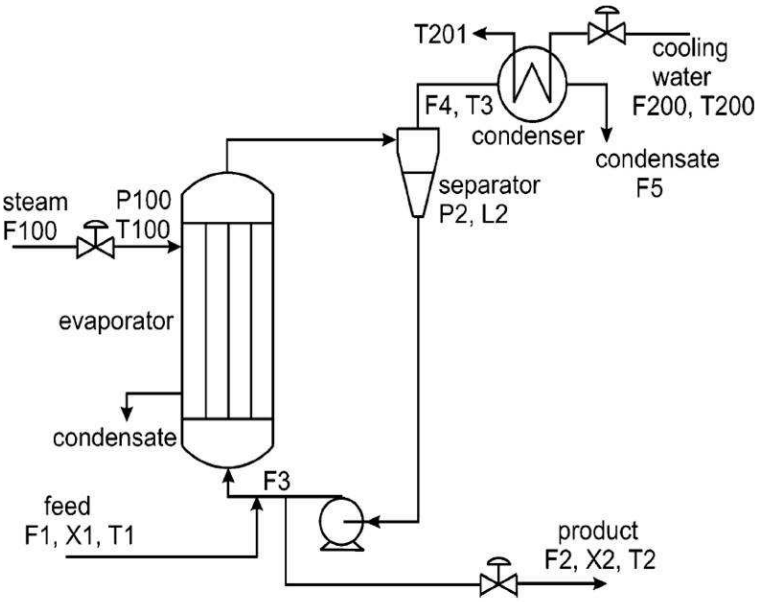

Figure B.1: Evaporator process

The economic objective is to maximize the operating profit [$/$h$], formulated as minimization of the negative profit (Kariwala et al., 2008).

$$J = 600F_{100} + 0.6F_{200} + 1.009(F_2 + F_3) + 0.2F_1 - 4800F_2 \tag{B.1}$$

The major constraints for this evaporator are product specification, safety and design limits

$$\begin{aligned} X_2 &\geq 35 + 0.5\% \\ 40kPa \leq P_2 &\leq 80kPa \\ P_{100} &\leq 400kPa \\ 0kg/min \leq F_{200} &\leq 400kg/min \\ 0kg/min \leq F_1 &\leq 20kg/min \\ 0kg/min \leq F_3 &\leq 100kg/min \end{aligned} \tag{B.2}$$

The evaporator process is optimized to maximize the profit (B.1) with process constraints (B.2) and the optimization data are given in Table B.1 The modified evaporator model equations are

$$20\frac{dL_2}{dt} = F_1 - F_4 - F_2 \tag{B.3}$$

$$20\frac{dX_2}{dt} = F_1X_1 - F_2X_2 \tag{B.4}$$

$$4\frac{dP_2}{dt} = F_4 - F_5 \tag{B.5}$$

$$T_2 = 0.5616P_2 + 0.3126X_2 + 48.43 \tag{B.6}$$

$$T_3 = 0.507P_2 + 55 \tag{B.7}$$

$$F_4 = \frac{Q_{100} - 0.07F_1(T_2 - T_1)}{38.5} \tag{B.8}$$

$$T_{100} = 0.1538P_{100} + 90 \tag{B.9}$$

$$Q_{100} = 0.16(F_1 + F_3)(T_{100} - T_2) \tag{B.10}$$

$$F_{100} = \frac{Q_{100}}{36.6} \tag{B.11}$$

$$Q_{200} = \frac{0.9576F_{200}(T_3 - T_{200})}{0.14F_{200} + 6.84} \tag{B.12}$$

$$T_{201} = T_{200} + \frac{13.68(T_3 - T_{200})}{0.14F_{200} + 6.84} \tag{B.13}$$

$$F_5 = \frac{Q_{200}}{38.5} \tag{B.14}$$

Table B.1: Evaporator example: variables at nominal optimum point

Variable	Description	Value
F_1	feed flow rate	9.469 kg/min
F_2	product flow rate	1.334 kg/min
F_3	circulating flow rate	24.721 kg/min
F_4	vapor flow rate	8.135 kg/min
F_5	condensate flow rate	8.135 kg/min
X_1	feed composition	5.000%
X_2	product composition	35.500%
T_1	feed temperature	40.000 C
T_2	product temperature	88.400 C
T_3	vapor temperature	81.066 C
L_2	separator level	1.000 m
P_2	operating pressure	51.412 kPa
F_{100}	steam flow rate	9.434 kg/min
T_{100}	steam temperature	151.520 C
P_{100}	steam pressure	400.000 kPa
Q_{100}	heat duty	345.292 kW
F_{200}	cooling water flowrate	217.738 kg/min
T_{200}	inlet temperature of cooling water	25.000 C
T_{201}	outlet temperature of cooling water	45.550 C
Q_{200}	condenser duty	313.210 kW

Bibliography

Kariwala, V., Cao, Y., Janardhanan, S., 2008. Local self-optimizing control with average loss minimization. Ind. Eng. Chem. Res. 47, 1150–1158.

Newell, R. B., Lee, P., 1989. Applied process control : A case study. Prentice-Hall of Australia, New York ; Sydney.

Appendix C

Distillation column model and assumptions

The distillation column case study is taken from Skogestad (1997)

C.1 Assumptions

The binary distillation column with 41 stages in LV-configuration is taken from Skogestad (1997) and reflux (L) and boil-up (V) are the remaining unconstrained steady state degrees of freedom (**u**) (Figure C.1). The assumptions in the model are binary mixture, constant pressure, constant relative volatility, constant molar flows, no vapor holdup, linear liquid dynamics, equilibrium on all stages, total condenser.

C.2 Notation

- L_i and V_i - liquid and vapor flow from stage i [kmol/min]
- x_i and y_i - liquid and vapor composition of light component on stage i [mole fraction]
- M_i - liquid holdup on stage i [kmol] D and B - distillate (top) and bottoms product flowrate [kmol/min]
- L and V - reflux flow and boilup flow [kmol/min]
- F and z_F - feed rate [kmol/min] and feed composition [mole fraction]
- q_F - fraction of liquid in feed

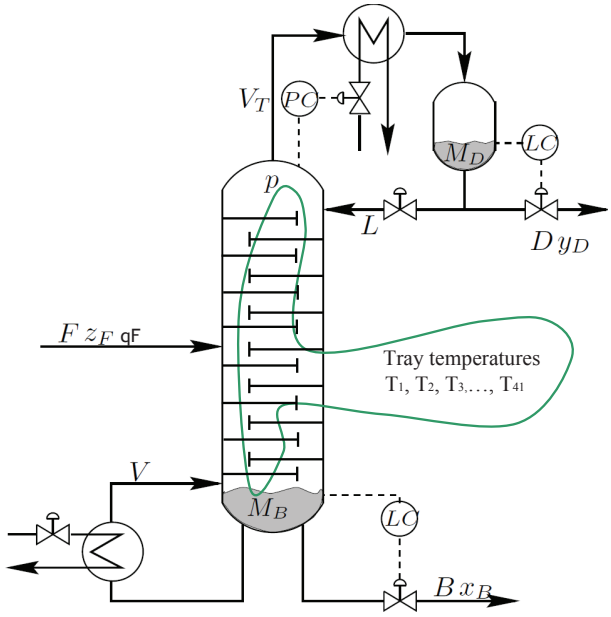

Figure C.1: Distillation column using LV-configuration

- i - stage no. (1=bottom. N_F=feed stage = 21, N_T=total condenser)
- α - relative volatility between light and heavy component
- τ_l - time constant [min] for liquid flow dynamics on each stage
- λ - constant for effect of vapor flow on liquid flow ("K2-effect")

C.3 Model equations

We will write the model such that the states are x_i and M_i $\forall i = 1, 2, \ldots, N_T$, a total of $2N_T$ states. The basic equations are

1. Total material balance on stage i

$$\frac{dM_i}{dt} = L_{i+1} - L_i + V_{i-1} - V_i \tag{C.1}$$

2. Material balance for light component on each stage i:

$$\frac{d(M_i x_i)}{dt} = L_{i+1}x_{i+1} + V_{i-1}y_{i-1} - L_i x_i - V_i y_i \tag{C.2}$$

which gives the following expression for the derivative of the liquid mole fraction

$$M_i \frac{dx_i}{dt} = \frac{d(M_i x_i)}{dt} - \frac{x_i dM_i}{dt} \tag{C.3}$$

3. Algebraic equations : The vapor composition y_i is related to the liquid composition x_i on the same stage through the algebraic vapor-liquid equilibrium

$$y_i = \frac{\alpha x_i}{1 + (\alpha - 1)x_i} \tag{C.4}$$

where α is the relative volatility. From the assumption of constant molar flows and no vapor dynamics we have the following expression for the vapor flows (except at the feed stage if the feed is partly vaporized), where $V_{N_F} = V_{N_F - 1} + (1 - q_F)F$:

$$V_i = V_{i-1} \tag{C.5}$$

4. The liquid flows depend on the liquid holdup on the stage above and the vapor flow as follows (this is a linearized relationship; we may alternatively use Francis' Weir formula etc.):

$$L_i = L0_i + (M_i - M0_i)\tau_l + (V - V0)_{i-1}\lambda \tag{C.6}$$

where $L0_i$ [kmol/min] and $M0_i$ [kmol] are the nominal values for the liquid flow and holdup on stage i. The vapor flow into the stage may also effect the holdup; λ may be positive because more vapor may give more bubbles and thus may push liquid off the stage. If λ is large (larger than 0.5) then the re-boiler holdup "flattens out" for some time in response to an increase in boil-up, and if $\lambda > 1$ we get an inverse response. λ may also be negative if the increased pressure drop caused by larger V results in a larger holdup in the down comers - in general it is difficult to estimate λ for tray columns. For packed columns λ is usually close to zero.
The above equations apply at all stages except in the top (condenser), feed stage and bottom (re-boiler).

5. Feed stage, $i = N_F$ (we assume the feed is mixed directly into the liquid at the feed stage):

$$\frac{dM_i}{dt} = L_{i+1} - L_i + V_{i-1} - V_i + F \tag{C.7}$$

$$\frac{d(M_i x_i)}{dt} = L_{i+1}x_{i+1} + V_{i-1}y_{i-1} - L_i x_i - V_i y_i + F z_F \tag{C.8}$$

6. Total condenser, $i = N_T$ ($M_{N_T} = M_D, L_{N_T} = L_T$)

$$\frac{dM_i}{dt} = V_{i-1} - L_i - D \tag{C.9}$$

$$\frac{d(M_i x_i)}{dt} = V_{i-1} y_{i-1} - L_i x_i - D x_i \tag{C.10}$$

7. Re-boiler, $i = 1$ ($M_i = M_B, V_i = V_B = V$)

$$\frac{dM_i}{dt} = L_{i+1} - V_i - B \tag{C.11}$$

$$\frac{d(M_i x_i)}{dt} = L_{i+1} x_{i+1} - V_i y_i - B x_i \tag{C.12}$$

C.4 Column data

- $N_T = 41$ stages including re-boiler and total condenser
- Feed at stage $N_F = 21$ counted from the bottom
- Nominal conditions: Feed rate F = 1 [kmol/min], Feed composition $z_F = 0.5$ [mole fraction units], Feed liquid fraction $q_F = 1$ (i.e., saturated liquid), Reflux flow $L_T = 2.706$ [kmol/min], Boilup V = 3.206 [kmol/min].
- The nominal liquid holdup on all 41 stages is $M0_i = 0.5$ [kmol] (including the re-boiler and condenser; for more realistic studies you may use $M0_1 = 10$ [kmol] (reboiler) and $M0_{N_T} = 32.1$ [kmol] (condenser)).
- The time constant for the liquid flow dynamics on each stage (except the reboiler and condenser) is $\tau_l = 0.063$ min. We assume that the vapor flow does not effect the liquid holdup, i.e. $\lambda = 0$.

This results in a distillate product with $D = 0.5$ [kmol/min] and composition $y_D = x_{N_T} = 0.99$ [mole fraction units], and a bottoms product with $B = 0.5$ [kmol/min] and composition $x_B = x_1 = 0.01$ [mole fraction units].

Bibliography

Skogestad, S., 1997. Dynamics and control of distillation columns: A tutorial introduction. Chemical Engineering Research and Design 75 (6), 539 – 562, distillation.

Appendix D

Steady state model between inputs for distillation column

Mass balances for binary distillation column assuming for the condenser and re-boiler at steady state yield (Häggblom and Waller, 1990)

$$\frac{dM_d}{dt} = 0 = V_{top} - L - D \tag{D.1}$$

$$\frac{dM_b}{dt} = 0 = L_{btm} - V - B \tag{D.2}$$

Here, at steady state and assuming constant molar flows

$$V_{top} = V + (1 - q_F)F \tag{D.3}$$

$$L_{btm} = L + q_F F \tag{D.4}$$

So we find at steady state

$$D = V - L + (1 - q_F)F \tag{D.5}$$

$$B = L + q_F F - V \tag{D.6}$$

Note that there is no effect of z_F in this case. Linearizing gives $\mathbf{G}^u$ and $\mathbf{G}_d^u$ as

$$\mathbf{G}^u = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -1 & 1 \\ 1 & -1 \end{bmatrix}, \quad \mathbf{G}_d^u = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 1 \end{bmatrix}$$

Bibliography

Häggblom, K. E., Waller, K. V., 1990. Control structures for disturbance rejection and decoupling of distillation. AIChE Journal 36 (7), 1107–1113.

Appendix E

Kaibel column model and assumptions

E.1 Model assumptions

The 4-product Kaibel column (Figure E.1) has high energy saving potential (Halvorsen and Skogestad, 2003), but presents a difficult control problem and serves as a good example to evaluate the quantitative methods developed in this thesis. The given 4-product Kaibel column arrangement separates a mixture of methanol (A), ethanol (B), propanol (C), butanol (D) into almost pure components. The Kaibel column model uses a stage-by-stage model (Strandberg, 2011).

E.2 Main assumptions

- Constant molar flows: That is $V_i = V_{i+1}$ and $L_i = L_{i-1}$ for stage i inside a column section.
- Constant pressure P.
- Equilibrium on each stage.
- No heat transfer across dividing wall.
- Linearized flow dynamics: The liquid flow dynamics are modeled as

$$L_i = L_{0,i} + \frac{M_i - M_{0,i}}{\tau_L} + (V_{i-1} - V_{0,i-1})\lambda \tag{E.1}$$

  where $L_{0,i}$ and $M_{0,i}$ are the nominal values for the liquid flow and holdup on stage i. τ_L is the liquid time constant and λ is the effect of

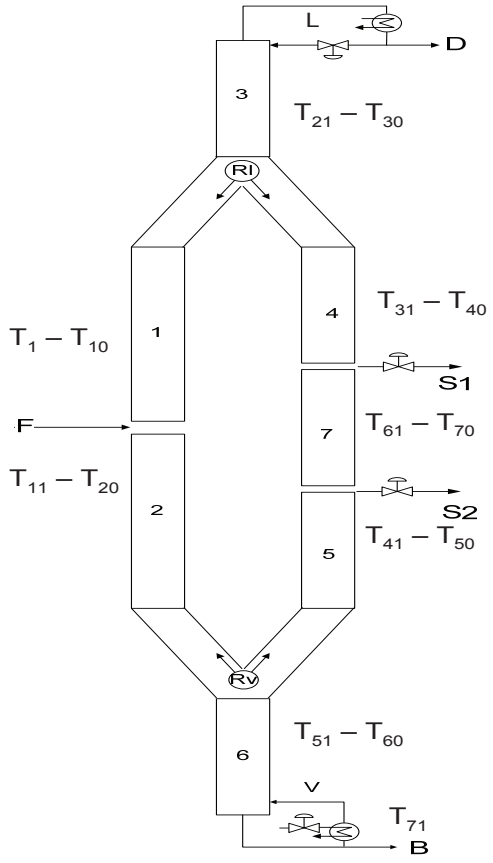

Figure E.1: The 4-product Kaibel column

vapor flow on the liquid flow ("K2"-effect). In this work $\lambda = 0$, which is a good assumption for a packed column (Skogestad, 1997).

E.3 Kaibel column model

The Kaibel column is modeled using 7 column sections. The first two sections are pre-fractionator column and the rest 5 sections are main column and each section has 10 stages. Liquid holdup volumes are included for the condenser, re-boiler, side product draws (S_1 and S_2) and the liquid split. We assume that the feed consists of an equimolar mixture of methanol (A), ethanol (B), propanol (C) and butanol (D). The liquid fraction of the feed has a nominal value of q = 0.9.

E.3.1 Vapour-liquid equilibria

Ideal vapour phase is assumed and the vapour-liquid equilibrium for component j is described by the equation:

$$Py_j = x_j \gamma_j P_j^s \tag{E.2}$$

where

$$P = \sum_{j=1}^{n=NC} x_j \gamma_j P_j^s \ [mmHg] \tag{E.3}$$

The vapour pressures (P^s) are given by the Antoine equation

$$log(P_j^s) = A_j - \frac{B_j}{T + C_j} \tag{E.4}$$

The activity coefficients (γ_j) are given by the Wilson equation with description and parameters taken from (Gmehling and Onken, 1997).

Bibliography

Gmehling, J., Onken, U., 1997. Vapor-liquid equilibrium data collection. DECHEMA Chemistry Data Series, Frankfurt am Main.

Halvorsen, I. J., Skogestad, S., 2003. Minimum energy consumption in multicomponent distillation. 3. more than three products and generalized petlyuk arrangements. Industrial & Engineering Chemistry Research 42 (3), 616–629.

Skogestad, S., 1997. Dynamics and control of distillation columns: A tutorial introduction. Chemical Engineering Research and Design 75 (6), 539 – 562, distillation.

Strandberg, J., 2011. Optimal operation of dividing wall columns. Ph.D. thesis, Norwegian University of Science and Technology, Department of Chemical Engineering,Trondheim, Norway.