REFERENCE MANAGEMENT FOR STEADY-STATE TRANSITIONS

REFERENCE MANAGEMENT FOR STEADY-STATE TRANSITIONS UNDER CONSTRAINED MODEL PREDICTIVE CONTROL

by

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ABSTRACT

There are increasing economic incentives within the chemical process industry towards demand driven operation with product diversification, requiring flexible operation in responsive plants. In continuous processes, this is realized through steady-state transitions but requires consideration of process dynamics arising from operation that is inherently transient in nature. The steady-state economic optimum is typically defined at the intersection of constraints, and requires multivariable control with optimal constraint handling capabilities. Thus, constrained model predictive control is well-suited to realize the profit potential at the economic optimum.

In this thesis, feasible and optimal steady-state transitions are achieved using reference management with consideration of the closed-loop dynamics of constrained model predictive control. The supervisory control scheme is used to determine the optimal setpoint trajectory which is subsequently tracked by regulatory control, incorporating feedback for the rejection of high frequency disturbances and eliminating steady-state offset in the presence of model mismatch. The separation of economic and control objectives enables the lower level to be tuned for stability and the upper level to be tuned for performance.

The mathematical formulation results in a multi-level optimization problem with an economic objective function at the upper level, and a series of control performance objective functions arising from constrained model predictive control at the lower levels. The solution strategy proposed converts the multi-level optimization problem into a single-level optimization problem using the Karush-Kuhn-Tucker conditions, and solves the resulting complementarity conditions using an interior point approach.

Alternative objective formulations are investigated based on maximizing profit during transient operation. The first formulation is typically based on a quadratic objective function minimizing the transition time, indirectly improving economic operation by reducing the amount of off-specification product produced. The second formulation is based on the explicit consideration of economics. The profit calculated during transient

operation is based on the difference between the revenue generated by the production of acceptable product within specified univariate product quality bands, and the operational costs of raw materials and utilities. The resulting linear objective function is further extended to incorporate control performance considerations to improve conditioning for gradient based optimization.

The proposed methodology is applied to a single-input single-output linear system, demonstrating the potential benefits of simultaneous rather than sequential optimization in terms of computational efficiency and solution reliability. Alternative objective function and constraint formulations are investigated, and the effect on the optimal solution assessed. In particular, the possibility of indeterminacy is shown and handled using hierarchical optimization. The methodology is also demonstrated on additional examples including non-minimum phase systems and multi-input multi-output linear systems.

Application to a multi-input multi-output nonlinear system corresponding to styrene polymerization using the proposed methodology is detailed. The set of differential and algebraic equations defining the process is discretized using orthogonal collocation on finite elements. The optimal operation during grade transitions based on explicit consideration of economics is determined, and additional improvements realized by manipulating the production rate.

Finally, reference management with online re-optimization is investigated for a single-input single-output linear system based on a bias update, and the improvement in closed-loop performance assessed for output disturbances and model mismatch. The methodology is also demonstrated on a multi-input multi-output system based on a linear model when applied to the nonlinear process.

The proposed methodology developed for steady-state transitions may also be applied to batch operation, startups and shutdowns. Future extensions include analysis of closed-loop stability due to the incorporation of feedback within the cascade control scheme, and the explicit consideration of uncertainty.

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Table of Contents

1 Introduction **1**

1.1 Motivation and Overview 1

1.2 Contributions to Research 4

1.3 Organization of Thesis 5

2 Literature Review **9**

2.1 Steady-State Real Time Optimization 9

2.2 Dynamic Models in Real Time Optimization 11

2.3 Constrained Model Predictive Control 13

2.4 Hard Output Constraints 16

2.5 Feasibility Based on Dynamic Backoff 17

2.6 Reference Management 19

2.6.1 Improvements in Stability and Performance 21

2.6.2 Incorporation of Uncertainty Considerations 22

2.6.3 Additional Comments 23

2.7 Optimization and Control Hierarchy 24

2.7.1 Two Layer Approach with LP/QP-MPC 25

2.7.2 Two Layer Approach with Consideration of Dynamics 28

3 Mathematical Formulation **29**

3.1 Constrained Model Predictive Control 29

3.2 Sequential Optimization 33

3.3 Simultaneous Optimization 36

3.4 Orthogonal Collocation on Finite Elements 38

3.5 Karush-Kuhn-Tucker Conditions 42

3.6 Interior Point Methods 45

4 Application to Linear Systems **49**

4.1 Single-Input Single-Output Systems 49

4.1.1 Comparison of Sequential and Simultaneous Optimization 52

4.1.2 The Effect of Input Saturation 55

4.1.3 The Effect of the Number of Allowable Changes 57

4.1.4 The Effect of the Setpoint Hold 59

4.1.5 The Effect of Objective Function Formulation 61

4.1.6 Two-Tiered Hierarchical Optimization 63

4.1.7 The Discrete Reference Filter 67

4.2 Non-Minimum Phase Systems 68

4.3 Multi-Input Multi-Output Systems 71

4.3.1 Application of Reference Management 74

4.3.2 Formulation with Alternative Objective Functions 76

4.3.3 Alternative Design and Control 77

4.4 Summary of Results 78

5 Application to Nonlinear Systems **80**

5.1 Optimal Grade Transitions in Literature 81

5.1.1 Feedback Control Required 82

5.1.2 Solution Strategies 83

5.1.3 Consideration of Economic Operation 84

5.1.4 Proposed Methodology 85

5.2 Process Description 85

5.2.1 The Importance of Temperature Control 91

5.2.2 Development of Regulatory Control 92

5.3 Reference Management with Linear Models 94

5.4 Reference Management with Reference Filters 96

5.5 Reference Management with Nonlinear Models 98

5.6 Reference Management with Dynamic Economics 103

5.6.1 Process Description 104

5.6.2 Development of the Economic Objective Function 106

5.6.3 Improvement in Profit in the Linear System 112

5.6.4 The Effect of the Weighting Parameter in Switching Functions . . . 113

5.6.5 Alternative Objective Function Formulations 114

5.6.6 Improvement in Profit in the Nonlinear System 116

5.6.7 Utilization of Additional Degrees of Freedom 117

5.6.8 Consideration of Initial Product Quality Bands 121

5.6.9 Alternative Switching Functions 123

5.7 Summary of Results 126

6 Online Implementation **128**

6.1 Single-Input Single-Output Systems 129

6.1.1 Step Disturbances in the Output 130

6.1.2 Model Mismatch 132

6.1.3 Pulse Disturbances 137

6.2 Multi-Input Multi-Output Systems 140

6.2.1 Online Reference Management 140

6.2.2 Enforcing the Successive Setpoint Change 142

6.2.3 Effect of Increasing Frequency of Re-optimization 144

6.3 Summary of Results 145

7 Conclusions and Recommendations **146**

7.1 Conclusions 146

7.2 Recommendations for Future Work 147

7.2.1 State-Space Model Predictive Control 147

7.2.2 Application to Startups and Shutdowns 148

7.2.3 Application to Batch Processes 148

7.2.4 Multivariate Quality Specifications 149

7.2.5 Integration of Optimization, Control and Design 149

7.2.6 Incorporation of Feedback 150

7.2.7 Explicit Consideration of Uncertainty 151

7.2.8 Suitable Model Development for Optimization 152

A KKT Conditions for QDMC **153**

References **159**

List of Figures

1.1 Conventional optimization and control hierarchy 2

1.2 Proposed optimization and control hierarchy for steady-state transitions . 3

1.3 Solution strategies for multi-level dynamic optimization 4

2.1 The error governor 20

2.2 The reference governor 20

3.1 Multi-level optimization arising from model predictive control 35

3.2 Orthogonal collocation on finite elements 42

4.1 Schematic of three continuously stirred tank reactors in series 50

4.2 Comparison of tuning for feasibility and performance 52

4.3 Sequential approach: Constraints satisfied with IC=1.00 $\alpha = 1$ $\beta = 0$ 53

4.4 Constraints satisfied with IC=1.50 NAC=100 SPH=2 $\alpha = 1$ $\beta = 0$ 57

4.5 Optimal reference trajectory dependent on the number of allowable changes 58

4.6 Optimal reference trajectory dependent on length of setpoint hold 60

4.7 Optimal reference trajectory with SPH=1 NAC=49 63

4.8 Optimal reference trajectory with SPH=5 NAC=9 63

4.9 Hierarchical formulation based on setpoint 65

4.10 Hierarchical formulation based on setpoint changes 66

4.11 Closed-loop response with first order low pass reference filter 68

4.12 Comparison of tuning for feasibility and performance 69

4.13 Enforcement of output constraints with IC=0 NAC=60 SPH=1 70

4.14 Schematic of distillation column 72

4.15 Closed-loop response for ethanol-water distillation column 74

4.16 Reference trajectory penalizing deviation between output and target . . . 75

4.17 Single setpoint change in temperature 75

4.18 Single setpoint change in composition 76

4.19 Reference trajectory penalizing deviation between setpoint and target . . . 77

4.20 Closed-loop response for optimal design of delay structure 78

5.1 Styrene polymerization in continuously stirred tank reactor 86

5.2 Closed-loop response of linear system to constant setpoint change 93

5.3 Closed-loop response of nonlinear system to constant setpoint change . . 93

5.4 Optimal reference trajectory for perfect linear model 95

5.5 Optimal reference trajectory with reduced setpoint variability 96

5.6 Discrete reference filters holding temperature setpoint constant 97

5.7 Discrete reference filters with adjustment in temperature setpoint 97

5.8 Discrete reference filters implementation on nonlinear system 98

5.9 Optimal input trajectory implemented on nonlinear system 99

5.10 Optimal reference trajectory implemented on nonlinear system 99

5.11 Optimal reference trajectory for perfect nonlinear model 100

5.12 Optimal reference trajectory with minimal setpoint variability 101

5.13 Optimal reference trajectory for perfect nonlinear model 102

5.14 Optimal reference trajectory with minimal setpoint variability 102

5.15 Grade transition on linearized system 105

5.16 Grade transition on nonlinear system 106

5.17 Polymerization univariate product quality specifications 106

5.18 Switching functions where $y = \frac{1}{2}\tanh \gamma x + \frac{1}{2}$ 107

5.19 Optimal economic operation for perfect linear model 113

5.20 Suboptimal solution resulting with $\gamma = 1.00$ 113

5.21 Optimal solution obtained with $\gamma = 0.05$ using end point constraints . . . 114

5.22 Suboptimal solution based on economics without conditioning 115

5.23 Suboptimal solution obtained with end point constraints 115

5.24 Optimal economic operation for perfect nonlinear model 117

5.25 Closed-loop response minimizing transient variability 118

5.26 Productivity minimized to reduce costs 119

5.27 Optimal operation with productivity maximization 120

5.28 Maximizing productivity 120

5.29 Arctangent switching functions where $y = \frac{1}{\Pi} \arctan \gamma x + \frac{1}{2}$ 123

5.30 Use of arctangent switching functions with $\gamma = 0.01$ 124

5.31 Use of arctangent switching functions with $\gamma = 0.05$ 124

5.32 Use of arctangent switching functions with $\gamma = 1.00$ 125

5.33 Sigmoidal switching functions where $y = \{1 + \exp\left[-6.9068\left(\frac{a+b-2x}{b-a}\right)\right]\}^{-1}$. 125

5.34 Use of the sigmoidal function with $a = 1.05NAMW_{tgt}$ $b = 1.07NAMW_{tgt}$. 126

6.1 Optimal reference trajectory without model mismatch 130

6.2 Implementation on the actual system with step disturbance 130

6.3 Optimal reference trajectory with perfect process and disturbance model . 131

6.4 Reference trajectory update with step disturbance estimate 132

6.5 Implementation on the actual system with model mismatch 133

6.6 Optimal reference trajectory with perfect model 134

6.7 Second model update enforcing 2 setpoint changes 135

6.8 Third model update enforcing 3 setpoint changes 136

6.9 Ninth model update enforcing 9 setpoint changes 136

6.10 Implementation on actual system with pulse disturbance 137

6.11 Reference trajectory with pulse disturbance under perfect model 138

6.12 First model update enforcing 1 setpoint change to pulse disturbance . . . 139

6.13 Third model update enforcing 3 setpoint changes to pulse disturbance . . 139

6.14 First model update enforcing two setpoint changes 141

6.15 Seventh model update enforcing fourteen setpoint changes 141

6.16 First model update enforcing two setpoint changes 142

6.17 Fifth model update enforcing ten setpoint changes 143

6.18 First model update enforcing one setpoint change 144

6.19 Tenth model update enforcing ten setpoint changes 145

List of Tables

4.1 Steady-state conditions for CSTRs in series 50

4.2 Sequential optimization under different initial conditions 54

4.3 Simultaneous optimization under different initial conditions 54

4.4 Sequential approach: Sensitivity under different initial conditions 56

4.5 Simultaneous approach: Insensitivity under different initial conditions . . 56

4.6 Simultaneous approach: Dependency on the number of allowable changes 59

4.7 Simultaneous approach: Dependency on the length of setpoint hold 61

4.8 Simultaneous approach minimizing output deviation 62

5.1 Styrene reactor initial conditions: Grade A 88

5.2 Styrene reactor parameters 89

5.3 Styrene reactor initial conditions: Grade B 105

Chapter 1

Introduction

1.1 Motivation and Overview

There are increasing economic incentives towards demand driven operation with product diversification in the chemical industry (Backx et al., 2000). Thus flexible operation in responsive plants is required (Rowe et al., 1997), and is realized through steady-state transitions in continuous processes. Since the operation is inherently transient in nature, achieving feasible and optimal steady-state transitions requires dynamic optimization with consideration of the process dynamics.

The determination of the open-loop input trajectory for optimal steady-state transitions has been proposed in literature, but may result in steady-state offset in the presence of model mismatch as discussed by McAuley and MacGregor (1992). An alternative approach is based on the determination of the optimal setpoint trajectory tracked by the underlying regulatory control layer. The resulting cascade-type control structure is capable of eliminating steady-state offset by incorporating feedback (McAuley and MacGregor, 1993), and is consistent with the standard control automation hierarchy shown in Figure 1.1.

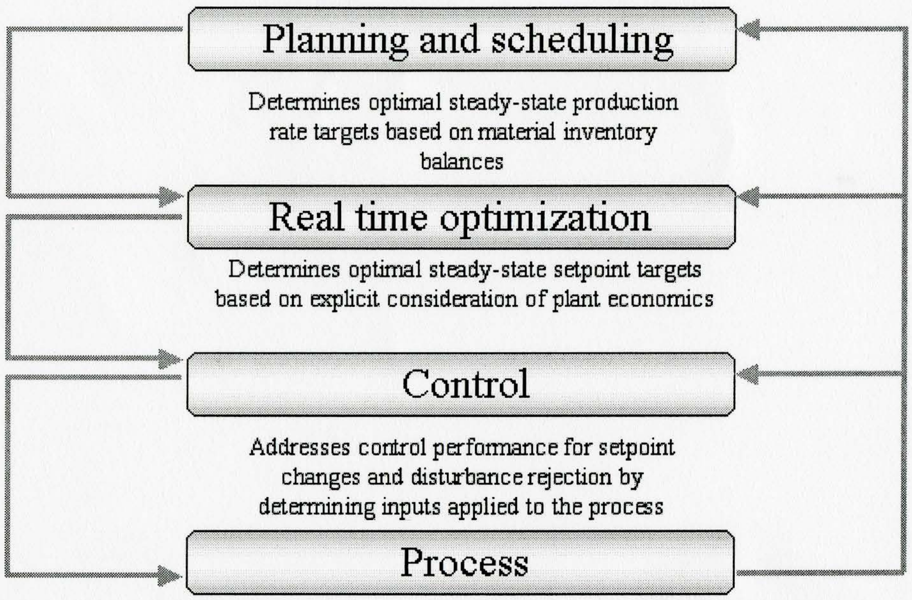


Figure 1.1: Conventional optimization and control hierarchy

In the conventional approach outlined by Marlin and Hrymak (1997), real time optimization is used to determine the steady-state economic optimum, typically defined at the intersection of active constraints. Thus, according to Cutler and Perry (1983), constrained multivariable control is required to hold the process at profitable operating conditions. Hence, constrained model predictive control is well-suited for achieving the maximum profit potential based on capabilities in the optimal handling of constraints (Qin and Badgwell, 2003).

However, consideration of dynamics is necessary for operations that are inherently transient in nature and requires the determination of the optimal setpoint *trajectory*. Furthermore, the setpoint trajectory is tracked by the underlying regulatory control layer, and thus the closed-loop dynamics must be considered in addition to the process dynamics. Thus while conventional real time optimization uses *steady-state models* to determine the optimal setpoint target, the proposed supervisory controller uses closed-loop *dynamic* models to determine the optimal setpoint trajectory required to achieve target specifications. The proposed optimization and control hierarchy for steady-state transitions is shown in Figure 1.2.

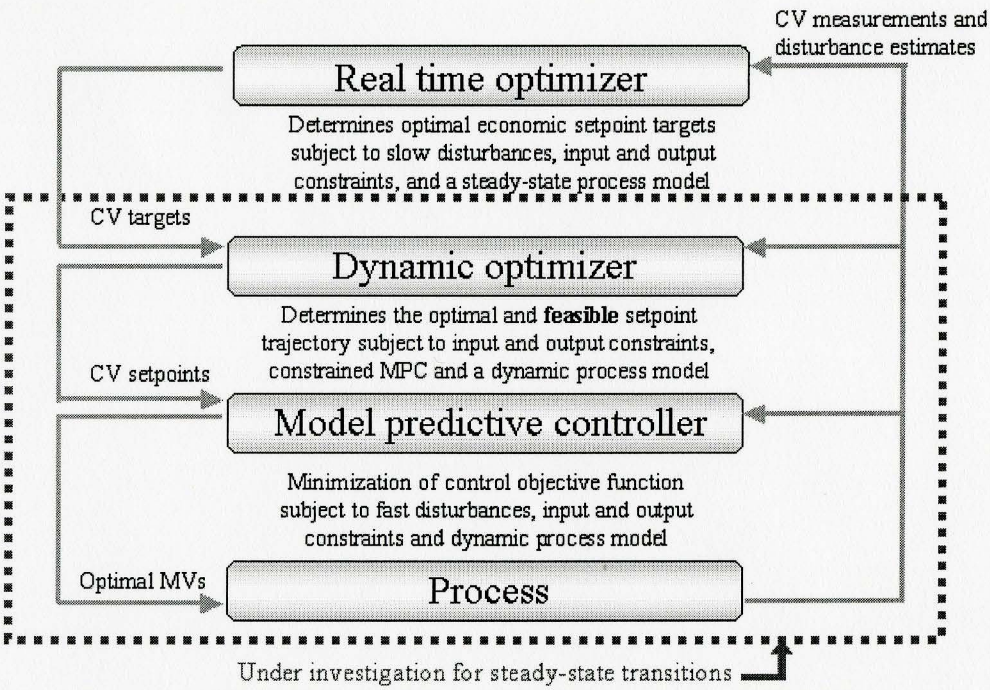


Figure 1.2: Proposed optimization and control hierarchy for steady-state transitions

The optimal setpoint trajectory is determined using reference management as developed by Kapasouris et al. (1989), and investigated by Gilbert et al. (1994) and Bemporad and Mosca (1994a). The cascade-type control structure enables tuning of the regulatory controller for stability, and the supervisory controller for performance.

In this thesis, the supervisory control scheme is used to achieve feasible and optimal operation during steady-state transitions. The optimal setpoint trajectory is determined using reference management with consideration of the closed-loop dynamics of constrained model predictive control, and results in a multi-level dynamic optimization problem. The solution may be obtained using the sequential approach based on separating optimization and integration of the closed-loop system, or the simultaneous approach based on reformulation into a single-level optimization problem. The alternative solution strategies are compared in Figure 1.3.

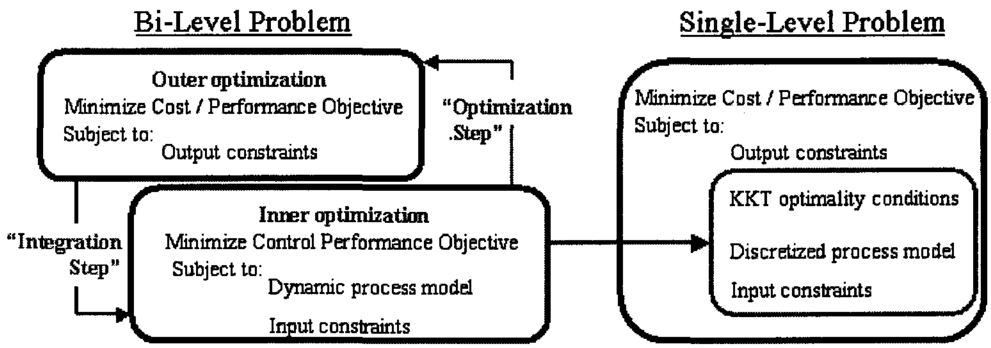


Figure 1.3: Solution strategies for multi-level dynamic optimization

The simultaneous approach is proposed, and is shown to result in reduced computational expense and increased solution reliability, particularly in the presence of derivative discontinuities introduced by input saturation. The solution strategy is based on discretization of the state profile using orthogonal collocation on finite elements and reformulation into a single-level optimization problem using the Karush-Kuhn-Tucker (KKT) conditions. The complementarity conditions arising from the optimality conditions are handled using an interior point approach.

1.2 Contributions to Research

Brengel and Seider (1992) investigated controllability of a fermentation process based on the closed-loop response under constrained model predictive control. The dynamic backoff from active steady-sate constraints was determined within the framework of integrated control and design, and the multi-level optimization problem reformulated into a single-level optimization problem using the Karush-Kuhn-Tucker (KKT) conditions. However, this was solved using differential arclength homotopy continuation methods and numerical difficulties were reported. Similarly, Soliman (2005) determined the dynamic backoff for steady-state operation of a fluid catalytic cracking (FCC) unit under constrained model predictive control, but solved the resulting multi-level optimization problem using mixed integer programming. Subsequently, Baker and Swartz (2005) determined the dynamic backoff by solving the complementarity constrained system using an interior point approach. A significant reduction in computational expense was demonstrated in comparison to mixed integer programming.

In this research, a similar interior point solution strategy is applied to reference management with consideration of the closed-loop dynamics of constrained model predictive control, and is extended to the determine the optimal setpoint *trajectory* during transient operations. The mathematical formulation of the resulting multi-level optimization problem is investigated with various objective function and constraint formulations, and applied to linear and nonlinear systems. One of the proposed formulations is based on minimizing the transition time to reduce the production of off-specification product, and is similar to investigations of optimal grade transitions in literature, for example by McAuley and MacGregor (1992) and Chatzidoukas et al. (2003). However, formulations that explicitly consider the economics of transition are also investigated.

Finally, a feedback mechanism was incorporated into the proposed methodology for updating the setpoint trajectory online to improve performance in the presence of disturbances and model mismatch.

1.3 Organization of Thesis

Chapter 2: Literature Review

This chapter details fundamental concepts in literature related to the motivation and development of this research. Conventional steady-state real time optimization is reviewed and incentives to incorporate dynamic considerations into the optimization and control hierarchy identified. Since the steady-state optimum is typically determined at the intersection of active constraints, constrained model predictive control is well-suited to realize optimal operation, and is briefly described. The treatment of hard output constraints and the dynamic backoff from active constraints required to ensure feasibility are also discussed. Finally, the development of reference management for feasible operation is reviewed and benefits in the decomposition of the optimization and control hierarchy summarized.

Chapter 3: Mathematical Formulation

This chapter details the mathematical formulation of reference management with consideration of the closed-loop dynamics of constrained regulatory control. The algorithm of constrained model predictive control is reviewed, and the methodology of reference management based on sequential and simultaneous optimization presented. Additional descriptions of mathematical concepts required in the simultaneous approach are also detailed: orthogonal collocation on finite elements used for discretization, the Karush-Kuhn-Tucker conditions for handling multi-level optimization, and the interior point approach to handling complementarity conditions arising from first order optimality conditions.

Chapter 4: Application to Linear Systems

This chapter details the application of the proposed methodology to linear dynamic systems. The objective function used in these simulations is based on maximizing economic operation indirectly, by minimizing the production of off-specification product with suitable hard output constraints based on economic considerations. A single-input single-output system is used to demonstrate the potential benefits of the simultaneous relative to the sequential approach in terms of computational efficiency and solution reliability. The effect of various constraint formulations on the optimal solution is explored, and alternative objective function formulations investigated. The discrete reference filter may be obtained from appropriate specification of setpoint constraints, and the effect on optimal operation is determined. The possibility of indeterminacy is shown and handled using a two-tiered approach, maximizing closed-loop performance. Finally, application of reference management to non-minimum phase and multi-input multi-output systems is demonstrated.

Chapter 5: Application to Nonlinear Systems

This chapter details the application of the proposed methodology to nonlinear dynamic systems. The multi-input multi-output control of styrene polymerization is described and grade transitions in literature summarized. The application of the methodology to the linearized system is demonstrated based on maximizing economic operation indirectly, by minimizing the production of off-specification product with suitable hard output constraints based on economic considerations. The offline optimal input trajectory is implemented on the nonlinear system to demonstrate steady-state offset, while the offline optimal setpoint trajectory is implemented to demonstrate online tracking of the constrained model predictive controller. The optimal reference trajectory is subsequently determined based on the nonlinear model discretized using orthogonal collocation on finite elements.

Finally, an objective function is formulated with explicit consideration of economics using product quality specification bands, and optimal economic operation during grade transitions determined. Further improvements are shown with the utilization of additional degrees of freedom, minimizing the production of off-specification product during transient operation.

Chapter 6: Online Implementation

This chapter details the online implementation of the proposed methodology using a bias update for disturbance estimation. The performance of the scheme is demonstrated on a single-input single-output system under step disturbances, model mismatch and pulse disturbances. In addition, application to a multi-input multi-output system is demonstrated.

Chapter 7: Conclusions and Recommendations

This chapter summarizes the results of this thesis, followed by a discussion of extensions for future research.

Simulation results were obtained using using Simulink in MatLab 7.0 for sequential optimization, and using *A Mathematical Programming Language* (AMPL) for simultaneous optimization with the solver IPOPT-C 2.2.1.d compiled November 2004. Computations were conducted on a 1.7 GHz Intel Pentium IV processor with 256 MB of RAM.

Chapter 2

Literature Review

This chapter details the motivation for the inclusion of dynamic models within the optimization and control hierarchy, and outlines the proposed solution strategy based on reference management. Conventional steady-state real time optimization is discussed in Section 2.1, and benefits in the incorporation of dynamic considerations stressed in Section 2.2. Constrained model predictive control is reviewed in Section 2.3 and hard output constraint formulations discussed in Section 2.4. The development of dynamic backoff from active constraints is summarized in Section 2.5, reference management described in Section 2.6, and decomposition of the optimization and control hierarchy discussed in Section 2.7.

2.1 Steady-State Real Time Optimization

Edgar (2004) reported substantial financial gains using steady-state optimization to reflect changes in operating conditions in industry since the 1970s. Successful application of steady-state optimization combined with control was detailed by (Cutler and Perry, 1983), with estimated benefits of 6-10% for a given process. Conventional steady-state real time optimization is based on nonlinear models consisting of several thousand variables, and the optimal setpoint targets passed to the underlying regulatory controller, typically based on linear dynamic models (Biegler, 2000).

However, Marlin and Hrymak (1997) remarked that steady-state real time optimization for increased profit is only possible in the presence of additional degrees of freedom after satisfying safety, product quality and production rate objectives. Furthermore, steady-state optimization requires data reconciliation and parameter estimation handled by the updater, and determination of optimal setpoint targets based on the updated process model, handled by the model optimizer. As described by Miletic and Marlin (1996), a results analyzer is required to ensure that input handles are still available for manipulation and that the system is still operating at steady-state before implementation of the optimal setpoint targets. Only significant changes are implemented, resulting in a reduction in the number of unnecessary changes, and an increase in profit as demonstrated by Miletic and Marlin (1998). This is particularly important if the dominant cause for a change in operation is a result of noise and ill-conditioned optimization. In fact, commercial real time optimization use trust region constraints to reduce unnecessary changes and increase profit (Zhang et al., 2001).

Successful implementation of steady-state real time optimization in industry has been reported in literature. An industrial application in a petrochemical power plant at Mitsubishi Chemicals was described by Emoto et al. (1998), and in an ethylene plant in Germany by Lauks et al. (1992). Implementation at the Hyundai Petrochemical Company in South Korea increased ethylene capacity by 4%, revenues by 12% and decreased energy and feedstock by 2.5% (Yoon et al., 1996). The steady-state effect of regulatory control was also considered in closed-loop steady-state real time optimization, and implemented in industry in an ethylene plant at the Mobil Chemical Company, yielding a payback period of less than 9 months (Georgiou et al., 1998), and at the Bayernoil refinery in Germany yielding an additional profit of $1.5 million a year (Besl et al., 1998). Thus, the application of steady-state real time optimization has been successfully implemented to improve economic operation in industry.

However, while steady-state real time optimization determines the optimal setpoint target, a separate optimization is required to determine the optimal dynamic trajectory (Forbes and Marlin, 1994). Thus, consideration of dynamic models in real time optimization would be required to determine optimal transient operation to realize the profit potential at the optimal steady-state target.

2.2 Dynamic Models in Real Time Optimization

Similar to the logistics and supply chain revolution in consumer electronics and automotive industries twenty years ago, Backx et al. (2000) identify incentives for the chemical process industry to adjust towards market driven operation, particularly in saturated markets with growing demands for product diversification. Currently, actual production is not correlated with actual demand due to a focus on supply driven operation with centralized production based on minimizing fixed costs through economies of scale. Thus, several production plants are constructed for product diversification to respond to changes in the market, but minimization of stock and maximization of margins is limited for production on demand.

According to Rowe et al. (1997), this shift towards market driven operation requires responsive plants satisfying instantaneous demand, but resulting in frequent transitions where feasibility of satisfying product specifications must be ensured to remain economically competitive. The design and operation of multi-product and distributed manufacturing plants for flexible operation has been receiving increased attention in the chemical process industry (Harold and Ogunnaike, 2000). Thus, there are economic incentives to achieve flexible operation to respond to market fluctuations but requiring consideration of dynamics to achieve optimal and feasible steady-state transitions.

Within the literature, desirable characteristics required for optimal and feasible market driven operation are discussed based on similar concepts such as switchability, flexibility, controllability and resiliency. White et al. (1996) and Vu et al. (1997) use switchability to define the ability for a process to move between operating points, implicitly combining the properties of feasibility and optimality. Mohideen et al. (1996) investigated both flexibility, the ability to adjust to changing steady-state conditions, and controllability, the ability to recover from disturbances and dynamic behaviour. Similarly, Weitz and Lewin (1996) used resiliency as a more general definition to describe the ability for a process to attain design objectives in the presence of disturbances and parametric uncertainty.

In addition to investigations in academia, a similar shift in focus toward dynamic considerations is evident in industry. Tosukhowong et al. (2004) demonstrated reduced performance with increasing frequency of conventional steady-state real time optimization without ensuring steady-state operation. Similarly, Singh et al. (2000) observed that while steady-state real time optimization has been successful at a refinery using blends from well mixed storage tanks, frequent execution and time varying feedstock provided incentives for real time optimization based on dynamic models. The incorporation of dynamic models into real time optimization was capable of minimizing quality giveaway and the number of re-blends required by using less expensive blend components, while meeting product specifications.

Thus while the majority of installed process optimization applications are based on steady-state models, organizational changes towards a rolling approach to planning for just-in-time production is driving the need for dynamic considerations (Kleinschrodt and Jones, 1996). Investigations in research has shifted to reflect the technology required by industry under such market conditions, and dynamic real time optimization (D-RTO) based on fundamental dynamic models proposed (Kadam and Marquardt, 2004).

Finally, frequent re-optimization and steady-state transitions provide strong incentives for the consideration of dynamics, but furthermore, conventional steady-state real time optimization is not applicable to batch operation. According to Rippin (1983) and Soroush and Kravaris (1993), batch processes are particularly flexible in operation and well-suited for adjustment to changing market conditions with fluctuations in product demand. However, the operation of batch processes is inherently transient in nature, and the inclusion of dynamic models into the optimization and control hierarchy is essential.

2.3 Constrained Model Predictive Control

Optimal economic conditions typically call for operation at higher capacity than design specifications, resulting in unit operation at capacity constraints (Skogestad, 2004). Hence the optimal operating conditions are typically defined at the intersection of active constraints, and require constrained multivariable control to hold the process at profitable operating conditions (Cutler and Perry, 1983).

Input and output constraints are particularly important, leading the list of the top five control objectives in industry as reviewed by Qin and Badgwell (2003), followed by driving outputs to steady-state optimal values and inputs to steady-state target values, preventing excessive input movement, and robustness to actuator failure. Thus, constrained model predictive control is well-suited for addressing these objectives, and is the advanced control algorithm of choice in the chemical process industry.

The general methodology of model predictive control is based on utilizing output predictions over a prediction horizon P using a dynamic model of the process to determine the optimal inputs over an input horizon M. The control performance objective function is typically formulated as a quadratic optimization problem based on minimizing the squared deviation of predicted outputs from target, weighted appropriately with penalty on input movement and subject to hard input constraints. The first input move calculated is implemented on the actual plant and the process is repeated at the subsequent sampling time, resulting in a receding horizon strategy with feedback to eliminate steady-state offset in the presence of uncertainty (Maciejowski, 2002).

Quadratic dynamic matrix control (QDMC) was originally proposed using the step response model (García and Morari, 1986) and is summarized for the single-input single-output case by the following equations:

$$\min_{\Delta u(k),\cdots,\Delta u(k+M-1)} \phi = \sum_{l=1}^{P} \|y_{sp}(k+l) - \hat{y}(k+l|k)\|_Q^2 + \sum_{l=1}^{M} \|\Delta u(k+l-1)\|_R^2 \tag{2.1}$$

where y_{sp} represents the setpoint, $\hat{y}(k+l|k)$ the predicted output at time $k+l$ with information available at time k, and $\Delta u(k+l) = u(k+l) - u(k+l-1)$ the optimal input move at time step $k+l$. Furthermore, $Q \in \Re^{P\times P}$ and $R \in \Re^{M\times M}$ are diagonal time invariant positive definite weighting matrices penalizing output deviation from setpoint and input moves respectively, where $\|x\|_Q^2 = x^T Q x$. The minimization problem in Equation 2.1 is subject to the following constraints:

$$\hat{y}(k+l|k) = \sum_{i=1}^{l} s_i \Delta u(k+l-i) + \sum_{i=l+1}^{n-1} s_i \Delta u(k+l-i) + s_n u(k+l-n) + \hat{d}(k+l|k) \tag{2.2}$$

$$\hat{d}(k+l|k) = y_m(k) - \sum_{i=1}^{n-1} s_i \Delta u(k-i) - s_n u(k-n) \tag{2.3}$$

$$\Delta u(k+l) = 0 \quad \forall l \geq M \tag{2.4}$$

$$u_{\min} \leq u(j) \leq u_{\max} \quad j = k, \cdots, k+M-1 \tag{2.5}$$

$$y_{\min} \leq \hat{y}(j|k) \leq y_{\max} \quad j = k+1, \cdots, k+P \tag{2.6}$$

where $s_i,\ i = 1..n$ represent the step response coefficients with truncation order n, $y_m(k)$ the measured output at time k, and $\hat{d}(k+l|k)$ the predicted value of additive disturbances in the output at time $k+l$ given information at time k. In conventional dynamic matrix control (DMC), the predicted disturbance is assumed constant in the future and is estimated from the difference between the measured and predicted output (García et al., 1989). The assumption of a step disturbance in the output is capable of eliminating steady-state offset but may result in sluggish disturbance rejection (Morari and Lee, 1991).

The inclusion of hard output constraints shown in Equation 2.6 is possible, but may result in infeasibility and may require constraint softening. A formulation for constraint softening is described by Zafiriou (1991) using slack variable ϵ_i for output constraint i, and is given by

$$y_{i,\min} - \epsilon_i \leq y_i\left(k+l\right) \leq y_{i,\max} + \epsilon_i \qquad l = 1, \cdots, P \tag{2.7}$$

A penalty term $w_i \epsilon_i^2$ is included in the quadratic control objective function where w_i represents constraint violation weighting for output i. Hard constraints are typically softened in commercial algorithms by the slack variable formulation (Morari and Lee, 1999).

The soft constraint formulation described is based on the penalty method and may result in constraint violation. A consistent set of penalty weightings must be determined experimentally while ensuring controller stability, robustness and performance (Qin and Badgwell, 2003). Hence, the soft constraint formulation introduces difficulty in distinguishing between optimization of the objectives and satisfaction of constraints, where the weightings are also dependent on scaling and changing operating conditions (García and Prett, 1986). Furthermore, stability problems are only minimized gradually and not eliminated by the softening of output constraints (Zafiriou, 1991).

While constrained model predictive control has been applied to large scale problems, the formulation of a reasonable objective function is increasingly complicated with an increasing number of variables and competing objectives (Ricker, 1991). Despite these apparent limitations, commercial products such as DMC-Plus from AspenTech, Shell Multivariable Optimizing Controller (SMOC) from Shell Global Solutions, and Process Perfector from Pavilion Technologies are popular in industry (Qin and Badgwell, 2003).

Thus, in this thesis, quadratic dynamic matrix control (QDMC) was chosen as the underlying regulatory controller to realize feasible and optimal steady-state transitions.

2.4 Hard Output Constraints

According to Marlin (2000), control systems are designed to maintain conditions within an operating window defined by constraints where soft output constraints are defined to reduce the production of poor quality product, and hard output constraints to ensure plant safety and prevent equipment damage. The consideration of hard output constraints is also included in commercial products such as Hierarchical Constraint Control (HIECON) from Adersa, and NOVA nonlinear controller (NOVA-NLC) from DOT Products (Qin and Badgwell, 2003).

However, the consideration of hard output constraints may result in infeasibility within the calculation of optimal inputs, and may require constraint softening (Brosilow and Joseph, 2002) as described in Section 2.3. Infeasibility results in suboptimality with the possibility of instability for open-loop unstable plants (Maciejowski, 2002). In fact, the inclusion of hard output constraints may result in closed-loop instability independent of tuning parameters (Oliveira and Biegler, 1994). In the event of infeasibility, Scokaert and Rawlings (1999) proposed relaxation of state constraints based on the minimum time or soft constraint approach. The minimum time approach identifies the minimum time beyond which state constraints may be enforced, leading to the earliest constraint satisfaction, but possibly resulting in large transient violations. The soft constraint approach penalizes constraint violations in the objective function with increasing weights to reduce the peak violation, but with sluggish return to the feasible region resulting in constraint violation over a longer period of time.

Zafiriou (1990a) demonstrated the possibility of instability in the closed-loop response under model predictive control as a result of including hard output constraints in the presence of disturbances, otherwise resulting in minimal constraint violation using the unconstrained formulation. Thus proper formulation of constraints and the effect of hard output constraints on closed-loop stability must be considered in control design (Zafiriou, 1990b).

In this work, hard input constraints are handled within regulatory control while hard output constraints arising from economic considerations are handled within the framework of supervisory control. Hard output constraints arising from safety considerations to ensure feasibility are only handled with a conservative formulation of constraints in developing an offline optimal operating strategy. Furthermore, the setpoint target is assumed to have incorporated dynamic backoff from active constraints to ensure feasibility in the presence of uncertainty as further discussed in Section 2.5.

2.5 Feasibility Based on Dynamic Backoff

Ensuring feasibility may be more important than optimality in the chemical process industry (Bonvin et al., 2002). However, since the steady-state economic optimum is typically defined at the intersection of active constraints (Cutler and Perry, 1983; García and Prett, 1986), backoff is required to ensure feasibility in the presence of disturbances. Narraway and Perkins (1993) estimated the maximum input and output constraint backoff using linear dynamic models and assuming perfect control in the context of control structure design. The backoff analysis was extended by Narraway and Perkins (1994) to nonlinear process models with dynamic path constraints. The resulting dynamic backoff was based on consideration of the dynamics of the underlying unconstrained regulatory control layer, and was used to ensure feasibility in the presence of disturbances.

The backoff required for feasibility under the worst case scenario was typically determined using a sequential approach, but requiring integration of differential algebraic equations and objective and constraint evaluations at each time step (Bandoni et al., 1994; Bahri et al., 1996a,b). While the integration error may be controlled using a sequential approach (Figueroa et al., 1996; Bahri et al., 1997), a reduction in computational expense may be obtained using a simultaneous approach as demonstrated by Bahri et al. (1995). The size of the resulting dynamic backoff was used in ranking economically viable controllers, but with the possibility of several control configurations, Young et al. (1996) determined the dynamic backoff based on Q-parametrization to produce the upper bound of achievable performance for all linear feedback controllers. Additional applications included consideration of state observers (Figueroa, 2000) and variable structure control (Contreras-Dordelly, 1999; Contreras-Dordelly and Marlin, 2000).

The application of backoff for control structure design was also extended to the design of online optimization schemes. Loeblein and Perkins (1996) determined the average deviation between the true and calculated optimum based on the size of backoff required under a given range of parametric uncertainty. The analysis was used to estimate the economic benefit of implementing online steady-state optimization, determining the model structure in addition to the optimal selection of measurements and parameters updated. A similar investigation on the economic benefit of using an approximate model for steady-state optimization was undertaken by Loeblein and Perkins (1998).

Loeblein et al. (1997) extended the analysis of average deviation to estimate the economic performance of batch optimization under parametric uncertainty. The size of the backoff required was reduced with increasing confidence in uncertain parameter estimates. However, due to the dynamic nature of batch operation, time varying backoff from active inequality constraints must be determined (Loeblein et al., 1999).

Thus the concept of average deviation from the optimum was further extended by Loeblein and Perkins (1999a), determining the dynamic backoff during transient operation with setpoint changes under unconstrained model predictive control. The dynamic economic assessment was capable of identifying an alternative control structure yielding improved performance for a fluid catalytic cracker (FCC) unit (Loeblein and Perkins, 1999b).

As investigated in literature, the determination of time varying dynamic backoff is useful for control structure design, but the concept is also particularly important in addressing feasibility and optimality during transient operation, and is further discussed in the context of reference management as described in Section 2.6.

2.6 Reference Management

Reference management is a methodology based on modifying the reference signal required to attain a desirable closed-loop response while ensuring feasibility. Findeisen et al. (1978) proposed feasible control generation (FCG) to predict future constraint violation for a given command input and modifying it before implementation to ensure feasibility, thus defining a set of constraint admissible reference signals. The set of constraint feasible trajectories enabling a plant to be driven from one point to another, is also defined as the reachability envelope (Backx et al., 1998).

Reference management was investigated in detail by Kapasouris et al. (1988), with the introduction of the error governor (EG) into the supervisory loop, as shown in Figure 2.1. The error governor is used to modify the control signal to maintain characteristics of linear control by preventing input saturation in multi-input multi-output open-loop stable plants. In addition to reset windup, input saturation induces change in the control vector direction resulting in oscillations and large overshoot in the output. Thus, reference management was initially proposed as a strategy to effectively handle input saturation within conventional linear feedback control.

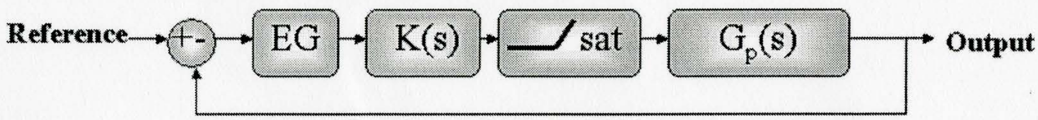


Figure 2.1: The error governor

An improvement in performance compared to the classical approach of bandwidth reduction was demonstrated using the error governor, where the input signal was modified by determining the maximum scalar gain restricted to [0,1]. The scheme was simulated on an F8 aircraft following pitch and flight path angle commands, and resulted in an increase in rise time but maintaining a linear response. An additional scalar gain to handle input rate constraints was introduced by Kapasouris and Athans (1990), and the minimum gain calculated applied to the process to prevent control saturation in magnitude and rate.

However, stability of the closed-loop compensated system could only be guaranteed for open-loop stable plants (Kapasouris et al., 1988), and hence an alternative formulation was proposed by Kapasouris et al. (1989) based on the reference governor (RG) as shown in Figure 2.2. The reference governor is a reference pre-filter that modifies the feedback error signal to prevent input saturation when necessary, such that the system under linear control is stable. An artificial saturation limit was also introduced, reserving control action for disturbance rejection in addition to reference tracking. The supervisory scheme was simulated on an AFTI-16 aircraft where sudden, large input moves were translated into slower commands to enable stabilization.

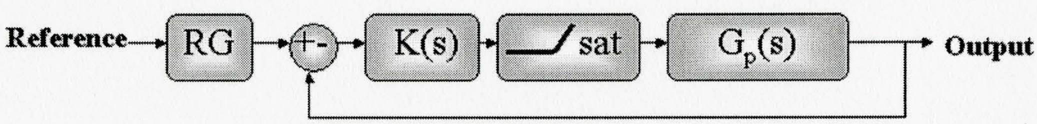


Figure 2.2: The reference governor

The discrete reference governor proposed by Gilbert et al. (1994) is a first order low pass filter with adjustable bandwidth gain, defined by a nonlinear relationship dependent on the states and reference target. At each time step, input and output constraint violations are predicted and the filter time constant modified to enforce point-wise in time constraints (Bemporad and Mosca, 1994a) based on an objective function minimizing the squared deviation between the setpoint and target (Bemporad and Mosca, 1995). The optimal filter time constant was determined using a grid approach (Bemporad and Mosca, 1994a,b) or using a bi-section algorithm (Bemporad, 1998b), but was extended by Bemporad et al. (1998) by solving a constrained quadratic programming (QP) problem.

Thus, reference management was originally proposed to maintain linear behaviour by preventing input saturation to improve linear control (Casavola et al., 2004). Industrial applications are expected to improve setpoint tracking for linear controllers in the presence of constraints, and has also been extended to closed-loop model predictive control under stochastic disturbances as described by Hessem and Bosgra (2004).

Since the development of the reference governor, research in reference management has increased under various terminology, such as the command governor (CG) as termed by Bemporad and Mosca (1995). Beneficial characteristics arising from the separation of objectives for feedback from constraint enforcement has been well discussed (Gilbert and Kolmanovsky, 1994), where constraint fulfillment is handled by the command governor while the primal controller is designed for stability and tracking in the absence of constraints (Angeli et al., 1998, 2000).

2.6.1 Improvements in Stability and Performance

Reference management may also improve closed-loop stability since instability may result for open-loop unstable systems in the presence of input saturation. This was demonstrated on a helicopter model by Gilbert et al. (1994), and in the control of an inverted pendulum by Gilbert and Kolmanovsky (1995), where instability was prevented by preventing input saturation.

Calamai et al. (2000) also used the command governor (CG) for stabilization of the cart position of an inverted pendulum with constraints on motor voltage and rod angle. A high gain controller resulted in instability for large setpoint changes, while a low gain controller avoiding input saturation resulted in large cart and rod angle displacements during disturbance rejection. However, application of the command governor (CG) was capable of improving transient and steady-state performance without instability by enabling a high gain controller to be used.

A similar scheme was proposed in adaptive control by Marroquin and Luyben (1972), where a cascade control structure adjusting the proportional gain of the slave controller according to the master loop error was shown to minimize the transition time and prevent overshoot for a batch process. However, while flexibility is obtained by defining the tuning parameters as a function of feedback error, the response is difficult to predict and tuning complicated (Bequette, 1991). A similar scheme using gain scheduling to reduce overshoot was also proposed by Leung and Romagnoli (2000), but based on heuristics, where stochastic control was used at 70% completion of the transition while deterministic control was used to initiate the steady-state transition.

Thus there are similarities between reference management and gain scheduling, with potential benefits in improving closed-loop stability and performance. Similar concepts have also been proposed in commercial products using filters to minimize overshoot and improve robustness to model mismatch by manipulation of the reference trajectory (Qin and Badgwell, 2003).

2.6.2 Incorporation of Uncertainty Considerations

The application of reference management must be capable of handling uncertainty, and is particularly important to realize applications in industry. Kolmanovsky et al. (1997) detailed the application of reference management to control the electric motor of turbo charged diesel engines during load changes to prevent engine stall and visible smoke emissions in the presence of unknown but bounded disturbances on the engine crankshaft. Additional applications to the soft landing nonlinear problem and a second order electromagnetic actuator in the presence of unknown bounded disturbances were considered by Kolmanovsky and Gilbert (2001).

Bemporad and Mosca (1998) considered the effects of uncertainty in reference management by utilizing bounded uncertainty in the impulse and step responses to determine the maximum lower bound and minimum upper bound restrictions on the filter time constant. The methodology was demonstrated in the control of a servomechanism model, where input constraint violations were prevented during transient operation in the presence of model uncertainty within the given bounds. An increase in the uncertainty range was shown to result in conservative control action and a reduction in response time. The system was also considered by Casavola et al. (2000) with additional state constraints, and the optimal solution determined using quadratic programming. Similarly, Gilbert and Kolmanovsky (1999) considered the effect of worst case disturbances within reference management to control open-loop unstable non-minimum phase systems including an inverted pendulum and a bank-to-turn missile.

Bemporad (1998a) extended the analysis with consideration of closed-loop predictions, where the effect of disturbances was reduced by regulatory control and taken into consideration in modifying the filter time constant. The objective function was based on minimizing the squared deviation of the setpoint from target with penalty on the steady-state tracking error and changes in the feedback gain.

2.6.3 Additional Comments

Hirata and Kogiso (2001) applied reference management on a position servomechanism, achieving an improvement in performance in addition to constraint fulfillment by minimizing the norm of the deviation between the output from target. Similarly, Sugie and

Yamamoto (2001) used a weighted objective function minimizing the squared deviation between the output from target in addition to the setpoint from target. Additional studies in reference management are also discussed by Casavola and Mosca (1996), Bemporad et al. (1997), Angeli et al. (1999), Miller et al. (2000), Angeli et al. (2001), Gilbert and Kolmanovsky (2001), Gilbert and Kolmanovsky (2002) Kogiso and Hirata (2002), Kogiso and Hirata (2003), Oh-Hara and Hirata (2003), Hirata and Minemura (2004), and Hatanaka and Takaba (2005).

Reference management was originally proposed to maintain linearity by preventing input saturation, thus improving closed-loop performance for linear control. However, subsequent research has extended the methodology to include consideration of output constraints and the effects of uncertainty. Computational strategies for the determination of the optimal scalar gain, or filter time constant in the low order reference filter were also investigated in literature. Conditions for convergence were developed and improved closed-loop stability and performance demonstrated.

2.7 Optimization and Control Hierarchy

According to Shobrys and White (2000), there are significant economic incentives for the integration of optimization and control in the chemical industry with oil companies estimating benefits at \$1 per barrel, and cost and inventory reductions of 20% reported by Exxon Chemicals. A strategy for integrating steady-state optimization and control was implemented by Guovêa and Odloak (1998) in a fluid catalytic cracker (FCC) unit at the Petrobras refinery in Brazil. The economic and control objectives were combined into a single objective function, where control performance was heavily weighted for robust stability resulting in a smooth but slow response to economic change. However, solving the optimization and control problem simultaneously in the single-level approach may be intractable for large scale nonlinear processes due to computational limitations (Kadam et al., 2002).

Furthermore, although model predictive control has obscured the distinction between optimization and control, the hierarchical decomposition is inherently related to the frequency of disturbances (Kookos and Perkins, 2004) and enables stationary and non-stationary disturbance rejection to be handled under two time scales (Morari et al., 1980). An additional advantage of multi-layer vertical decomposition is decomposition by functionality, thus simplifying regulatory control structure design and enabling intuitive interpretation of plant operation by operating personnel.

2.7.1 Two Layer Approach with LP/QP-MPC

The two layer approach of separating economic and control objectives is also implemented in commercial products as described by Qin and Badgwell (2003), based on steady-state target optimization using linear programming (LP) or quadratic programming (QP). Cascading steady-state optimization to update the setpoints used in model predictive control has been used in industry for several years for dynamic tracking of the optimum in the presence of disturbances (Ying and Joseph, 1999). In the presence of additional degrees of freedom, ideal resting values for inputs are also determined by optimization (Maciejowski, 2002). Thus the setpoint and input targets are typically updated based on a linear or quadratic economic objective function resulting in LP-MPC and QP-MPC respectively (Ying et al., 1998). The sub-optimization within the controller influences economic performance while ensuring feasible operation (Mizoguchi et al., 1995). The higher frequency compared to real time optimization is required to ensure the economic model and setpoints are consistent with current operating conditions (Tenny et al., 2004).

The mathematical formulation for QP-MPC is given by Brosilow and Joseph (2002) as shown below,

$$\min_{y_{sp}, u_{tgt}} \|y_{tgt} - y_{sp}\|^2_{W_y} + \|u_{tgt} - u_r\|^2_{W_u} \tag{2.8}$$

$$y_s = A_s u_s + d_s \tag{2.9}$$

$$u_{min} \leq u_r \leq u_{max} \tag{2.10}$$

$$y_{min} \leq y_{sp} \leq y_{max} \tag{2.11}$$

where W_y and W_u are symmetric positive definite weighting matrices given to outputs and inputs based on relative costs. The steady-state optimizer based on economic or minimum movement objectives, is embedded within model predictive control, and may improve stability by providing feasible steady-state setpoints in the presence of unmeasured disturbances (Sorensen and Cutler, 1998). Furthermore, the economic objective may be based on unit objectives not considered by real time optimization (Becerra et al., 1998), and ensures feasibility based on local constraints (Yousfí and Tourier, 1991).

Nominal stability of LP-DMC and QP-DMC was discussed by Ying et al. (1998) and Ying and Joseph (1999), concluding that linear or quadratic programming with time invariant active constraints would not affect stability given stability of the underlying regulatory control layer. The theorem proposed was used to justify tuning the regulatory control for stability and subsequently using LP/QP optimization to improve performance without affecting stability. However, while used in industry (Lee and Xiao, 2000), LP/QP-DMC may result in suboptimal operation due to the absence of input saturation considerations within the regulatory controller (Ramos et al., 2002).

Optimal economic performance is important in industry, particularly in the presence of changing disturbances. The industrial approach in the application of steady-state optimization to systems affected by persistent disturbances, is based on relaxing steady-state assumptions, otherwise resulting in lost opportunity with low frequency of re-optimization (Nath et al., 2000). However, suboptimality may result during transient operation due to violation of the steady-state assumption (Moro and Odloak, 1995). Thus, increasing the frequency of optimization, may not necessarily improve performance.

Kozub (1997) described the industrial implementation of a monitoring scheme for a model predictive controller with an embedded LP steady-state optimizer, and identified stability problems arising from chattering as a result of rapid changes in the controller dimension due to frequent re-optimization. Similar trends were observed by Kassmann and Badgwell (2000) with inputs cycling at opposite ends of the feasible region as a result of model mismatch arising from optimization based on steady-state objectives under dynamic operation. A similar conclusion was drawn by Zanin et al. (2000) at a fluid catalytic cracking (FCC) unit in Brazil, attributing the noisy closed-loop response to conflicting steady-state economic and dynamic control objectives. Thus there are incentives to incorporate dynamic models within optimization.

Despite the shortcomings of LP-MPC and QP-MPC, the ability to yield significant return on investment is recognized in industry. Vermeer et al. (1997) estimated benefits of \$0.50 per m^3 of gasoline produced as a result of lower value blend components, and reduced the number of re-blends from 12% to less than 1% at Sunoco in Canada. Similar benefits at British Petroleum Amoco in Australia estimated benefits of \$1 million per year (Verne et al., 1999), and a composite LP steady-state optimizer in the Toledo refinery at Sunoco resulted in performance benefits of 30% (Jakhete et al., 1999). Several commercial products are also available as detailed by Qin and Badgwell (2003). Commercial implementation of LP-MPC is used in such products as Control and Identification (Connoisseur) from Invensys, but susceptible to uncertainty which is partially addressed through filtering, detuning and move suppression. Commercial implementation of QP-MPC is used in such products as Robust Model Predictive Control (RMPCT) from Honeywell Hi-Spec, Predictive Functional Control (PCF) from Adersa, Aspen Target from AspenTech, Multivariable Control (MVC) from Continental Controls Inc. and Processs Perfector from Pavilion Technologies, where the quadratic objective function used is expected to reduce solution sensitivity to uncertainty.

2.7.2 Two Layer Approach with Consideration of Dynamics

As discussed, the incorporation of dynamics may yield additional benefits and enable increased frequency of re-optimization. Thus, Kadam et al. (2002) proposed the two layer approach where the upper level determines the optimal trajectory based on a dynamic nonlinear economic model, tracked by lower level unconstrained model predictive control based on a dynamic linear or nonlinear model. The resulting dynamic real time optimization (D-RTO) scheme was capable of meeting target objectives for the production of methyl acetate in a semi-batch reactive distillation column. The proposed scheme based on plantwide dynamic optimization was also applied by Brempt et al. (2004) to improve grade transitions in polyethylene polymerization. The economically optimal reference trajectory was determined based on a rigorous dynamic nonlinear model, and model predictive control used for tracking.

In this work, a similar decomposition is proposed where the upper level determines the optimal setpoint trajectory based on a closed-loop dynamic model, but tracked at the lower level by *constrained* model predictive control, which is taken into account in the computation of the optimal setpoint trajectory.

Chapter 3

Mathematical Formulation

This chapter details the mathematical formulation and solution strategy for reference management based on closed-loop dynamic models. The calculation of the optimal setpoint trajectory results in a multi-level optimization problem when the closed-loop dynamics of constrained model predictive control are taken into account. The setpoint trajectory is optimized at the upper level using an economic or dynamic performance objective function while the plant inputs are determined at the lower level using the control performance objective function. The algorithm of quadratic dynamic matrix control is reviewed in Section 3.1, and the sequential and simultaneous solution strategies for the proposed methodology presented in Sections 3.2 and 3.3 respectively. For further details on implementing the simultaneous approach, orthogonal collocation on finite elements is described in Section 3.4, the Karush-Kuhn-Tucker (KKT) conditions in Section 3.5, and interior point methods in Section 3.6.

3.1 Constrained Model Predictive Control

The general formulation of constrained model predictive control was discussed in Section 2.3. Model predictive control is a model based receding horizon control algorithm, calculating a sequence of inputs over a control horizon M of which only the first is implemented. Optimal inputs are determined by minimizing a least squares control performance objective function by penalizing the squared deviation between output predictions from setpoint, input deviation from the ideal resting value, and penalty on input movement over a prediction horizon P subject to a linear dynamic model, and input and output constraints.

The algorithm for quadratic dynamic matrix control (QDMC) based on the finite step response for open-loop stable systems is briefly outlined in Equations 3.1-3.12 for a single-input single-output system, with further details provided in García and Morari (1986) and Bequette (2003).

$$\min_{\Delta u} \phi = (y_{sp} - \hat{y})^T Q (y_{sp} - \hat{y}) + \Delta u^T R \Delta u \tag{3.1}$$

where $Q \in \Re^{P \times P}$ and $R \in \Re^{M \times M}$ are positive definite weighting matrices, $\hat{y} \in \Re^P$ a vector of output predictions over the prediction horizon P, and $u \in \Re^M$ and $\Delta u \in \Re^M$ are vectors comprising of future inputs and input changes respectively.

$$\hat{y} = [\hat{y}_{k+1}, \cdots, \hat{y}_{k+P}]^T \tag{3.2}$$

$$u = [u_k, \cdots, u_{k+M-1}]^T \tag{3.3}$$

$$\Delta u = [\Delta u_k, \cdots, \Delta u_{k+M-1}]^T \tag{3.4}$$

The minimization in Equation 3.1 is subject to the following constraints,

$$\hat{y} = y_f + A\Delta u + \hat{d} \tag{3.5}$$

$$y_{\min} \leq \hat{y} \leq y_{\max} \tag{3.6}$$

$$u_{\min} \leq u \leq u_{\max} \tag{3.7}$$

$$\Delta u_{\min} \leq \Delta u \leq \Delta u_{\max} \tag{3.8}$$

where $y_f \in \Re^P$ represents the free response depending only on past inputs, and $A \in \Re^{P\times M}$ represents the dynamic matrix given by

$$A = \begin{bmatrix} s_1 & 0 & \cdots & 0 \\ s_2 & s_1 & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ s_P & s_{P-1} & \cdots & s_{P-M+1} \end{bmatrix} \tag{3.9}$$

where s_i are the unit step response coefficients. The estimated disturbance is given as follows, with the standard conventional assumption of uncorrelated integrated random walk disturbances in the outputs (Morari and Lee, 1991),

$$\hat{d} = \begin{bmatrix} \hat{d}_{k+1} \\ \vdots \\ \hat{d}_{k+P} \end{bmatrix} = \begin{bmatrix} d_k \\ \vdots \\ d_k \end{bmatrix} = \begin{bmatrix} y_k - \hat{y}_k \\ \vdots \\ y_k - \hat{y}_k \end{bmatrix} \tag{3.10}$$

where y_k denotes the actual measured output, and $\hat{d}$ denotes the predicted disturbance assumed to be constant over the prediction horizon P. By recognizing that

$$\hat{y} = y_f + A\Delta u + \hat{d} \tag{3.11}$$

$$u_{k+l} = u_{k-1} + \sum_{i=1}^{l+1} \Delta u_{k+i-1} \qquad l = 0, \cdots, M-1 \tag{3.12}$$

Equations 3.1-3.8 may be expressed in terms of the vector of input changes Δu as given by García and Morari (1986),

$$\min_{\Delta u} \phi' = \frac{1}{2}\Delta u^T H \Delta u - g^T \Delta u \tag{3.13}$$

$$C\Delta u \leq b \tag{3.14}$$

$$\Delta u_{\text{min}} \leq \Delta u \leq \Delta u_{\text{max}} \tag{3.15}$$

where C and b refer to a matrix and vector corresponding to inequality constraints respectively, and the Hessian H and gradient g of the objective function given by

$$H = A^T Q A + R \tag{3.16}$$

$$g = A^T Q \left(y_{sp} - y_f - \hat{d}\right) \tag{3.17}$$

Equations 3.13-3.17 constitutes a quadratic programming (QP) problem and may be further simplified using slack variables and reformulated as

$$\min_{x} x^T \bar{H} x + \bar{g}^T x \tag{3.18}$$

$$Ax = b \tag{3.19}$$

$$x \geq 0 \tag{3.20}$$

where A and b refer to a matrix and vector corresponding to equality constraints respectively. The Karush-Kuhn-Tucker (KKT) conditions may be applied to the standard quadratic optimization given in Equations 3.18-3.20, resulting in the following first order optimality conditions, yielding the optimal solution for quadratic dynamic matrix control (QDMC),

$$\bar{H}x + \bar{g} - A^T v - w = 0 \tag{3.21}$$

$$Ax = b \tag{3.22}$$

$$w_i x_i = 0 \tag{3.23}$$

$$(w, x) \geq 0 \tag{3.24}$$

where v and w refer to the equality and inequality Lagrange multipliers respectively. The ability to handle input constraints is characteristic of second generation quadratic dynamic matrix control (Qin and Badgwell, 2003), while hard output constraints are typically softened in commercial algorithms by slack variables penalized in the objective function (Morari and Lee, 1999).

In this thesis, inequality constraints on outputs and input changes are not considered at the regulatory control level. Furthermore, the controller formulation was based on the assumption of a constant setpoint trajectory over the future prediction horizon, since specification of a dynamic setpoint trajectory is not common in practice (Bemporad et al., 2004) and the focus of this research is the application of reference management with consideration of the existing regulatory control system. However, the general formulation for model predictive control is capable of utilizing information about the future setpoint trajectory to improve setpoint tracking.

3.2 Sequential Optimization

The application of reference management to determine the optimal setpoint trajectory such that the output attains target based on a cost objective function subject to hard input and output constraints, requires solution to a multi-level optimization problem due to consideration of the closed-loop dynamics of input constrained model predictive control.

Sequential optimization may be used to solve the multi-level problem, essentially separating optimization in the upper level from integration in the lower level performed in MatLab 7.0 (Bemporad et al., 2004) via closed-loop simulations. The solution strategy parameterizes the setpoint profile using control vector parameterization with piecewise constant setpoints, but the state profile is determined at every iteration by the integration of the set of differential and algebraic equations (DAE) representing the process. Thus the feasible path method enables integration solvers to control the discretization error by adjusting the integration step (Vassiliadis et al., 1994). The mathematical formulation of the two-layered algorithm to indirectly improve economic operation by minimizing the amount of off-specification product produced is given by

$$\min_{y_{sp}} \phi = \sum_{i=1}^{N} \left[\alpha_i \left(y_{sp,i} - y_{tgt}\right)^2 + \beta_i \left(y_i - y_{tgt}\right)^2\right] \tag{3.25}$$

$$x_{i+1} = f\left(x_i, u_i, d\right) \tag{3.26}$$

$$y_i = g\left(x_i, u_i, d\right) \tag{3.27}$$

$$u_i = h\left(y_i, u_p, y_{sp}\right) \tag{3.28}$$

where y_{tgt}, y_{sp} and y represent the target, setpoint and the measured output respectively over the simulation horizon N with weighting factors α and β to penalize the squared deviation between the setpoint and output from target. The states x given by Equation 3.26 are determined from the integration of a system of differential and algebraic equations. The implemented inputs u are generated through the solution of an open-loop optimal control problem using constrained model predictive control and represented by Equation 3.28, where u_p represents the inputs previously applied to the process.

In addition, hard output constraints and constraints on the admissible setpoints may be included at the upper level:

$$y_{\min} \leq y_i \leq y_{\max} \tag{3.29}$$

$$y_{sp,\min} \leq y_{sp,i} \leq y_{sp,\min} \tag{3.30}$$

where $\min$ and $\max$ represent minimum and maximum values. Thus determination of the optimal setpoint trajectory using reference management results in a multi-level optimization problem as seen in Figure 3.1. The outer optimization problem is based on an economic or control performance objective function, and a series of inner optimization problems are solved at each time instant along the simulation horizon arising from the consideration of constrained model predictive control.

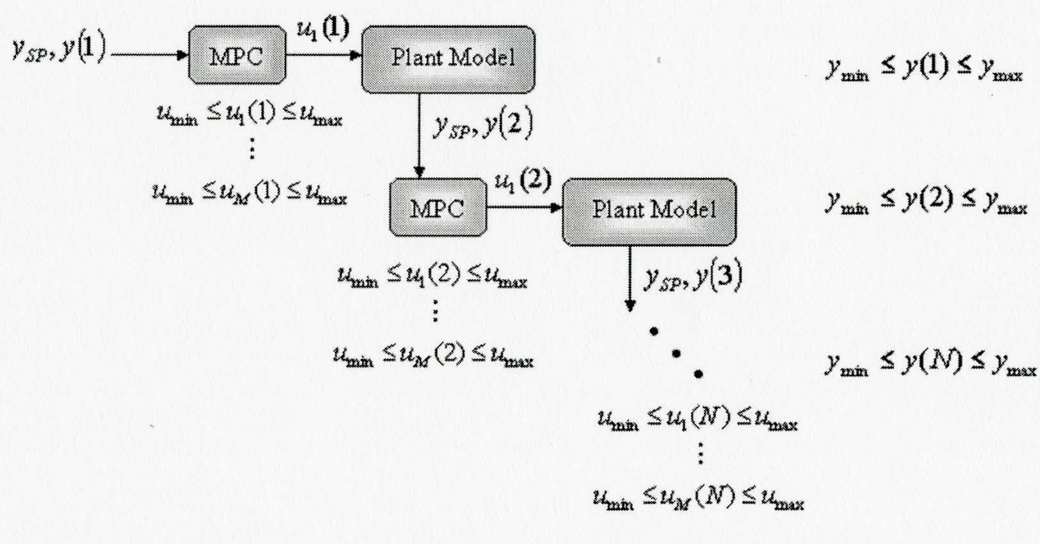


Figure 3.1: Multi-level optimization arising from model predictive control

The sequential approach separates optimization of the setpoint trajectory and integration of a continuous state profile, solving the constrained regulatory control optimization problems within the integration step through closed-loop simulations. However, the sequential approach may be computationally expensive with 90% of the computational time attributed to model integration (Abel et al., 2000). Furthermore, handling path constraints directly within the optimizer and indirectly within the integrator may be inefficient requiring several iterations to ensure feasible states (Feehery and Barton, 1996, 1998). The activation of inequality path constraints also introduces derivative discontinuities, slowing convergence of the optimization algorithm as a result of step length restrictions (Chen and Vassiliadis, 2005).

However, according to Bloss et al. (1999), the main bottleneck in sequential dynamic optimization is the calculation of objective function and constraint gradients by finite differencing or techniques based on sensitivity and adjoint equations. The computational expense incurred by the sensitivity equation approach is proportional to the number of decision variables, while the adjoint equation approach is proportional to the number of constraints. Furthermore, inefficiency in numerical integration at intermediate solutions also increases computational expense particularly for stiff systems (Tjoa and Biegler, 1991) and infeasibility may result with integration failure resulting from unstable intermediate points despite a stable final solution (Biegler, 1998).

3.3 Simultaneous Optimization

Simultaneous optimization, or direction transcription, is used to solve the multi-level problem by formulating the multi-level programming problem into a single-level programming problem using the Karush-Kuhn-Tucker (KKT) conditions, similar to the solution strategy used by Clark and Westerberg (1990). The solution strategy proposed parameterizes the setpoint and state profiles producing a large sparse system of algebraic constraints solved using an interior point approach. The general mathematical formulation is given as follows,

$$\min_{y_{sp}} \phi = \sum_{i=1}^{N} \left[\alpha_i \left(y_{sp,i} - y_{tgt}\right)^2 + \beta_i \left(y_i - y_{tgt}\right)^2\right] \tag{3.31}$$

$$x_{i+1} = f\left(x_i, u_i, d\right) \tag{3.32}$$

$$y_i = g\left(x_i, u_i, d\right) \tag{3.33}$$

$$u_i = h\left(y_i, u_{i-1}, y_{sp,i}\right) \tag{3.34}$$

$$y_{\min} \leq y_i \leq y_{\max} \tag{3.35}$$

$$y_{sp,\min} \leq y_{sp,i} \leq y_{sp,\min} \tag{3.36}$$

where y_{tgt}, y_{sp} and y represent the target, setpoint and the measured output respectively over the simulation horizon N with weighting factors α and β to penalize the squared deviation between the setpoint and output from target. Equation 3.32 represents the linear or possibly nonlinear dynamic process model, and Equation 3.34 represents the lower level optimization problem of constrained model predictive control. Hard output constraints are given in Equation 3.35, and constraints on the admissible setpoints in Equation 3.36. Constraints on the change between successive setpoints are not shown, but may also be included if desired, and are typically used in conventional steady-state real time optimization to enable time for the plant to move to the new operating point while preventing large changes in operation (Bailey et al., 1993).

The reformulation of the multi-level optimization problem by replacing the inner problem with stationary conditions results in a mathematical program with equilibrium constraints (MPEC) as defined by Raghunathan and Biegler (2003), and is similar to the integrated control and design formulation used to handle input saturation by Baker and Swartz (2004a). The single-level formulation of the nested optimization problem results in a non-convex (Clark and Westerberg, 1990), and highly constrained problem (Raspanti et al., 2000).

In this work, the complementarity conditions are solved using an interior point approach, where the complementarity conditions are relaxed with a positive barrier parameter which is gradually decreased to zero to obtain the optimal solution, thus recovering the original complementarity constraints (Terlaky and Boggs, 2000).

Thus the simultaneous approach is proposed to determine the optimal setpoint trajectory by reference management, and quadratic dynamic matrix control implemented in AMPL (Fourer et al., 2002) based on development from Baker (2004) and Soliman (2005).

3.4 Orthogonal Collocation on Finite Elements

The simultaneous approach requires discretization of the state and output profiles, handled through techniques such as orthogonal collocation on finite elements. For systems described by a linear dynamic model, the principle of superposition of finite step response coefficients may be used at the desired sampling interval for discretization of the output, similar to dynamic matrix control. However, for systems described by a nonlinear dynamic model, orthogonal collocation is used to convert differential equations corresponding to state variables into algebraic equations over finite intervals by polynomial approximation as detailed by Biegler (1984). The time axis is scaled over each finite element $k = 1, \cdots, nFE$:

$$\tau = \frac{t - t_{k-1}}{\delta} \in [0, 1] \tag{3.37}$$

where nFE is the number of finite elements, and δ the time interval between finite elements. The state over each finite element is approximated by

$$\tilde{x}(t) = \sum_{j=0}^{nCOL+1} x[k, j]\, \phi[j, \tau] \tag{3.38}$$

where $nCOL$ is the number of collocation points, and $\tilde{x}$ the approximate state. The collocation points defined within the normalized intervals of each finite element were chosen to correspond with the zeros of the Legendre polynomial, and an additional collocation point was enforced at the finite element boundary. The n degree Jacobi polynomial of the form,

$$P_n^{(\alpha,\beta)}(x) = 2^{-n} \sum_{k=0}^{n} \begin{pmatrix} n+\alpha \\ k \end{pmatrix} \begin{pmatrix} n+\beta \\ n-k \end{pmatrix} (x-1)^{n-k} (x+1)^k \tag{3.39}$$

is given by Funaro (1992), where $\alpha, \beta > -1$ defines an orthogonal polynomial, thus ensuring the existence of n distinct real zeros in the interval $[-1, 1]$ for $n \geq 1$ (Villadsen and Michelsen, 1978; Datta and Mohan, 1995). Equidistant placement of collocation points may result in divergence problems, while orthogonality ensures real and distinct zeros, although alternative polynomials may be used based on different weighting functions with slight differences in accuracy and convergence (Villadsen and Stewart, 1967; Villadsen, 1970). Improved accuracy in the approximation is obtained with an increase in the number of collocation points.

The Legendre polynomial is classified as a Genebauer or ultraspherical ($\alpha = \beta$) Jacobi polynomial with $\alpha = \beta = 0$ (Funaro, 1992) and the zeros determined from the following,

$$P_0^{(0,0)}(x) = 0 \tag{3.40}$$

$$P_1^{(0,0)}(x) = \frac{1}{2}(\alpha+\beta+2)x + \frac{1}{2}(\alpha-\beta) = x \tag{3.41}$$

$$P_2^{(0,0)}(x) = \frac{3}{2}x^2 - \frac{1}{2} \tag{3.42}$$

$$P_3^{(0,0)}(x) = \frac{5}{3}x\left(\frac{3}{2}x^2 - \frac{1}{2}\right) - \frac{2}{3}x = \frac{x}{2}\left(5x^2 - 3\right) = 0 \Rightarrow z = 0, \pm\sqrt{\frac{3}{5}} \tag{3.43}$$

$$P_n^{(0,0)}(x) = \frac{2n-1}{n}xP_{n-1}^{(0,0)}(x) - \frac{n-1}{n}P_{n-2}^{(0,0)}(x) \tag{3.44}$$

Hence, the state profile within a finite element with 3 collocation points is approximated by the 3rd degree Legendre polynomial with zeros determined at $z = -0.775, 0, 0.775$ as calculated in Equation 3.43. According to Vasantharajan and Biegler (1990), two or three collocation points are generally sufficient for an accurate approximation given a sufficient number of finite elements, although the approximation error may be further controlled using adaptive placement of finite elements.

The Jacobi polynomials are defined within the interval $|P_n^{(\alpha,\beta)}(x)| \leq 1$ for a bounded state $|x| \leq 1$ (Funaro, 1992), and within each finite element, the collocation points may be normalized to an arbitrary interval by linear transformation (Datta and Mohan, 1995). Thus, the collocation points were normalized within the range of $[0, 1]$ resulting in collocation points at $\tau = 0.113, 0.500, 0.887$. In addition to the interior quadrature points, the residuals of the differential equation are made to vanish at the element boundary at $\tau = 0, 1$. The Lagrange interpolation polynomial relative to the Legendre zeros, was used for approximation of the solution (Biegler, 1984).

$$\phi[j, \tau] = \prod_{l=0, l\neq j}^{nCOL+1} \frac{\tau - \tau_l}{\tau_j - \tau_l} \tag{3.45}$$

$$\phi[j, \tau_i] = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases} \tag{3.46}$$

Residual constraints are applied at each collocation point $i = 1, \cdots, nCOL$ and at knots defining the boundary of finite elements

$$\sum_{j=0}^{nCOL+1} \left(x\left[k,j\right] \frac{d\phi\left[j,\tau_i\right]}{d\tau_i} \right) - f\left(x\left[k,i\right]\right)\delta = 0 \tag{3.47}$$

However, superelements consisting of collocation points on several finite elements may be used with breakpoint boundaries, and the adaptive placement of knots may be used to improve the accuracy of approximation without excessive increase in the number of additional finite elements (Cuthrell and Biegler, 1987).

The derivative of the Lagrange polynomial function given in Equation 3.45 is required to evaluate the residuals and may be obtained using the Chain Rule with $l \neq j$ and $n = nCOL$, given by

$$\begin{aligned} \frac{d\phi\left[j,\tau_i\right]}{d\tau_i} = \left(\frac{1}{\tau_j - \tau_1}\right)\left(\frac{\tau_i - \tau_2}{\tau_j - \tau_2}\right)\cdots\left(\frac{\tau_i - \tau_n}{\tau_j - \tau_n}\right) + \cdots \\ + \left(\frac{1}{\tau_j - \tau_n}\right)\left(\frac{\tau_i - \tau_1}{\tau_j - \tau_1}\right)\cdots\left(\frac{\tau_i - \tau_{n-1}}{\tau_j - \tau_{n-1}}\right) \end{aligned} \tag{3.48}$$

Furthermore, function continuity constraints are imposed for smooth state profiles between finite elements at $\tau = 0$ and $\tau = 1$,

$$x\left[0,0\right] = x_0 \tag{3.49}$$

$$x\left[k,0\right] = \sum_{j=0}^{nCOL+1} x\left[k-1,j\right]\phi\left[j,\tau=1\right] \qquad k \geq 2 \tag{3.50}$$

The discretization of the state profile through the use of orthogonal collocation on finite elements is schematically presented in Figure 3.2.

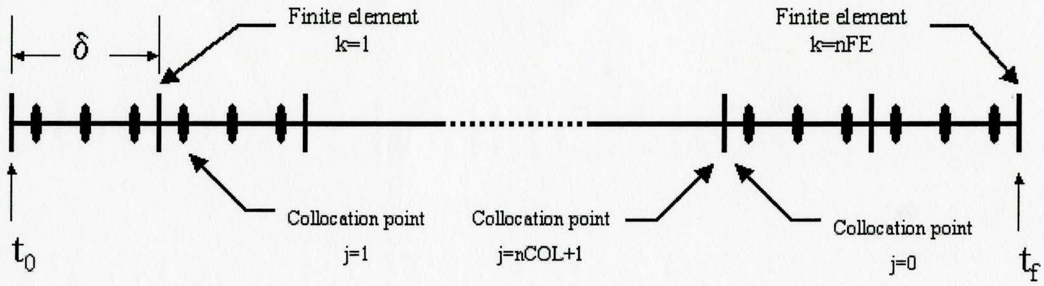


Figure 3.2: Orthogonal collocation on finite elements

3.5 Karush-Kuhn-Tucker Conditions

The general formulation of the minimization problem is given by Nash and Sofer (1996),

$$\min_{x} \quad f(x) \tag{3.51}$$

$$h_i(x) = 0 \tag{3.52}$$

$$g_j(x) \geq 0 \tag{3.53}$$

where $i = 1, \cdots, m$ and $j = 1, \cdots, r$ denote equality and inequality constraints respectively. The Karush-Kuhn-Tucker (KKT) conditions are used to transform a constrained optimization problem into a corresponding set of algebraic equations based on the Lagrangian defined by,

$$L(x, \lambda, \nu) = f(x) - \sum_{i=1}^{m} \lambda_i^T h_i(x) - \sum_{j=1}^{r} \nu_j^T g_j(x) \tag{3.54}$$

The Karush-Kuhn-Tucker (KKT) first order necessary conditions for optimality are given by Nash and Sofer (1996) and Luenberger (1984),

$$\nabla_x L(x^*, \lambda^*, \nu^*) = \nabla f(x^*) - \lambda^{*T} \nabla h(x^*) - \nu^{*T} \nabla g(x^*) = 0 \tag{3.55}$$

$$\nabla_\lambda L(x^*, \lambda^*, \nu^*) = h(x^*) = 0 \tag{3.56}$$

$$g_j(x^*) \geq 0 \tag{3.57}$$

$$\nu_j^* g_j(x^*) = 0 \tag{3.58}$$

where λ^* the lagrange multiplier for equality constraints, ν^* is the lagrange multiplier for inequality constraints and is sign restricted $\nu_j^* \geq 0$, and x^* is the local extremum point of f and a regular point of constraints. The regularity condition ensures that the gradients of active constraints are linearly independent, and is also known as linear independence constraint qualification (Nocedal and Wright, 1999). Violation of the regularity conditions may result in an iterate that is the only feasible point within its neighbourhood (Bell and Sargent, 2000) and may cause failure for global convergence particular interior point algorithms caused by iterates approaching their bounds prematurely (Wächter and Biegler, 2000; Byrd et al., 2004).

The inequality constraints may be reformulated into equality and bound constraints using slack variables s_j as follows,

$$g_j(x) - s_j = 0 \qquad s_j \geq 0 \tag{3.59}$$

According to Forsgren et al. (2002), the reformulation results in additional expense only in storing and updating the slack variables. Although the introduction of slack variables increases the problem dimension, with interior point methods, it is simple to retain feasibility with bound constraints since the step to the boundary may be calculated exactly, while several iterations are required for general inequality constraints. Also it enables interior point methods requiring a feasible initial point to be applied despite an unknown initial point, thus the computational burden is shifted from inequality to equality constraint satisfaction, changing the behaviour of alternative formulations of interior point methods. Thus converting general inequality constraints into equality and bound constraints may improve the efficiency of interior point algorithms as also used by Vanderbei and Shanno (1999), but resulting in an infeasible slack-based interior point method (Byrd et al., 2003).

Optimization problems consisting of a quadratic objective function and linear equality constraints with variable bound constraints may be described by the standard quadratic programming problem of the form,

$$\min_{x} f(x) = \frac{1}{2}x^T H x + g^T x \tag{3.60}$$

$$Ax = b \tag{3.61}$$

$$x \geq 0 \tag{3.62}$$

where A and b correspond to equality constraints, and H is a symmetric positive semi-definite matrix. Thus, the Lagrangian is given by

$$L = \frac{1}{2}x^T H x + x^T g + \lambda^T (Ax - b) - \nu^T x \tag{3.63}$$

The corresponding Karush-Kuhn-Tucker (KKT) first order optimality conditions are given by

$$Hx + g + A^T\lambda - \nu = 0 \tag{3.64}$$

$$Ax - b = 0 \tag{3.65}$$

$$\nu_j x_j = \nu^T x = 0 \tag{3.66}$$

$$(x, \nu) \geq 0 \tag{3.67}$$

where λ_i and ν_j are the equality and inequality lagrange multipliers. Thus the methodology described by Edgar et al. (2001) may be applied to quadratic dynamic matrix control (QDMC) which consists of a convex minimization problem based on a quadratic control performance objective function, linear equality constraints and variable bound constraints on inputs. Furthermore, the second order conditions for optimality are not required since convexity ensures a global minimum with the additional restrictions on H being positive semi-definite (Nocedal and Wright, 1999). Note that the complementarity condition given in Equation 3.66 may be written in vector notation due to non-negativity conditions on $\nu_j \geq 0$ and $x_j \geq 0$.

3.6 Interior Point Methods

The resulting complementarity conditions shown in Equation 3.66 arising from the Karush-Kuhn-Tucker conditions may be efficiently handled using interior point methods, which are used in commercial linear programming with additional applications in linear and nonlinear programming with complementarity conditions (Wright, 1998). The complementarity conditions with Lagrange multipliers ν corresponding to inequality constraints are relaxed with a positive barrier parameter μ,

$$\nu_j x_j = \nu^T x = \mu \tag{3.68}$$

which is gradually decreased to zero to obtain the optimal solution, thus recovering the original complementarity constraints (Terlaky and Boggs, 2000). The barrier parameter is updated by

$$\mu_{k+1} = \theta \mu_k \quad 0 \leq \theta < 1 \tag{3.69}$$

Interior point methods are based on barrier functions imposing a penalty on reaching the boundary of an inequality constraint (Nash and Sofer, 1996). The nonlinear constrained problem considered is given by

$$\min_x \quad f(x) \tag{3.70}$$

$$g_j(x) \geq 0 \tag{3.71}$$

where $j = 1, \cdots, r$ denotes inequality constraints. The barrier term prevents iterates from reaching the boundary by growing unbounded as approached from the interior, and may be implemented with the logarithmic function,

$$\min_x \beta(x, \mu) = f(x) - \mu \sum_{i=1}^{m} \log(g_i(x)) \tag{3.72}$$

or alternatively, with the inverse function,

$$\min_x \beta(x, \mu) = f(x) - \mu \sum_{i=1}^{m} \frac{1}{g_i(x)} \tag{3.73}$$

As the barrier parameter is decreased, it approaches the boundary such that the original complementarity conditions are closer to being satisfied, thus approaching the optimal primal-dual solution. However, the problem becomes increasingly difficult to solve due to ill-conditioning and numerical errors resulting in poor search directions where Newton's method is only effective in finding the approximate optimal solution at each iteration. Hence, line search and trust region mechanisms with good initial starting points are required to improve convergence. Furthermore, convergence criteria may be specified with the assumption of the existence of continuously parameterized families of approximate solutions asymptotically converging to the exact solution (Wright, 2004).

Primal-dual interior point methods use a central path (Nocedal and Wright, 1999),

$$C_{pd} = \left[x^*\left(\mu\right), \lambda\left(\mu\right), \nu\left(\mu\right), s\left(\mu\right) | \mu > 0\right] \tag{3.74}$$

to bias iterates such that complementarity products are decreased towards zero at the same rate, thus improving identification of the active set (Rico-Ramírez and Westerberg, 2002). According to Roos et al. (1997) decreasing μ by a small amount at each iteration forces iterates to remain close to the primal-dual central path but resulting in slow convergence in practice. A large update reduces the barrier parameter at a much faster rate ($\theta = 0.75$) although resulting in iterates further away from the central path, thus reducing the efficiency of Newton's method.

According to Forsgren et al. (2002), primal-dual interior point methods are increasingly popular for solving general nonlinear programming problems, and efficient for non-convex nonlinear programming with possible applications for large scale optimization as described Biegler et al. (2002). Interior point methods appear to be insensitive to problem size (Biegler, 1998), supported by experimental results obtained by Baker and Swartz (2004b), demonstrating a significant increase in computational expense with increasing number of binary variables used to represent logical conditions in comparison to a modest increase in solution time using an interior point approach. Similar experimental results were obtained by Baker and Swartz (2005) in the application of an interior point approach to handle complementarity conditions arising from the solution of multi-level optimization problems, and reliability in obtaining the global optimum demonstrated.

The interior point algorithm IPOPT was developed by Wächter (2002) to solve nonlinear programming (NLP) problems. Raghunathan and Biegler (2003) extended the algorithm to address mathematical programming problems with complementarity constraints (MPCCs) by developing IPOPT-C, and applied to determine optimal startup of batch distillation columns and multi-component separation of natural gas by Raghunathan et al. (2004). Additional details of the implementation of the primal-dual interior point algorithm are given by Wächter and Biegler (2004), and the handling of complementarity conditions by Raghunathan and Biegler (2005).

In this work, IPOPT-C 2.2.1.d was used to determine the optimal reference trajectory using the simultaneous approach. The solver was compiled November 2004 from open source code available by Wächter and Biegler (2004) under Common Public Licence (CPL) from the Computational Infrastructure for Operations Research (COIN-OP) repository, using Fortran subroutines available by Duff (2004) through the Harwell Subroutine Library (HSL) archive from Hyprotech UK Ltd.

Chapter 4

Application to Linear Systems

This chapter details the application of reference management under constrained model predictive control for steady-state transitions in linear systems. A single-input single-output system is investigated in Section 4.1 demonstrating the benefits of the simultaneous rather than sequential approach in terms of reduced computational expense and increased solution reliability, particularly in the presence of input saturation. The simultaneous strategy is further investigated to determine the sensitivity of the optimal solution to the formulation of the objective function and constraints. The possibility of indeterminacy, resulting in non-unique solutions is shown and a two-tiered hierarchical approach is proposed to determine optimal operation. The discrete reference filter is also applied, and the limitations and potential benefits discussed. Reference management is also applied to non-minimum phase systems in Section 4.2, and multi-input multi-output systems in Section 4.3.

4.1 Single-Input Single-Output Systems

This case study is based on a single-input single-output nonlinear system modified from Marlin (2000), consisting of three continuously stirred tank reactors in series as shown in Figure 4.1, with steady-state conditions summarized in Table 4.1. A given setpoint target of x_{A3}=4 %, representing the mole fraction of component A in the product, was assumed for all simulations.

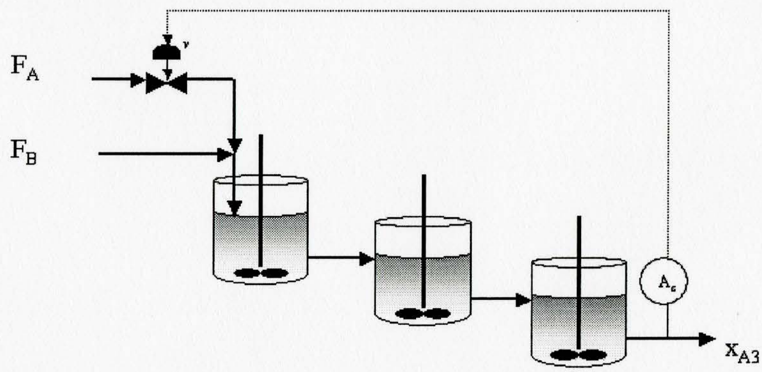


Figure 4.1: Schematic of three continuously stirred tank reactors in series

The steady-state conditions in Table 4.1 are represented by the inlet valve position v, the volume of the reactor V, the flow rate F, and the mole fraction of component A in stream A, x_{AA0}, the mole fraction of component A in stream B, x_{AB0}, and the mole fraction of component A in the final product stream, x_{A3}.

Table 4.1: Steady-state conditions for CSTRs in series

Variables	Value
v	20 % open
V_i	35 m^3
F_A	0.14 m^3/min
F_B	6.9 m^3/min
x_{AA0}	100 %
x_{AB0}	0.5 %
x_{A3}	3.0 %

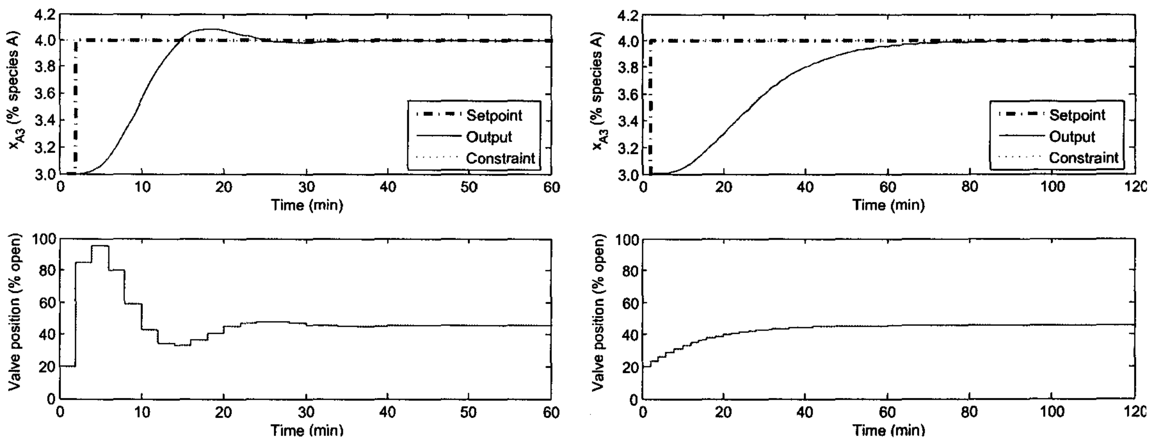
The mole fraction of component A in the outlet stream of the third mixing tank is controlled by manipulating the valve controlling the inlet flow rate of stream A. The process transfer function given by

$$x_{A3}(s) = G_p(s)\, v(s) = \frac{0.039}{(5s+1)^3} v(s) \tag{4.1}$$

An open-loop simulation in MatLab 7.0 resulted in a settling time of 60 minutes. In this case study, an output constraint in product quality of x_{A3}=4.0 % species A was assumed, based on economic considerations. The target was assumed to have incorporated dynamic backoff based on worst-case disturbance considerations, such that placing the constraint at target would prevent constraint violation resulting from aggressive control. Thus the constraint would be enforced assuming similar disturbances during transient operation as steady-state operation. The output constraint may also be related to operational constraints, possibly arising from concentration limitations to prevent equipment damage due to precipitation.

The system was controlled using constrained model predictive control such that the manipulated variable was constrained to $[0, 100]$ % open, and the rate of input change unconstrained. The controller was executed every 2 minutes with a prediction horizon of 30 and an input horizon of 10. The initial tuning with an output to input move weighting ratio of 100:1 resulted in 8.72% overshoot relative to the setpoint change as seen in Figure 4.2(a).

The output constraint violation resulting from the nominal controller tuning may be considered undesirable, and addressed by detuning the controller. However, while an output to input move weighting ratio of 100:30 is capable of preventing constraint violation, an increase in the transition time from 45 minutes to 100 minutes resulted as shown in Figure 4.2(b).



(a) Aggressive control (b) Detuned control

Figure 4.2: Comparison of tuning for feasibility and performance

Thus, output constraint violation may be addressed by detuning, but at the expense of increased transition times and reduced controller performance in disturbance rejection. However, an alternative solution retains aggressive controller tuning while enforcing output constraints, through manipulation of the setpoint trajectory during transient operation using reference management.

4.1.1 Comparison of Sequential and Simultaneous Optimization

The application of reference management is demonstrated based on the mathematical formulations detailed in Chapter 3, and the objective function based on minimizing the squared deviation between the setpoint and target.

Sequential optimization is used to solve the multi-level problem in MatLab 7.0 where the setpoint trajectory is optimized using sequential quadratic programming via the 'fmincon' function, and closed-loop simulations of constrained model predictive control using the the 'mpc' block in Simulink.

The resulting setpoint trajectory is shown in Figure 4.3, with a reduction in the transition time t_s to 30 minutes. The optimal solution was obtained in 215.3 CPU seconds with initial conditions (IC) based on a constant setpoint trajectory.

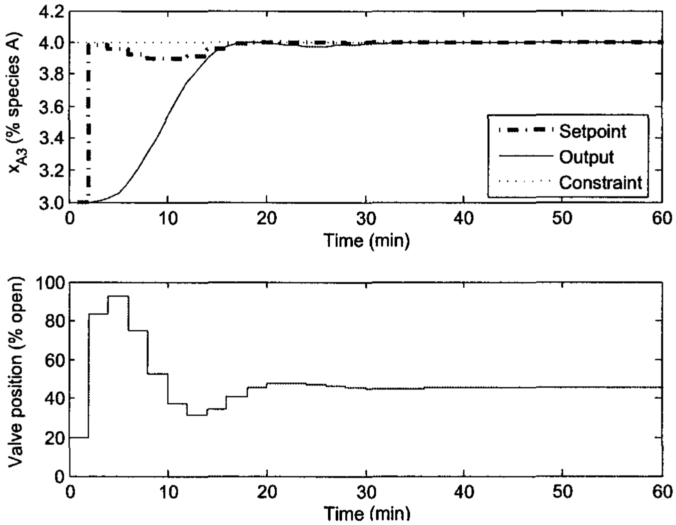


Figure 4.3: Sequential approach: Constraints satisfied with IC=1.00 $\alpha = 1$ $\beta = 0$

Solution sensitivity to the initial conditions was not evident, but computational efficiency was affected as summarized in Table 4.2, where the response was simulated for 100 minutes at a sampling time of 1 minute and with an objective function ϕ ($\alpha = 1$ and $\beta = 0$).

Identical results were obtained using simultaneous optimization, but requiring only 13.4 CPU seconds. The optimal solution was also found to be insensitive to initial conditions for optimization but the computational expense was significantly reduced as summarized in Table 4.3, where the response was simulated for 100 minutes at a sampling time of 1 minute and with an objective function ϕ ($\alpha = 1$ and $\beta = 0$).

Table 4.2: Sequential optimization under different initial conditions

IC	ϕ	Number of Iterations	Number of Evaluations	Computational Time (CPU seconds)
0.00	1.037924	18	1044	315.8
0.25	1.037925	11	635	186.1
0.50	1.037924	17	961	289.6
1.00	1.037924	13	727	215.3
1.50	1.037924	27	1535	460.6

Table 4.3: Simultaneous optimization under different initial conditions

IC	ϕ	Number of Iterations	Number of Evaluations	Computational Time (CPU seconds)
0.00	1.037916	40	69	13.6
0.25	1.037916	36	57	11.5
0.50	1.037916	40	90	13.4
1.00	1.037916	42	62	13.4
1.50	1.037916	47	106	16.0

Thus the results obtained by simultaneous optimization are identical to results obtained by sequential optimization but at a fraction of the computational cost by avoiding the need to integrate a system of differential algebraic equations over the simulation horizon at each iteration. The formulation of quadratic dynamic matrix control (QDMC) was based on step response coefficients of the linear process, but memory and computational expense may be significantly reduced using a state-space model representation (Lundström et al., 1995).

4.1.2 The Effect of Input Saturation

Steady-state transitions were next investigated with the input valve bounds restricted to $[20, 80]$ % open. Under such circumstances, the maximum constraint violation for a constant setpoint change was reduced to 7.14% of the setpoint change as a result of restrictions on allowable input action.

The restricted input bounds may represent safety margins, also used by Glemmestad et al. (1997) for steady-state optimization of heat exchanger networks in the presence of uncertainty. Thus, restricting the inputs within optimization to reserve capacity for disturbance rejection is a viable but suboptimal alternative to the explicit consideration of uncertainty. The safety margins required under worst case disturbances may be determined as detailed by Lear et al. (1995), based on the backoff from output constraints under open-loop operation, and backoff from input constraints under closed-loop operation. The use of safety margins is particularly important to maintain feasibility of operational constraints, but not required under economic considerations where suboptimal operation would be obtained in the presence of uncertainty in any event. Furthermore, in this work, dynamic backoff from active constraints was assumed to be incorporated into the target specifications. However, the restricted input bounds were chosen to investigate the effect of input saturation on solution reliability.

However, the presence of input saturation resulted in derivative discontinuities in the objective function, reducing the reliability of gradient based optimization algorithms. Furthermore, the use of the sequential approach in the presence of input saturation may result in failure as seen in Table 4.4, where the response was simulated for 100 minutes at a sampling time of 1 minute and with an objective function ϕ ($\alpha = 1$ and $\beta = 0$). Non-uniqueness in the solutions was also present when comparing the results under initial conditions (IC) based on a constant setpoint of 1.0 to the results obtained for a constant setpoint of 0.50; despite the same objective function value, differences in the setpoint trajectory were present.

Table 4.4: Sequential approach: Sensitivity under different initial conditions

IC	ϕ	Number of Iterations	Number of Evaluations	Computational Time (CPU seconds)
0.00	1.025797	30	1692	456.5
0.25	1.127200	10	580	159.1
0.50	1.025797	27	1561	466.1
1.00	1.025797	8	467	138.1
1.50	failure	18	998	305.7

However, the results obtained by *simultaneous* optimization under the restricted inputs bounds, demonstrated solution insensitivity to initial conditions (IC) as summarized in Table 4.5, where the response was simulated for 100 minutes at a sampling time of 1 minute and with an objective function ϕ ($\alpha = 1$ and $\beta = 0$).

Table 4.5: Simultaneous approach: Insensitivity under different initial conditions

IC	ϕ	Number of Iterations	Number of Evaluations	Computational Time (CPU seconds)
0.00	1.024462	49	50	16.1
0.25	1.024625	61	102	21.8
0.50	1.024625	54	78	17.4
1.00	1.024625	61	90	21.6
1.50	1.024625	54	78	17.4

While initial conditions (IC) based on a constant setpoint trajectory of 1.50 resulted in failure using the sequential approach, the simultaneous approach determined the optimal solution in 17.4 CPU seconds as shown in Figure 4.4.

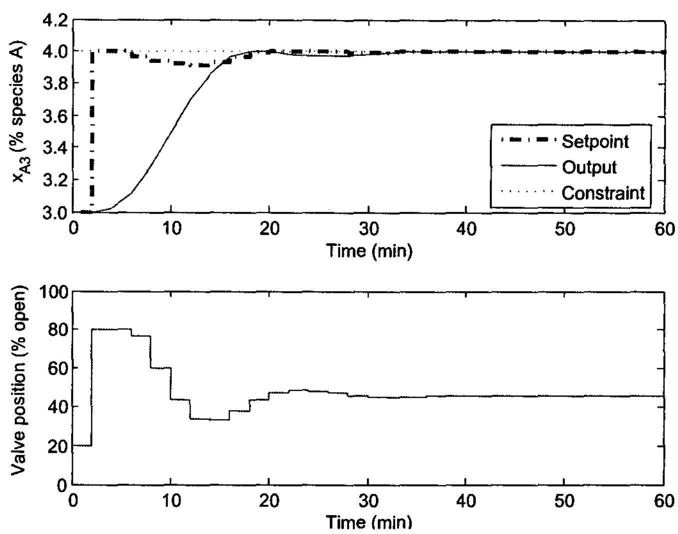
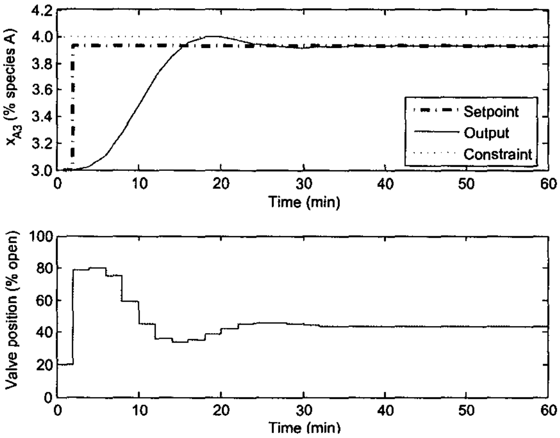


Figure 4.4: Constraints satisfied with IC=1.50 NAC=100 SPH=2 $\alpha = 1$ $\beta = 0$

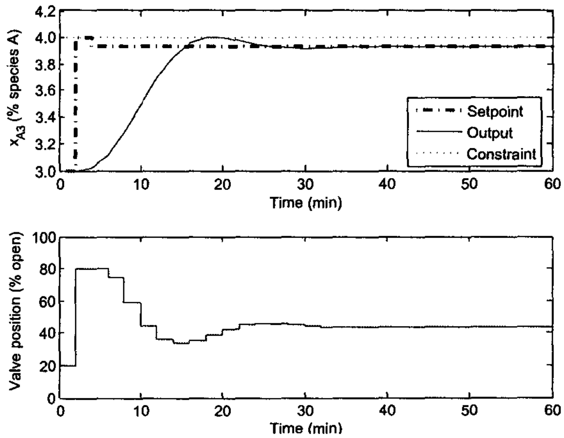
Thus under certain conditions, particularly in the presence of input saturation, the simultaneous approach may be computationally efficient and more reliable compared to the sequential approach.

4.1.3 The Effect of the Number of Allowable Changes

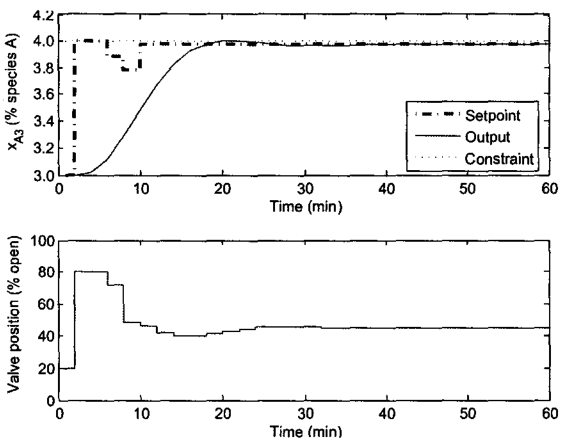
The simultaneous formulation with restricted input bounds was further explored under varying conditions in the number of allowable changes (NAC) in the setpoint trajectory as shown in Figures 4.5(a)-4.5(d). Thus, for a given setpoint hold (SPH) where the setpoint is held constant over a specified number of sampling times, the number of successive setpoint changes was manipulated to determine the effect on the optimal solution obtained.



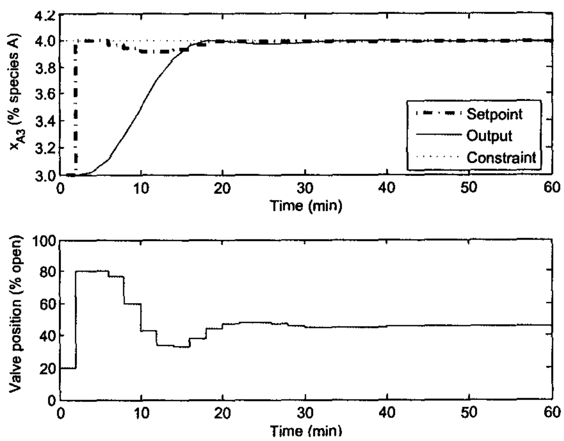
(a) NAC=1



(b) NAC=2



(c) NAC=5



(d) NAC=10

Figure 4.5: Optimal reference trajectory dependent on the number of allowable changes

The results are summarized in Table 4.6, where the response was simulated for 100 minutes at a sampling time of 1 minute to calculate the integral square error (ISE) and integral absolute error (IAE) based on the deviation between the output and target, IC=1.00, SPH=1, and an objective function ϕ ($\alpha = 1$ and $\beta = 0$).

In the absence of end point constraints enforcing the desired steady-state transition, increasing the time available for setpoint manipulation increased the flexibility of the system to improve performance by reducing the dynamic backoff from steady-state active constraints. The dynamic backoff from active constraints was expressed as a percentage of the desired setpoint change and represented the steady-state offset from the setpoint target required to ensure output constraint satisfaction during transient operation. Thus the steady-state offset may be eliminated by ensuring adequate degrees of freedom for setpoint trajectory manipulation.

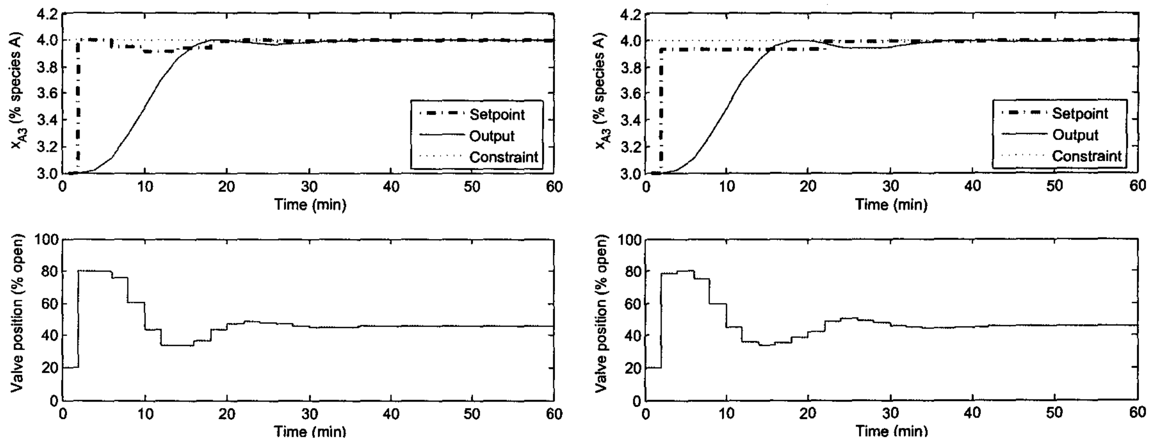
Table 4.6: Simultaneous approach: Dependency on the number of allowable changes

NAC	ϕ	ISE	IAE	t_s (min)	Dynamic Backoff (%)	Computational Time (CPU seconds)
1	1.2204	9.1643	15.9233	40	6.64	14.8
2	1.2141	9.1300	15.8686	40	6.61	37.1
5	1.0956	8.9254	13.0363	38	2.74	20.8
10	1.0251	8.7702	10.8768	35	0.02	25.7
20	1.0246	8.7682	10.8768	35	0.02	20.6
30	1.0246	8.7682	10.8717	35	0.00	20.7

Further increasing the number of allowable changes is not expected to improve performance, but may result in increased computational expense. Significantly decreasing the number of allowable changes may result in suboptimal transitions by reducing the capacity of the dynamic optimizer to avoid output constraint violation while attaining the desired setpoint target. Thus, a sufficiently large time horizon available for setpoint trajectory manipulation must be ensured such that the desired setpoint target may be attained.

4.1.4 The Effect of the Setpoint Hold

The simultaneous formulation with restricted input bounds was also explored under varying conditions in the length of the setpoint hold (SPH), an integer multiple of the control sampling time. Reducing the length of the setpoint hold improved performance and reduced the transition time, since the effective deadtime for a corrective response is reduced as seen in Figures 4.6(a)-4.6(b).



(a) SPH=2 (b) SPH=5

Figure 4.6: Optimal reference trajectory dependent on length of setpoint hold

The results are summarized in Table 4.7, where the response was simulated for 100 minutes at a sampling time of 1 minute to calculate the integral square error (ISE) and integral absolute error (IAE) based on the deviation between the output and target, IC=1.00, NAC=9, and an objective function ϕ ($\alpha = 1$ and $\beta = 0$).

However, while optimality would not impose artificial, arbitrary constraints on the setpoint hold, it may be desirable for operators to implement less aggressive setpoint trajectories. These additional constraints may also enable the optimizer to be invoked less frequently when implemented online with smoother profiles for tracking, and may prevent inciting process dynamics by reducing sensitivity to model mismatch through a less aggressive setpoint trajectory. However, the effect of uncertainty on solution sensitivity under the proposed methodology was not investigated.

Table 4.7: Simultaneous approach: Dependency on the length of setpoint hold

SPH	ϕ	ISE	IAE	t_s (min)	Computational Time (CPU seconds)
2	1.0256	8.7758	10.9036	35	23.7
3	1.0281	8.7654	10.9404	40	20.5
4	1.0338	8.7960	10.9661	40	15.5
5	1.0444	8.8381	11.3386	45	16.4

4.1.5 The Effect of Objective Function Formulation

The simultaneous formulation with restricted input bounds was also explored by penalizing combinations of the deviation between the output and setpoint and target as shown in Table 4.8, where the response was simulated for 100 minutes at a sampling time of 1 minute to calculate the integral square error (ISE) and integral absolute error (IAE) based on the deviation between the output and target, IC=1.00, and with an objective function ϕ.

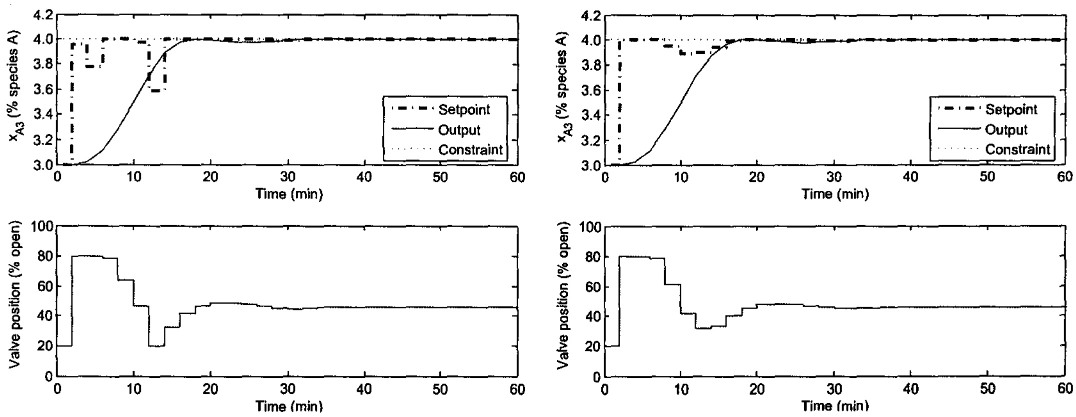
Note that the objective function based on minimizing the squared deviation between the *output* and target resulted in an increase in computational time, possibly resulting from indeterminacy in the setpoint trajectory. The objective function based on minimizing the squared deviation between the *setpoint* and target may improve conditioning of the optimization problem by increasing sensitivity of the objective function to the decision variables, and thus improving the efficiency of gradient based optimization algorithms.

Table 4.8: Simultaneous approach minimizing output deviation

SPH	NAC	α	β	ISE	IAE	t_s (min)	Computational Time (CPU seconds)
1	49	1	0	8.7682	10.8717	35	31.2
1	49	0	1	8.7284	10.7482	35	126.5
1	49	1	1	8.7436	10.7619	35	22.6
5	9	1	0	8.8381	11.3386	45	16.4
5	9	0	1	8.8333	11.5872	50	17.1
5	9	1	1	8.8379	11.3402	45	18.7

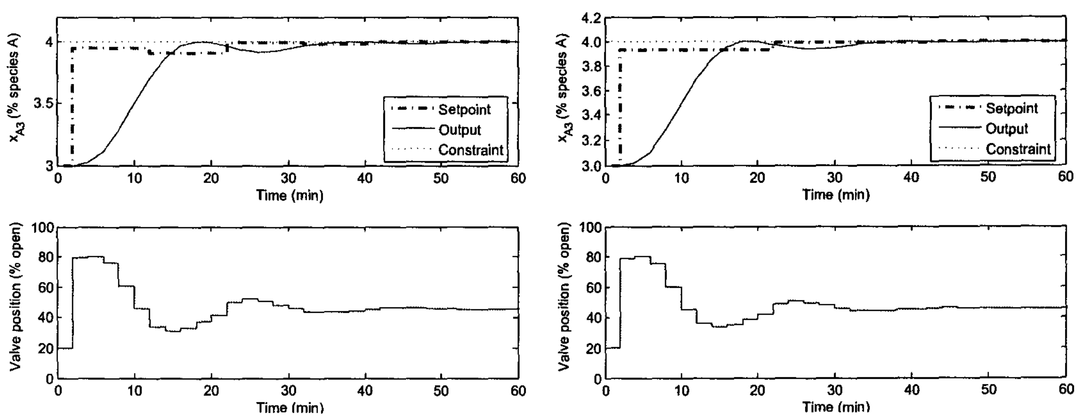
In the first set of simulations seen in Figures 4.7(a)-4.7(b), an objective function based on minimizing the squared deviation between the output and target reduced the integral squared error (ISE), but with a significant increase in computational expense with minimal improvement in performance despite a more aggressive setpoint trajectory. In fact, performance may be reduced as a result of an increase in settling time as seen in the second set of simulations shown in Figures 4.8(a)-4.8(b).

Simulations attempting to penalize the settling time based on a specified output tolerance bound about the desired steady-state increased computational expense without significant reduction in the settling time. In contrast, penalizing the squared deviation between the setpoint and target improved computational performance with minimal effect on the integral squared error, reducing the settling time indirectly. Thus the optimal solution is only optimal with respect to the objective function, hence indicating the importance and difficulty in defining and mathematically translating performance objectives into the optimization framework.



(a) $\alpha = 0\ \beta = 1$ (b) $\alpha = 1\ \beta = 1$

Figure 4.7: Optimal reference trajectory with SPH=1 NAC=49



(a) $\alpha = 0\ \beta = 1$ (b) $\alpha = 1\ \beta = 1$

Figure 4.8: Optimal reference trajectory with SPH=5 NAC=9

4.1.6 Two-Tiered Hierarchical Optimization

Investigation in the mathematical formulation of objective function and constraints indicated the possibility of non-unique solutions, particularly when the objective was based on minimizing the squared deviation between the output and target. According to Gill et al. (2004), indeterminacy may yield identical objective function values with convergence to different optimal solutions based on initial conditions for the solution, while less robust optimization algorithms may fail to yield a solution.

Thus, additional specifications are required for defining a unique solution, and a hierarchical approach, similar to the strategy used by Bathazaar (2005), was proposed to preserve optimal closed-loop performance followed by minimizing the squared deviation between the setpoint and target. The hierarchical formulation enables prioritization by introducing constraints into subsequent optimization problems without affecting solution feasibility (Swartz, 1995).

In this work, the initial conditions (IC) based on a constant setpoint trajectory were not altered, and thus the tolerance specified for constraints introduced into the subsequent optimization problem was relaxed to enable the hierarchical formulation to determine an optimal solution based on reducing setpoint variability with minimal degradation in the closed-loop performance. This is similar to multiple criteria decision making (MCDM) problems described by Alhammadi and Romagnoli (2004), consisting of multiple conflicting objectives and a set of alternative Pareto optimal solutions. One possible solution strategy utilizes scalarizing functions such as the parametric weighting function, where the multiple objectives are combined in a single objective function and weighted appropriately. However, the hierarchical ϵ constraint method enabling objective prioritization was used, where one objective function is optimized while the other objectives are transformed into constraints with defined upper bounds. Thus, the hierarchical multi-objective formulation was used where the squared deviation between the output and target is minimized by

$$\min_{y_{sp}} \phi_1 = \sum_{i=1}^{N} (y_i - y_{tgt})^2 \tag{4.2}$$

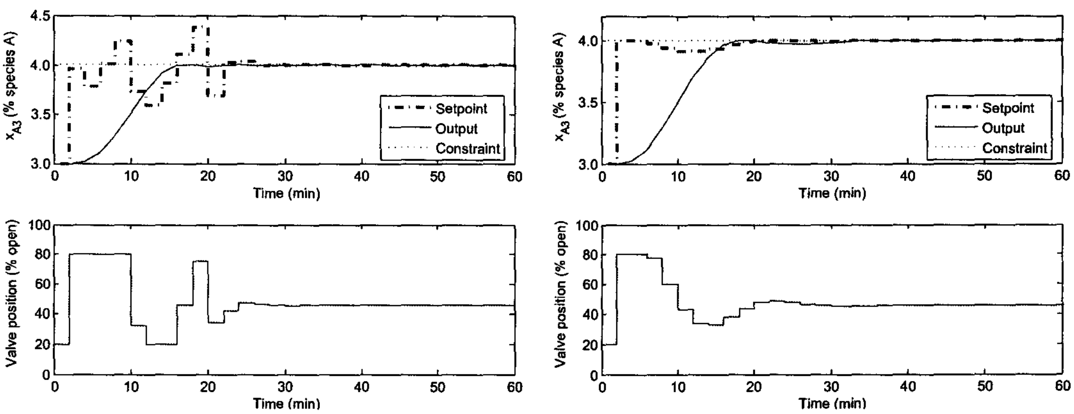
Subject to the closed-loop response. The subsequent optimization requires an additional constraint satisfying the previous objective function value within a given tolerance of $\epsilon \geq 0$, and is given by

$$\min_{y_{sp}} \phi_2 = \sum_{i=1}^{N} \left(y_{sp,i} - y_{tgt}\right)^2 \tag{4.3}$$

$$\phi_1 \leq \phi_1^* + \epsilon \tag{4.4}$$

in addition to constraints on the closed-loop response, and where ϕ_1^* is the optimal solution to Equation 4.2.

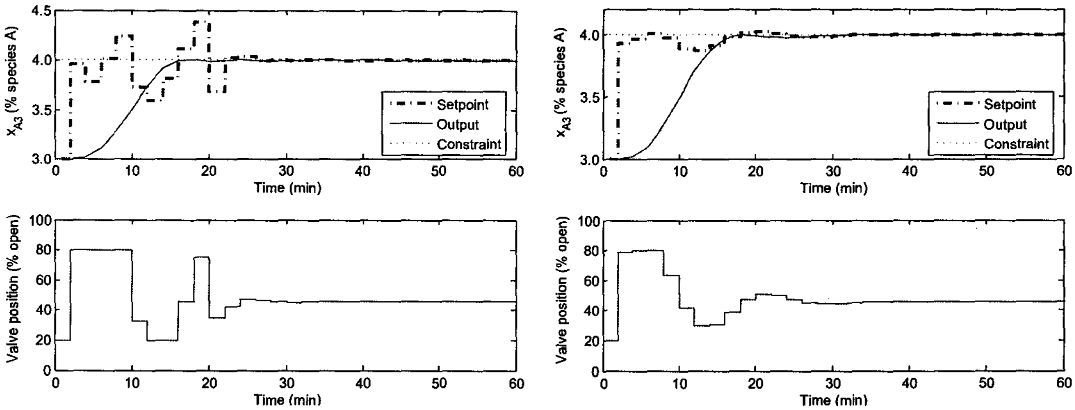
Relaxation of the constraints on allowable setpoints from $y_{sp} \in [0, 4]$ to $[0, 5]$, resulted in a non-unique and aggressive setpoint trajectory based on the first optimization problem given in Equation 4.2. The optimal solution was obtained in 111.5 CPU seconds, and the closed-loop response shown in Figure 4.9(a). Thus a hierarchical multi-objective optimization problem was solved, with the subsequent optimization problem based on Equations 4.3-4.4. The previous objective function value was satisfied within a given tolerance of $\epsilon = 0.01\phi_1^*$, reducing variability in the setpoint trajectory without a significant reduction in the closed-loop performance. The final solution was obtained in an additional 27.5 CPU seconds, and shown in Figure 4.9(b).



(a) First optimization problem (b) Second optimization problem

Figure 4.9: Hierarchical formulation based on setpoint

A modification of the subsequent objective function minimizing the *squared setpoint change* resulted in an optimal solution obtained in 18.8 CPU seconds, and a similar closed-loop response as shown in Figure 4.10(b). However, in comparison to Figure 4.9(b), the settling time was increased and the input does not reach steady-state for an additional 5 minutes. Hence, setpoint change suppression may result in a less desirable closed-loop response, while minimizing the setpoint from target directly reflects the overall objective of attaining target specifications and indirectly reduces the transition time.



(a) First optimization problem (b) Second optimization problem

Figure 4.10: Hierarchical formulation based on setpoint changes

However, while the formulation ensures optimal performance in terms of minimizing the squared deviation between the output and target, additional computational expense is required to solve multiple optimization problems. Thus, an objective function based on minimizing the squared deviation between the setpoint and target is adequate for near optimal performance of the dynamic optimizer for this particular single-input single-output system.

4.1.7 The Discrete Reference Filter

An alternative mathematical formulation for reference management is based on the introduction of additional constraints on the setpoint trajectory. The first order low pass exponential reference filter is similar to the structure discussed within traditional reference management literature and in two degrees of freedom internal model control, and is given by

$$y_{sp}(z) = \frac{1 - f_i}{1 - f_i z^{-1}} y_{tgt}(z) \tag{4.5}$$

where the optimal closed-loop filter time constant f_i is determined to detune the closed-loop response. The tuning parameter is very appealing because it offers simplicity of design and tuning, and easily tuned online, but the arbitrary structure of the first order filter may limit performance. The difference equation in the time domain is given by

$$y_{sp}(k) = (1 - f_i)\, y_{tgt} + f_i y_{sp}(k-1) \tag{4.6}$$

The discrete reference filter in Equation 4.6 was implemented on the linearized system using the simultaneous formulation with restricted input bounds, and the optimal solution obtained in 20.6 CPU seconds. The closed-loop response resulting from implementing the optimal filter time constant of $f_i = 0.6856$ is shown in Figure 4.11.

The use of the reference filter resulted in less aggressive input moves but comparable transition times. However, hard output constraints were relaxed by 0.01% to prevent numerical instability arising from the specification of hard constraints at target. Alternatively, slight offset in the final steady-state may be acceptable to improve numerical conditioning. Thus while the filter may produce smooth reference profiles, the additional constraints on the setpoint structure may reduce the region of numerical stability within the dynamic optimizer.

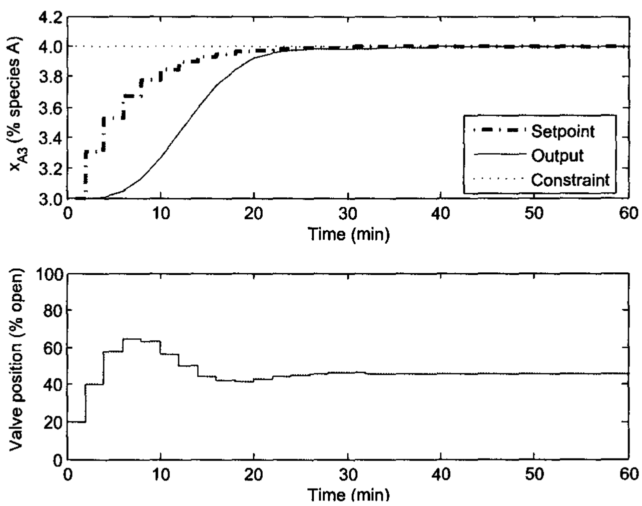


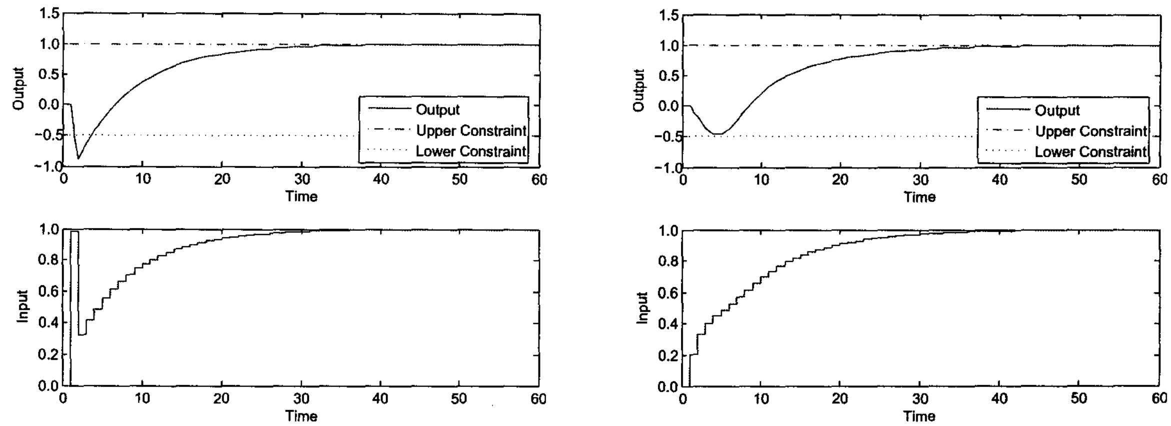
Figure 4.11: Closed-loop response with first order low pass reference filter

4.2 Non-Minimum Phase Systems

The single-input single-output non-minimum phase system,

$$G_p(s) = \frac{-1.20s + 0.1601}{s^2 + 0.40s + 0.16} \tag{4.7}$$

was taken from Bemporad et al. (1997). The system is controlled using input constrained model predictive control without consideration of output constraints. The open-loop simulation resulted in a settling time of 30 minutes, thus a prediction horizon of 30 and an input horizon of 10 were chosen with a sampling time of 1 minute. The model predictive control tuning used an output to input move weighting ratio of 100:1, but the presence of inverse response characteristics resulted in output constraint violation. Detuning to an output to input move weighting ratio of 1:4 ensured the closed-loop response was within the range $[-0.50, 1.0]$ but slightly increased the transition time by an additional 5 minutes as seen in Figures 4.12(a)-4.12(b).



(a) Output to input move weighting of 100:1

(b) Output to input move weighting of 1:4

Figure 4.12: Comparison of tuning for feasibility and performance

While detuning under such circumstances is a possibility, the nominal tuning was retained to demonstrate the application of reference management to systems with non-minimum phase characteristics, where output constraints were enforced and setpoint adjustment made possible every 1 minute. The dynamic optimizer determined an optimal setpoint trajectory based on minimizing the squared deviation between the setpoint and target, such that the closed-loop response did not violate output constraints. The optimal solution using sequential optimization was obtained in 224.8 CPU seconds, and the closed-loop response shown in Figure 4.13. Slight violations of 2% of the setpoint change between sampling times were eliminated by reducing the output sampling time to 0.1 minutes and enforcing hard constraints at additional points in time without significant additional computational expense.

Note that the sequential approach used the 'fmincon' function in MatLab 7.0 to determine the optimal setpoint trajectory at the upper level, and the 'mpc' block in Simulink for closed-loop simulations at the lower level.

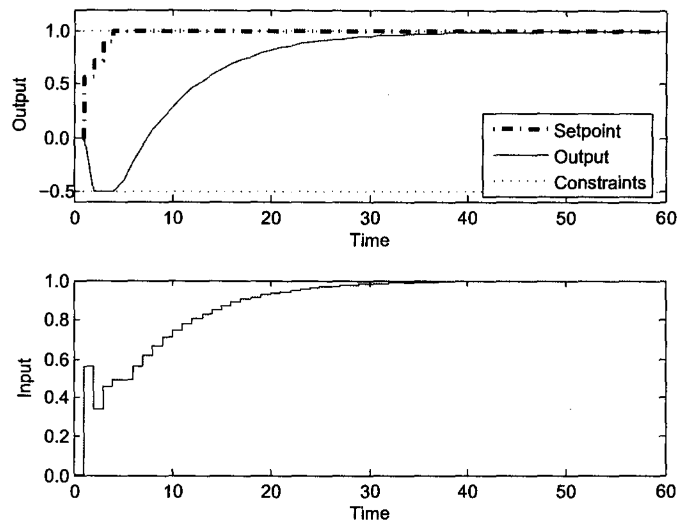


Figure 4.13: Enforcement of output constraints with IC=0 NAC=60 SPH=1

However, in the absence of input saturation, an explicit expression may be derived for unconstrained model predictive control, given by

$$\min_{\Delta u} \phi = (y_{sp} - \hat{y})^T Q (y_{sp} - \hat{y}) + \Delta u^T R \Delta u \tag{4.8}$$

$$\hat{y} = A\Delta u + y_f + \hat{d} \tag{4.9}$$

Consequently, the closed-loop simulation does not require the solution of quadratic programming sub-problems. The solution is given by

$$\Delta u = \left(A^T Q A + R\right)^{-1} A^T Q \left(y_{sp} - y_f - \hat{d}\right) \tag{4.10}$$

The application of the explicit formulation resulted in a comparable settling time, but at a computational cost of 28.4 CPU seconds compared to 224.8 CPU seconds.

Further improvement in computational efficiency was demonstrated using simultaneous optimization, with the optimal solution, identical to Figure 4.13, obtained in 15.9 CPU seconds. However, enforcement of output constraints at a sampling time of 0.10 time steps increased the computational expense significantly, providing an optimal solution in 419.7 CPU seconds. This was implemented by discretizing the process model at a different sampling rate than the sampling interval used by model predictive control, and enforcing output constraints on sub-sampled output predictions.

The application of additional structural constraints on the setpoint trajectory based on the first order exponential reference filter was also investigated using the simultaneous approach. The optimal filter time constant of $f_i = 0.5575$ was determined in 39.3 CPU seconds resulting in a similar optimal setpoint trajectory and comparable transition times. However, the computational expense exceeds that required using the general formulation for reference management, despite a reduction in the dimension of decision variables.

4.3 Multi-Input Multi-Output Systems

The British Petroleum Company determined offline open-loop optimal control profiles in the operation of a distillation column using nonlinear dynamic models, determining the optimal switching time to introduce setpoint changes (Sargent and Sullivan, 1979). The transition time was reduced by minimizing the squared deviation between the output and target, indirectly minimizing profit loss through a reduction in the amount of off-specification product produced. A direct economic objective function was not used because instantaneous product values were difficult to estimate before blending operations and fuel costs dependent on other units not considered. A similar study minimizing transition time as an indirect economic objective function was conducted by Elf Company during distillation column changeovers (Fikar et al., 1999).

Similarly, this section details the application of reference management based on an objective function improving economic operation indirectly during setpoint transitions in the control of distillation columns. The pilot scale ethanol and water distillation column shown in Figure 4.14 was taken from Psarris and Floudas (1991). The linearized system is characterized by poor closed-loop response due to the presence of infinite right half plane zeros close to the origin.

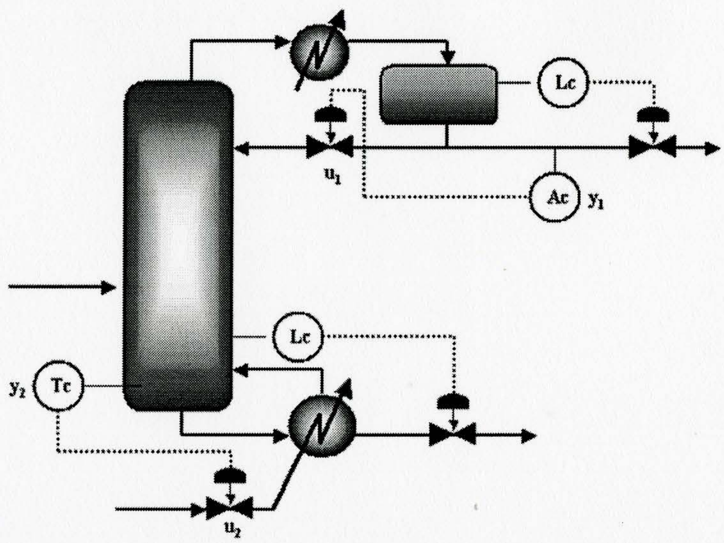


Figure 4.14: Schematic of distillation column

The multi-input multi-output system is represented by the linear transfer function model

$$\begin{bmatrix} y_1(s) \\ y_2(s) \end{bmatrix} = G(s) \begin{bmatrix} u_1(s) \\ u_2(s) \end{bmatrix} = \begin{bmatrix} \frac{0.66e^{-6s}}{6.7s+1} & \frac{-0.005}{9.06s+1} \\ \frac{-34.7e^{-4s}}{8.15s+1} & \frac{0.87(11.6s+1)e^{-2s}}{(3.9s+1)(18.8s+1)} \end{bmatrix} \begin{bmatrix} u_1(s) \\ u_2(s) \end{bmatrix} \quad (4.11)$$

where the outputs y_1 and y_2 represent the overhead ethanol mole fraction and the bottom tray temperature (^{0}C) respectively, controlled by inputs u_1 and u_2 representing the reflux flow rate (gpm) and the reboiler steam pressure (psig). The system was also studied by Ross (1997) and Ross and Swartz (1997) using the input constraints

$$-0.112 \leq u_1 \leq 0.065 \tag{4.12}$$

$$-4.40 \leq u_2 \leq 14.00 \tag{4.13}$$

The output constraints proposed for investigation are given by

$$-0.050 \leq y_1 \leq 0.050 \tag{4.14}$$

$$0.000 \leq y_2 \leq 4.000 \tag{4.15}$$

and are similar to constraints considered by Prett and García (1987), where the top draw composition was bounded by economic constraints and the bottom column temperature by operating constraints. Total reflux operation for startups is common but may cause problems for products sensitive to high temperatures due to thermal degradation as a result of long residence times, and hence temperature constraints are particularly important during transient operation (Kruse et al., 1996). Hard constraints were enforced by Brosilow (1990) using hierarchical ranking based on the severity of maintaining the temperature constraint. Diverting control action to enforce the temperature constraint increased variation in the top draw composition, but such variations may be significantly reduced if temporary violations are tolerable. Thus meaningful formulation of constraints is important, but not investigated further in this case study.

The system was controlled using input constrained model predictive control without consideration of output constraints. The open-loop settling time was approximately 60 minutes, thus a prediction horizon P of 30 and an input horizon M of 10 was used, executed every 2 minutes to attain the desired target specifications of $y_1 = -0.035$ and $y_2 = 3.0$ given by Psarris and Floudas (1991). The relative output to input move weighting ratio of $[1000, 5]$ was used, also accounting for variable scaling. A settling time of 30 minutes was obtained, but overshoot in the temperature was observed in the closed-loop response as shown in Figure 4.15.

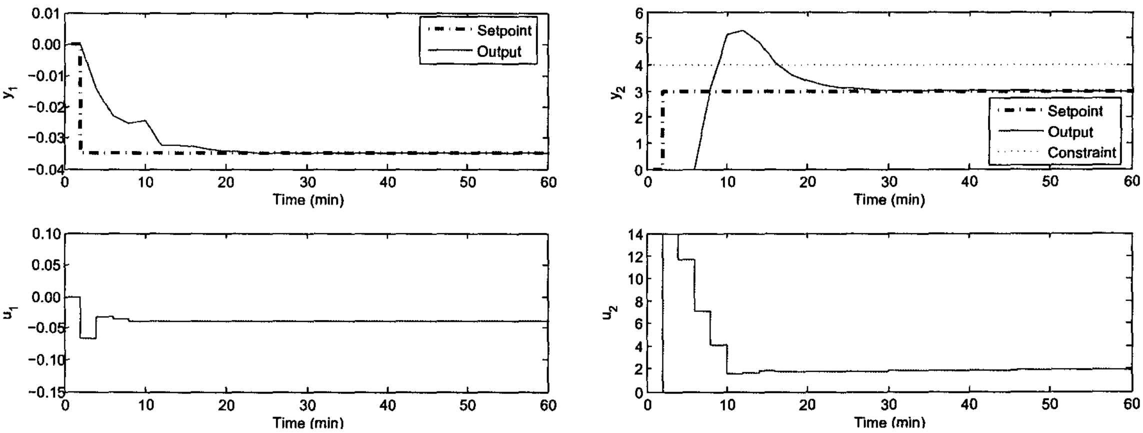


Figure 4.15: Closed-loop response for ethanol-water distillation column

Ying and Joseph (1999) demonstrated reduced overshoot using LP-MPC for the Shell Control Problem, thus similar benefits may be expected for reference management based on closed-loop dynamic models.

4.3.1 Application of Reference Management

Reference management was applied with hard output constraints to limit temperature overshoot. The objective function used a relative weighting of 100:1 for the ethanol mole fraction compared to the bottom tray temperature, noting that variables were not scaled while minimizing the squared deviation between the output and target. Both setpoint trajectories were manipulated, and the optimal solution obtained in 22.1 CPU seconds, with the resulting closed-loop response shown in Figure 4.16. In addition to satisfying the upper temperature constraint, the settling time was also reduced from 25 minutes to 20 minutes.

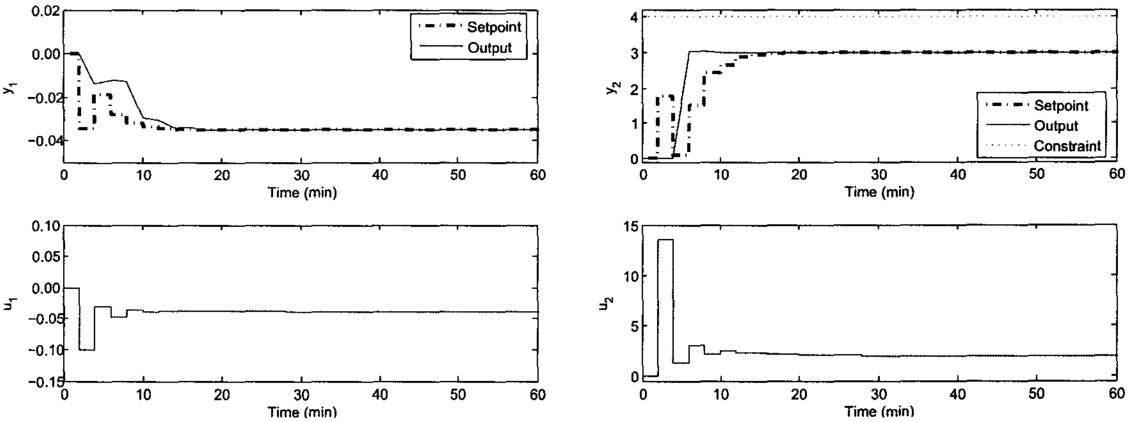


Figure 4.16: Reference trajectory penalizing deviation between output and target

Enforcing a single setpoint change in temperature resulted in a more aggressive closed-loop response as seen in Figure 4.17.

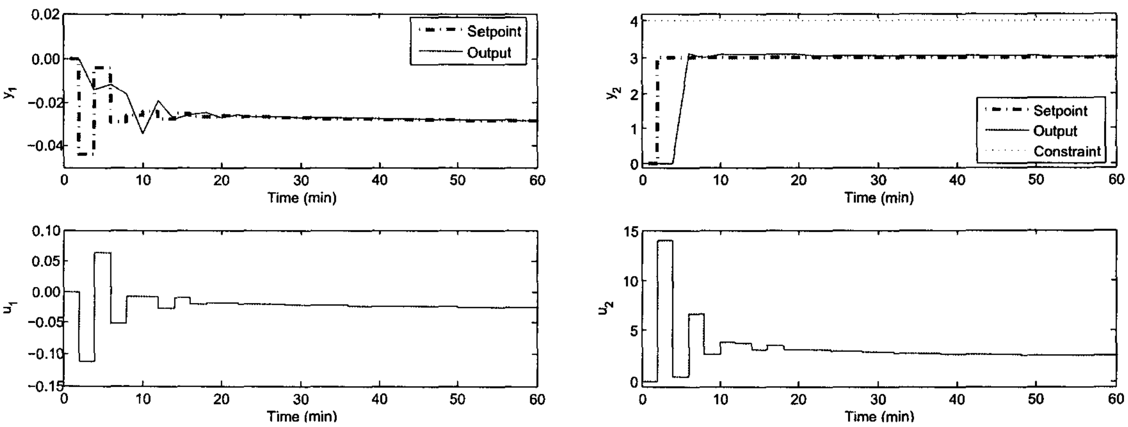


Figure 4.17: Single setpoint change in temperature

However, enforcing a single setpoint change in composition resulted in a highly aggressive oscillatory closed-loop response as seen in Figure 4.18, with an increase in settling time to 80 minutes.

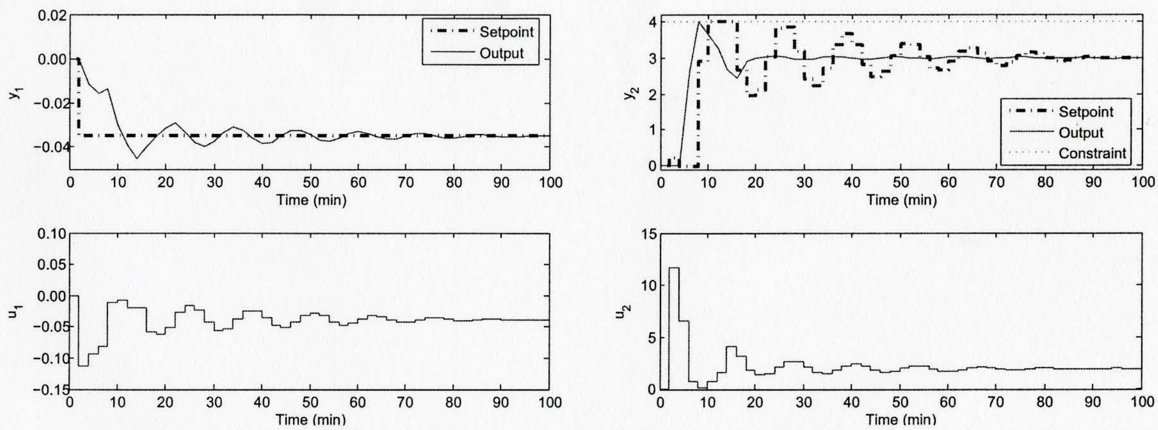


Figure 4.18: Single setpoint change in composition

Thus improved closed-loop performance may be achieved by utilizing all available degrees of freedom and manipulating the setpoint trajectory of all controlled variables.

4.3.2 Formulation with Alternative Objective Functions

The formulation of the objective function was also investigated for multi-input multi-output systems. The objective function was modified to minimize the squared deviation between the setpoint and target while manipulating both setpoint trajectories. The solution was obtained using simultaneous optimization in 52.8 CPU seconds, and the closed-loop response shown in Figure 4.19 with a settling time of 25 minutes.

Comparing Figure 4.16 with Figure 4.19, the closed-loop performance may be significantly improved when minimizing the squared deviation between the output and target compared to minimization of the squared deviation between the setpoint and target for this multi-input multi-output system.

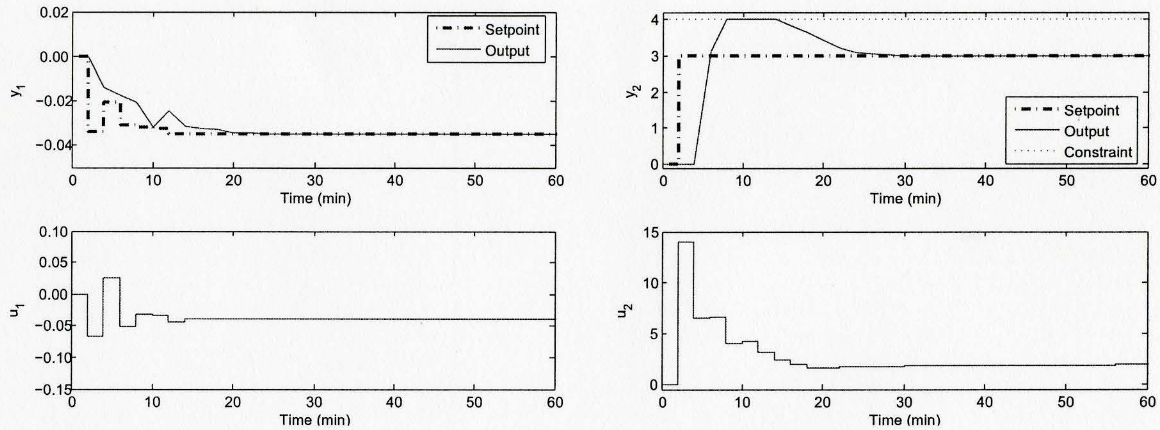


Figure 4.19: Reference trajectory penalizing deviation between setpoint and target

4.3.3 Alternative Design and Control

Finally, reference management is a form of advanced control that is capable of improving closed-loop performance by manipulating the setpoint trajectory. However, additional benefits to improve dynamic operability may exist at the design stage. Psarris and Floudas (1991) used a delay compensation scheme to determine the minimal increase in delay in off-diagonal elements required to reduce interaction and improve performance for disturbance rejection and setpoint changes. A similar analysis on the achievable closed-loop performance based on delay compensation resulted in a system of the following form as discussed by Ross (1997):

$$\begin{bmatrix} y_1(s) \\ y_2(s) \end{bmatrix} = \begin{bmatrix} \frac{0.66e^{-6s}}{6.7s+1} & \frac{-0.005e^{-6s}}{9.06s+1} \\ \frac{-34.7e^{-6s}}{8.15s+1} & \frac{0.87(11.6s+1)e^{-2s}}{(3.9s+1)(18.8s+1)} \end{bmatrix} \begin{bmatrix} u_1(s) \\ u_2(s) \end{bmatrix} \tag{4.16}$$

The closed-loop response for the optimal delay distribution is shown in Figures 4.20(a)-4.20(b). Thus, while advanced process control may improve closed-loop performance, design considerations may yield further benefits resulting in simple solutions without the implementation of more complex control schemes.

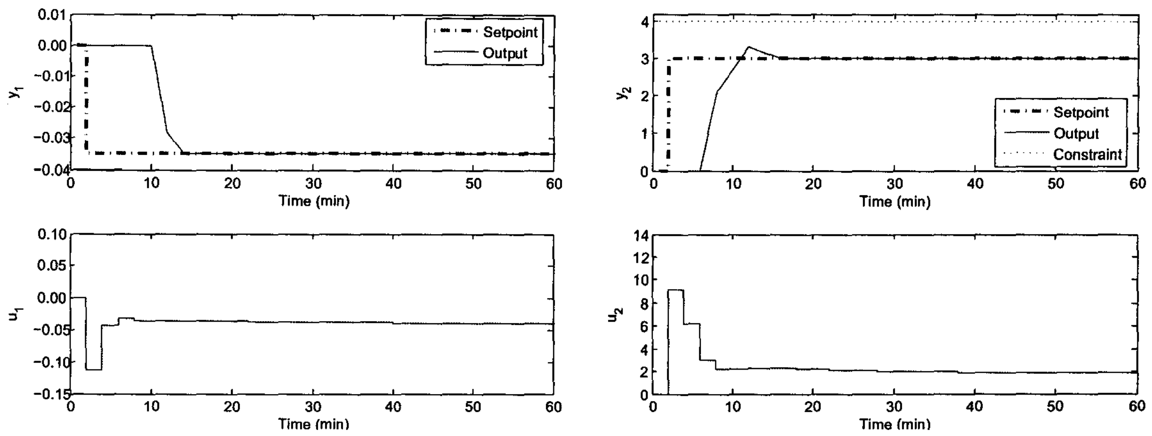


Figure 4.20: Closed-loop response for optimal design of delay structure

Similarly, classical feedback control in a series of continuously stirred tank reactors may result in overshoot, but may be avoided using a single reactor (Subramanian et al., 2001). Ross et al. (2001) described a high purity industrial distillation column with 15 years of operational problems, and demonstrated through integrated control and design with optimal equipment sizing and control tuning, savings of 6% corresponding to $300,000 per year. Thus the incorporation of dynamic considerations for design and control is particularly important for realizing optimal economic operation, and may result in reduced operational difficulty and substantial savings.

4.4 Summary of Results

This chapter detailed the application of the proposed methodology to linear dynamic systems. The objective function used in these simulations was based on maximizing economic operation indirectly, by minimizing the production of off-specification product with suitable hard output constraints based on economic or operational considerations. Furthermore, the enforcement of hard output constraints at target during steady-state transitions ensures feasibility assuming the disturbances during transient operation are similar to the disturbances encountered during steady-state operation.

A single-input single-output system was used to demonstrate the potential benefits of the simultaneous relative to the sequential approach in terms of computational efficiency and solution reliability, particularly in the presence of derivative discontinuities. The effect of various constraint formulations on the optimal solution was determined, including adjusting the number of allowable setpoint changes, and the length of the setpoint hold in the parameterized piecewise constant setpoint trajectory. Alternative objective function formulations penalizing the output or setpoint from target were also investigated. The possibility of indeterminacy was demonstrated and handled using a two-tiered approach based on maximizing closed-loop performance. Additional structural constraints on the setpoint trajectory were enforced resulting in the implementation of the discrete reference filter, similar in structure to the development of reference management discussed in literature. Applications to non-minimum phase and multi-input multi-output systems were also demonstrated.

Chapter 5

Application to Nonlinear Systems

This chapter details the application of reference management to multi-input multi-output nonlinear systems using the simultaneous formulation presented in Chapter 3. A discussion on optimal grade transitions for polymerization systems in literature is detailed in Section 5.1. A fundamental model for styrene polymerization is then detailed in Section 5.2, reference management applied based on a linear model in Section 5.3, using the discrete reference filter in Section 5.4, and based on a nonlinear model in Section 5.5.

Finally, the explicit consideration of economics during transient operation is presented in Section 5.6, and shown to result in further economic benefits by minimizing the cost of raw materials and the production of off-specification product. The formulation of the dynamic economic objective function is detailed and conditioned to consider control performance. Additional improvement in economic operation is also demonstrated with the manipulation of the production rate.

5.1 Optimal Grade Transitions in Literature

According to Xie et al. (1994), polyethylene is the largest synthetic polymer in production and is produced exclusively in continuous processes. As many as 50 different grades must be produced in the same reactor in response to market demand, thus requiring regular grade changeover operations. A kinetic model was developed by McAuley et al. (1990), predicting the production rate, melt index and polymer density. Model reduction enabled the prediction of instantaneous properties online based on temperature and gas composition measurements (McAuley and MacGregor, 1991).

Optimal grade transitions were investigated by McAuley and MacGregor (1992), minimizing an objective function based on the squared deviation of cumulative output properties from target and the squared deviation of inputs from target,

$$\Phi = \int_{t_0}^{t_f} \left[\sum_i w_i \left(y_i\left(t\right) - y_{tgt}\right)^2 + \sum_j w_j \left(u_j\left(t\right) - u_{tgt}\right)^2 \right] dt \tag{5.1}$$

The minimization of the squared deviation of instantaneous output properties from target was also included to minimize overshoot. Excessive overshoot may result in a degradation in quality since old polymer contained in the reactor is mixed with the new polymer leading to the undesirable broadening of the cumulative molecular weight distribution in the end product. Narrow molecular weight distributions are particularly important in polyethylene film and injection molded applications, and thus the instantaneous rather than cumulative properties were chosen for control to improve the consistency of the product and to reduce variability in the end-use polymer properties (McAuley, 1991).

5.1.1 Feedback Control Required

The dynamic optimization problem corresponding to the objective function given in Equation 5.1 was solved using sequential optimization, to determine the optimal input trajectory. McAuley and MacGregor (1992) used soft constraints to minimize overshoot but indicated consideration of hard output constraints may be desirable but may be more effectively handled through simultaneous optimization. The optimal input trajectory was implemented but significant deviation from the predicted response was demonstrated in the presence of disturbances and model mismatch, thus requiring feedback control.

Thus, McAuley and MacGregor (1993) developed a nonlinear controller based on controlling the instantaneous properties, tracking the offline optimal setpoint trajectory while the offline optimal trajectory for additional inputs was tracked open-loop. Similarly, BenAmor et al. (2004) proposed nonlinear model predictive control for tracking the offline optimal setpoint trajectory in the presence of disturbances, assumed to be determined by dynamic optimization.

Similar concepts of tracking the offline optimal trajectory for grade transitions may be found in literature with different variations. For example, Seki et al. (2001) developed nonlinear model predictive control for grade transitions in high density polyethylene polymerization where the optimal setpoint and input trajectories were determined at the upper level using a nonlinear model and unconstrained inputs, and feedback control implemented at the lower level with input constraints. A similar strategy was used by Wang et al. (2000), but the optimal input trajectory signals were used as feedforward elements in conjunction with feedback corrections from regulatory control in the presence of disturbances.

In the presence of uncertainty, the implementation of the optimal input trajectory without feedback may result in significant production of off-specification product; this is particularly important, but often neglected in literature. Lee et al. (1997) proposed a two level hierarchical controller for vinyl-acetate polymerization during grade transitions. The upper level determined the optimal steady-state inputs corresponding to the desired steady-state and an upper bound on the transition time, while the lower level determined the optimal input trajectory using genetic algorithms forced to approach the steady-state input. Lee et al. (1999) improved the calculation of the optimal inputs by using local search algorithms based on differencing to reduce computational expense. A similar strategy was demonstrated for grade transitions in polyethylene polymerization by Yi et al. (2003). However, feedback control was not incorporated to ensure the optimal input trajectory would be capable of attaining the desired target specifications in the presence of uncertainty. Takeda and Ray (1999) also determined the offline optimal input trajectory for grade transitions in olefin polymerization, but recognized the need for an online strategy due to the presence of disturbances.

5.1.2 Solution Strategies

The use of sequential optimization for dynamic optimization is prevalent in determining optimal grade transitions for polymerization processes in literature. However, the use of simultaneous optimization based on orthogonal collocation on finite elements was investigated for low density polyethylene polymerization by Cervantes et al. (2000). The optimal input trajectory was determined using interior point methods, based on minimizing the the squared deviation between the output and target, and was capable of reducing the transition time by 30%. However, significant computation time was required to calculate derivative information based on finite difference perturbations within their implementation of the primal-dual interior point method (Cervantes et al., 2002).

5.1.3 Consideration of Economic Operation

The objective function used for dynamic optimization in literature is typically based on minimizing the squared deviation between the output and target to minimize the transition time, thus improving economic operation indirectly by minimizing the production of off-specification product (McAuley and MacGregor, 1992; Chatzidoukas et al., 2003).

However, the explicit use of an economic function has also been investigated in literature. Schot et al. (1999) proposed the use of an economic objective function to determine the optimal input trajectory using sequential optimization for optimal grade transitions in high density polyethylene polymerization. Similarly, Tousain and Bosgra (2000) proposed an economic cost function based on minimizing raw material costs and maximizing production, with different pricing given to different operating regimes at fixed points in time, and further extended to include product quality specification bands by Tousain (2002). However, the objective function used for optimization combined economic and control objectives using arbitrary weightings.

Brempt et al. (2001) proposed dynamic optimization of a high density polyethylene reactor based on an economic cost function to determine the optimal setpoint trajectory without consideration of the underlying regulatory controller. The optimal trajectory was tracked by a model based controller, successively linearized depending on current operation, to compensate for deviations from the setpoint trajectory. The dynamic optimization was based on the sequential approach, and Backx (2002) demonstrated improvements of up to €117,330 and subsequent applications investigated for a polystyrene plant in Belgium by Brempt et al. (2003). Bosgra et al. (2004) also investigated optimal economic operation during grade transitions in the production of high density polyethylene using mixed integer linear programming (MILP), where the offline optimal reference trajectory was tracked by model predictive control.

5.1.4 Proposed Methodology

Thus the dominant methodology in optimal grade transitions for continuous polymerization processes discussed in literature is based on developing an offline optimal trajectory using nonlinear dynamic models, subsequently tracked using feedback control. The methodology for dynamic optimization prevalent for polymerization grade transitions is based on sequential optimization, minimizing a quadratic cost objective based on the squared deviation of controlled variables from target.

The research undertaken and detailed in this chapter investigates the use of simultaneous optimization based on minimizing a quadratic cost objective with hard output constraints to minimize product variability caused by overshoot. The solution is obtained using reference management based on closed-loop linear and nonlinear dynamic models. In particular, the closed-loop dynamics of quadratic dynamic matrix control (QDMC) is considered, and subsequently used for tracking the offline optimal setpoint trajectory. Finally, the explicit consideration of economics is also investigated and an alternative formulation of combining economic and control objectives is discussed and implemented.

5.2 Process Description

The free radical polymerization of styrene in a jacketed continuously stirred tank reactor considered and shown in Figure 5.1 is taken from Maner et al. (1996), and based on work done originally by Hidalgo and Brosilow (1990). The objective used by Maner et al. (1996) is based on controlling the number average molecular weight $NAMW$ and the reactor temperature T by manipulating the initiator flow rate Q_i and the coolant flow rate Q_c at the lower stable steady-state. The rate of polymerization is constrained by a large reactor inventory, resulting in slow product changeovers and increased production of off-specification product (Meister and Cummings, 2003).

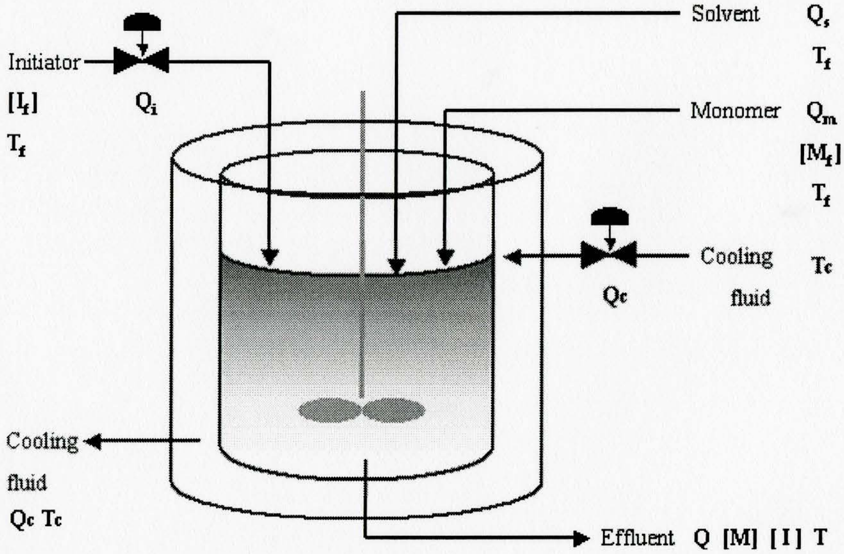


Figure 5.1: Styrene polymerization in continuously stirred tank reactor

The system of equations describing the nonlinear process is given below. The change in the initiator concentration $[I]$ and monomer concentration $[M]$ are determined from

$$\frac{d[I]}{dt} = \frac{Q_i [I_f] - Q[I]}{V} - k_d [I] \tag{5.2}$$

$$\frac{d[M]}{dt} = \frac{Q_m [M_f] - Q[M]}{V} - k_p [M][P] \tag{5.3}$$

where $[I_f]$ and $[M_f]$ represent the initiator and monomer feed concentration, $[P]$ the concentration of growing polymer, and V the reactor volume. The total reactor flow rate Q is determined according to

$$Q = Q_i + Q_m + Q_s = Q_i + Q_m + (1.5Q_m - Q_i) = 2.5Q_m \tag{5.4}$$

where Q_m represents the monomer flow rate and Q_s the solvent flow rate. The simplification used by Maner et al. (1996) in Equation 5.4 adjusts the solvent flow rate to avoid nonlinearity caused by the gel effect (Hidalgo and Brosilow, 1990).

The kinetic parameters k_i follow Arrhenius' Equation with frequency factor A_i and activation energy E_i for $i = d, p, t$ given by

$$k_i = A_i \exp\left[-E_i/T\right] \tag{5.5}$$

where k_d represents the overall chain dissociation rate constant, k_p the overall chain propagation rate constant, and k_t the overall chain termination rate constant.

The reactor temperature T and the coolant temperature T_c are determined from

$$\frac{dT}{dt} = \frac{Q\left(T_f - T\right)}{V} + \frac{\left(-\Delta H_r k_p \left[M\right]\left[P\right]\right)}{\rho C_p} - \frac{hA}{\rho C_p V}\left(T - T_c\right) \tag{5.6}$$

$$\frac{dT_c}{dt} = \frac{Q_c\left(T_{cf} - T_c\right)}{V_c} + \frac{hA}{\rho C_{pc} V_c}\left(T - T_c\right) \tag{5.7}$$

where T_f and T_{cf} represent the reactor and coolant feed temperatures, ρ and ρ_c the mean density of the reactor and coolant fluids, C_p and C_{pc} the heat capacity of the reactor and coolant fluids, V_c the volume of the cooling jacket, ΔH_r the heat of reaction, A the heat transfer area, and h the overall heat transfer coefficient. The number average molecular weight may be determined from

$$NAMW = \frac{D_1}{D_0} \tag{5.8}$$

$$\frac{dD_0}{dt} = 0.50 k_t \left[P\right]^2 - \frac{QD_0}{V} \tag{5.9}$$

$$\frac{dD_1}{dt} = M_m k_p [M][P] - \frac{QD_1}{V} \tag{5.10}$$

$$[P] = \left(\frac{2fk_d[I]}{k_t}\right)^{0.50} \tag{5.11}$$

where D_0 and D_1 represent the zeroth and first moment of chain length distribution for dead and living polymers respectively, M_m is the molecular weight of the monomer, and f the initiator efficiency.

The initial conditions of operation are summarized in Table 5.1, and the reactor parameters given in Table 5.2, taken from Maner et al. (1996) and Hidalgo and Brosilow (1990). The development of the process model and assumptions are detailed in Hidalgo and Brosilow (1990).

Table 5.1: Styrene reactor initial conditions: Grade A

Variable	Initial Value	Units
$[I]$	6.6832x10^{-2}	mol/L
$[M]$	3.3245	mol/L
T_c	305.17	K
D_0	2.7547x10^{-4}	mol/L
D_1	16.110	g/L
Q_i	0.03	L/s
Q_c	0.131	L/s
$NAMW$	58.481	kg/mol
T	323.5558	K

Table 5.2: Styrene reactor parameters

Parameter	Value	Units
A_d	5.95x10^{13}	s^{-1}
A_p	1.06x10^{7}	L/mol s
A_t	1.25x10^{9}	L/mol s
E_d	14897	K
E_p	3557	K
E_t	843	K
f	0.60	
hA	70	cal/K s
M_m	104.14	g/mol
Q_s	0.1275	L/s
Q_m	0.105	L/s
V	3000	L
V_c	3312.4	L
T_f	330	K
T_{cf}	295	K
$-\Delta H_r$	16700	cal/mol
ρC_p	360	cal/K L
ρC_{pc}	966.3	cal/K L
$[I_f]$	0.5888	mol/L
$[M_f]$	8.6981	mol/L

According to Kozub and MacGregor (1992), feedback causing overshoot and oscillations may not be desirable since the cumulative properties are not corrected by the production of off-specification product in the opposite direction. Thus, the instantaneous properties may be used for uniform quality control in free radical polymerization where the growth of co-polymer chains is short relative to the time constant of the reactor. In contrast, the polymer continues to grow throughout the reactor in condensation reactions, and using instantaneous properties to control cumulative properties is no longer valid. Thus, the production of polymer of constant number average molecular weight at each instant in time results in a narrow molecular weight distribution (Tsoukas et al., 1982). McAuley and MacGregor (1993) similarly used instantaneous rather than the cumulative properties for nonlinear control since the current operation can only affect newly produced polymer. Similarly, in this work, the instantaneous properties developed are used for control.

The system of equations was simulated in MatLab 7.0, linearized at the initial steady-state averaging positive and negative 25% input step tests as a percentage of the original steady-state values, and approximated by first order plus deadtime transfer function models. The scaled linear transfer functions, with time units in the order of hours, are given by

$$G_{11}(s) = \frac{NAMW(s)}{Q_i(s)} = \frac{-0.4191e^{-1.89}}{6.1024s+1} \tag{5.12}$$

$$G_{12}(s) = \frac{NAMW(s)}{Q_c(s)} = \frac{0.03705e^{-4.58}}{10.292s+1} \tag{5.13}$$

$$G_{21}(s) = \frac{T(s)}{Q_i(s)} = \frac{0.0353e^{-0.91}}{6.8485s+1} \tag{5.14}$$

$$G_{22}(s) = \frac{T(s)}{Q_c(s)} = \frac{-0.01431e^{-2.06}}{9.0275s+1} \tag{5.15}$$

Furthermore, the following constraints were imposed:

$$u_1 \in [0,150], \quad u_2 \in [0,500] \tag{5.16}$$

$$y_1 \in [50,80], \quad y_2 \in [323,324] \tag{5.17}$$

The hard input constraints given in Equation 5.16 were assumed, with upper and lower bounds based on valve limitations. The hard output constraints given in Equation 5.17 were assumed, based on economically desirable specifications similarly discussed by McAuley (1991). Furthermore, according to Ohshima and Tanigaki (2000), time optimal operation with drastic changes in instantaneous properties may reduce the transition time but may also increase the production of off-specification material when the total product quality is taken into consideration, emphasizing the importance in maintaining the instantaneous properties within a certain range. Thus, hard output constraints were defined to maintain the instantaneous properties within the range spanned by the initial and final steady-states.

5.2.1 The Importance of Temperature Control

Safety constraints to prevent reaction runaway is also important, and temperature control for a semi-batch polymerization reactor within 1^0C was proposed by Clarke-Pringle and MacGregor (1997). Temperature limits are also based on an upper limit for thermal degradation and a lower limit based on the transition temperature. High temperature sensitivity for polymers is also known, where even the effects of short term exposure to high temperatures may be substantial (McKenna and Malone, 1990). The temperature must also remain above the lower limit to ensure adequate catalyst activity and above the dew point of reactants to prevent condensation, and below the upper limit of the melting point of the polymer to prevent particle agglomeration (McAuley and MacGregor, 1992). Tight temperature control is particularly important for commercial gas phase ethylene polymerization, which otherwise results in low catalyst productivity and off-specification product (Dadebo et al., 1997), and is required to prevent instability, limit cycles and excursion toward high temperature steady-states (McAuley et al., 1995).

According to Crowley and Choi (1996), temperature control is also important for product quality in methyl methacrylate polymerization where conventional controllers are detuned to prevent overshoot during rapid temperature transitions, but resulting in longer batch times. The activation of a temperature overshoot controller when operating close to the temperature setpoint was proposed to reduce conservatism in detuning. Campbell (1985) proposed gradually stepping up the setpoint to prevent temperature overshoot while maintaining a reasonable closed-loop response, and once stabilized, controlling the temperature within 0.50^{0}C. The narrow control band is desirable since consistent temperature results in high product quality with narrow molecular weight distributions and high transparency (Niessner and Gausepohl, 2003). Thus, while operational constraints exist, tight temperature control may be directly related to economics through demands for reduced variability in product quality specifications.

5.2.2 Development of Regulatory Control

The open-loop settling time for the system was approximately 40 hours. According to Maner et al. (1996), the order of the response time was comparable to studies by Congalidis et al. (1989), and results due to operation at the lower steady-state with lower conversion and a large reactor volume. Thus linear model predictive control was designed with a prediction horizon P of 20 and an input horizon M of 5, and relative output to input move suppression weighting of $[10, 100]$, executed every 2 hours to attain the desired target specifications for the number average molecular weight of 80 kg/mol and reactor temperature of 323.6 K given by Maner et al. (1996). The controller was input constrained but did not consider output constraints.

Maner et al. (1996) used a sampling time of 0.03 hours for linear model predictive control and 1 hour for nonlinear model predictive control based on a truncated model. The step response model is typically approximated by truncating the step response at the time step with negligible change in the outputs. The sampling time used for this case study was chosen assuming lower level regulatory control such as proportional integral (PI) control is used for high frequency disturbance rejection, but not modelled.

An overall settling time of 35 hours was obtained when the desired setpoint change was implemented on the linearized system, but undershoot in the temperature response was observed as shown in Figure 5.2.

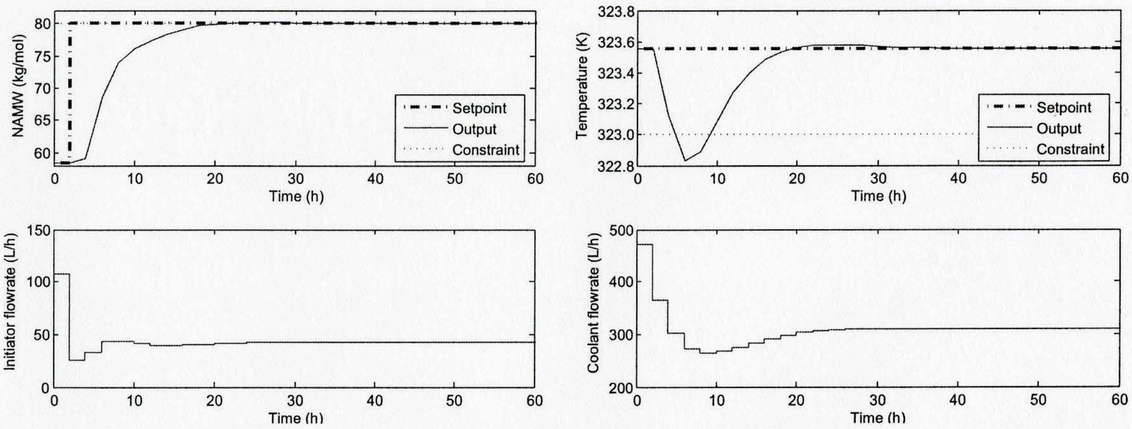


Figure 5.2: Closed-loop response of linear system to constant setpoint change

The effect of undershoot in the reactor temperature and overshoot in the number average molecular weight are more pronounced when linear model predictive control was applied to the actual nonlinear system, as seen in Figure 5.3.

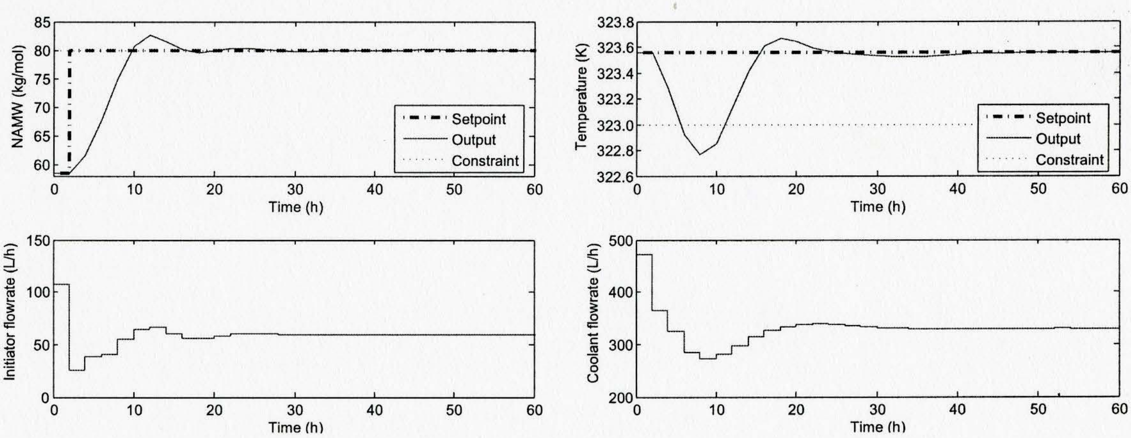


Figure 5.3: Closed-loop response of nonlinear system to constant setpoint change

Linear model predictive control is used in industry to control nonlinear systems but may result in poor performance (Lu and Arkun, 2002). Hence, applications of nonlinear model predictive control based on process gain scheduling have been developed for small multivariable polymerization systems in industry , and solutions offered through commercial products such as Process Perfector from Pavilion Technologies (Henson, 1998).

Similarly, Sriniwas et al. (1995) demonstrated improved performance with nonlinear control when applied to an α-olefin polymerization reactor due to nonlinearity arising from slow purging rates. According to Doyle et al. (1995), nonlinear control may be used for more accurate approximation of nonlinearity to improve control performance for highly nonlinear systems. Second order volterra models integrated into model predictive control based on input-output data was implemented with reduced overshoot in the number average molecular weight when applied to the styrene case study by Maner et al. (1996). However, several parameters were required to model nonlinearity, and model validity must be monitored due to changes in curvature inherent in second order models. In contrast, the stability of linear model based control is maintained over a broad regime and may be less computationally expensive.

5.3 Reference Management with Linear Models

The offline approach for reference management was implemented to enforce output constraints by manipulating both setpoint trajectories determined through minimization of the squared deviation of the output from target, weighting deviations in the reactor temperature 100:1 relative to deviations in the number average molecular weight.

The solution was obtained by simultaneous optimization in 35.0 CPU seconds, where setpoint changes were enabled at the control sampling time. Furthermore, setpoint changes near the end of the simulation horizon were held constant, similar to the technique used by Sargent and Sullivan (1979), since the process delay would result in indeterminacy. The closed-loop response of the discrete linear system assuming a perfect model is shown in Figure 5.4.

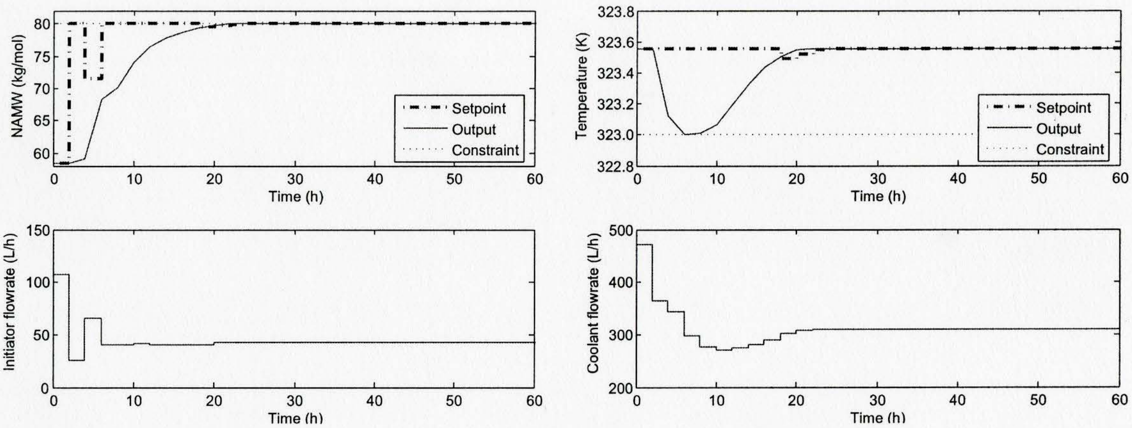


Figure 5.4: Optimal reference trajectory for perfect linear model

The temperature setpoint was available for manipulation, but was not adjusted extensively indicating that effective prevention of constraint violation requires detuning the setpoint change in the number average molecular weight.

To further minimize variability in the setpoint trajectory, the two-tiered hierarchical approach was used as discussed in Section 4.1.6. The subsequent objective function was based on minimizing the squared deviation between the setpoint and target, and subject to an additional constraint satisfying the the previous optimal objective function value of 1773.48 within a numerical tolerance of 1%. The optimal solution was obtained in 56.8 CPU seconds, and the closed-loop response shown in Figure 5.5.

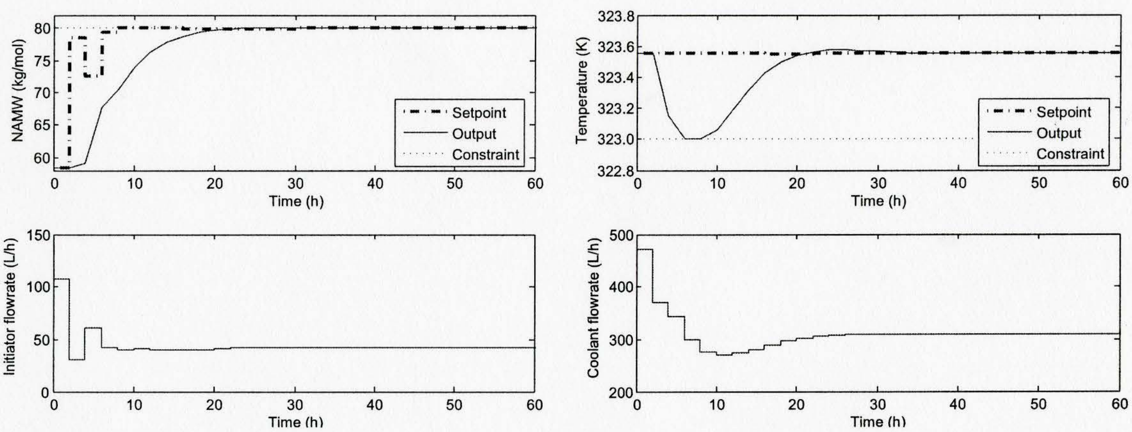


Figure 5.5: Optimal reference trajectory with reduced setpoint variability

The application of reference management based on minimizing the squared deviation between the setpoint and target was also investigated. The optimal solution obtained resulted in a similar closed-loop response without the two-tiered approach, thus reducing computational expense.

5.4 Reference Management with Reference Filters

The discrete reference filter was implemented for setpoint changes in the number average molecular weight, minimizing the squared deviation between the output and target while holding the temperature setpoint constant. The closed-loop response seen in Figure 5.6 was obtained in 319.8 CPU seconds with an optimal filter time constant of $f_{i1} = 0.5153$ and a feasible setpoint target of $y_{tgt} = 79.89$. Implementation of the reference filter resulted in a smooth setpoint trajectory requiring less aggressive input movement.

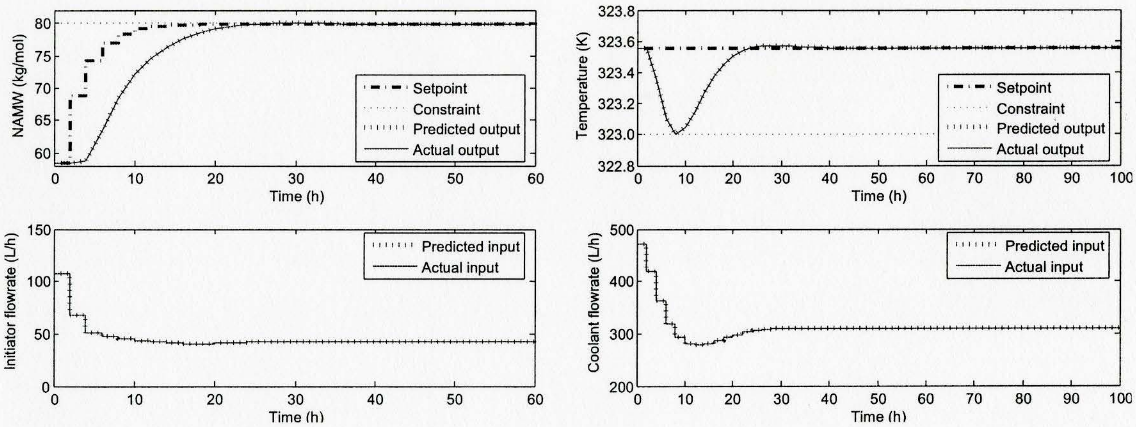


Figure 5.6: Discrete reference filters holding temperature setpoint constant

Allowing adjustments in the temperature setpoint, the actual target may be achieved with a slightly more aggressive filter time constant of $f_{i1} = 0.5200$. The optimal solution was obtained in 212.5 CPU seconds, and the resulting closed-loop response shown in Figure 5.7.

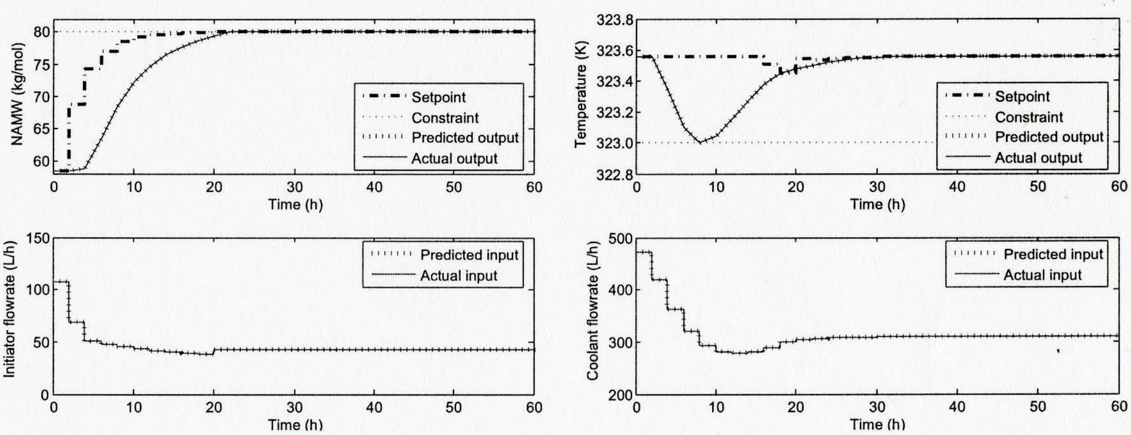


Figure 5.7: Discrete reference filters with adjustment in temperature setpoint

Implementation of the optimal solution shown in Figure 5.6, on the actual nonlinear system resulted in the closed-loop response seen in Figure 5.8.

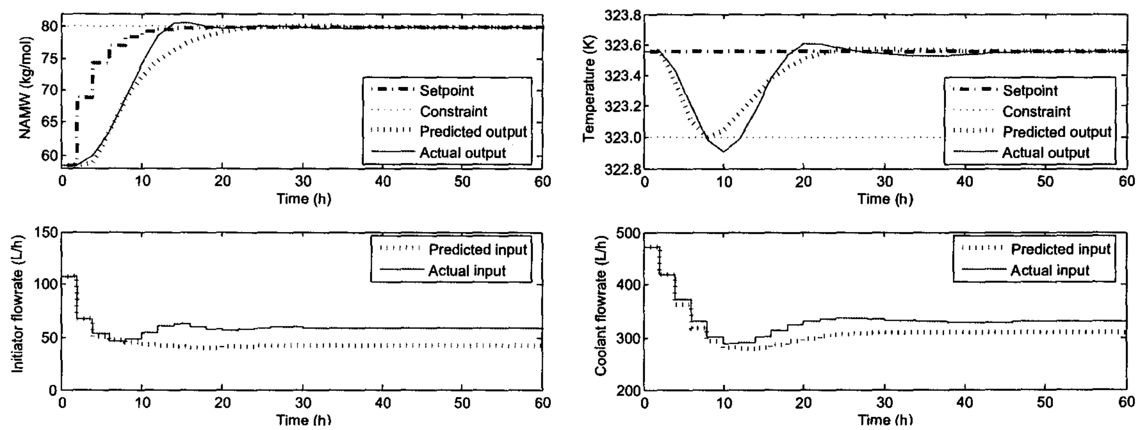


Figure 5.8: Discrete reference filters implementation on nonlinear system

The implementation of the offline optimal solution of reference management based on a linear model on the actual nonlinear system did not result in steady-state offset due to feedback handled by the regulatory controller, but undesirable characteristics in the closed-loop response was present due to model mismatch.

5.5 Reference Management with Nonlinear Models

The optimal solutions for reference management based on a linear model was developed in Section 5.3, but the application of the offline optimal solution to the actual nonlinear system results in model mismatch. However, several proposals for optimal grade transitions discussed in literature, detailed in Section 5.1, were based on determining the optimal input trajectory. Thus, while a regulatory controller has been constructed, steady-state offset due to model mismatch in the absence of feedback was demonstrated when the offline optimal input trajectory based on a linear model was implemented on the actual nonlinear system, as shown in Figure 5.9.

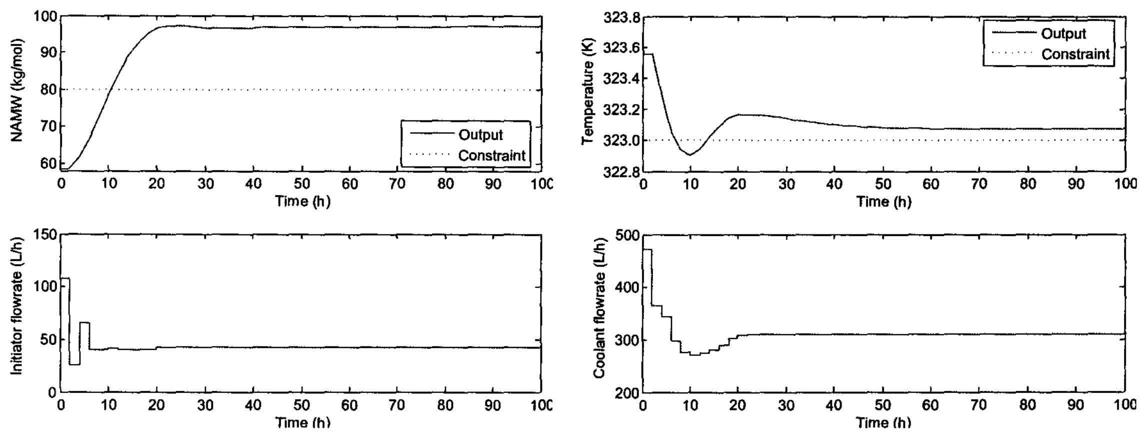


Figure 5.9: Optimal input trajectory implemented on nonlinear system

In contrast, steady-state offset was eliminated when the offline optimal setpoint trajectory based on a linear model was implemented on the actual nonlinear system, as shown in Figure 5.10. However, the closed-loop response was not accurately predicted due to model mismatch, resulting in undesirable characteristics.

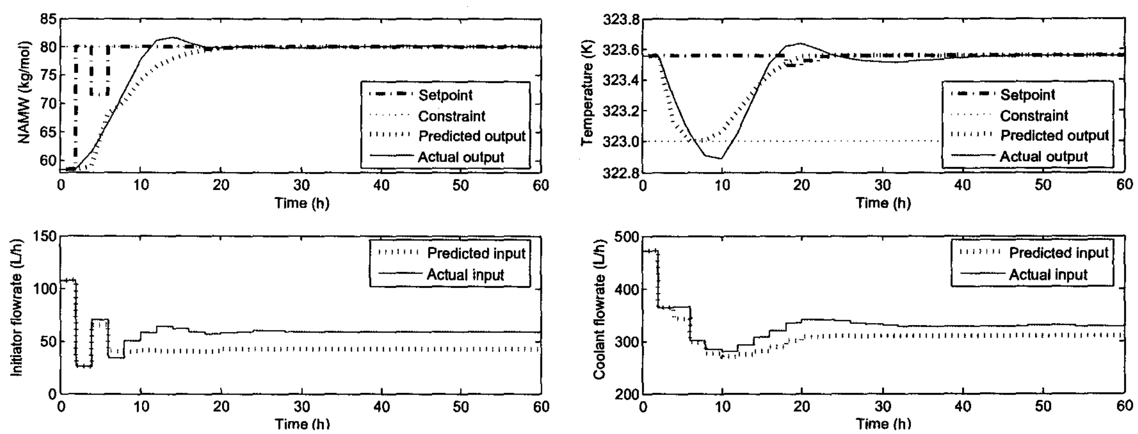


Figure 5.10: Optimal reference trajectory implemented on nonlinear system

Thus assuming the availability of a nonlinear model, reference management based on a nonlinear process model using linear model predictive control was implemented. The set of differential and algebraic equations was discretized using orthogonal collocation on finite elements, and the objective function based on minimizing the squared deviation between the output and target. The optimal solution was obtained in 1835.4 CPU seconds, and the closed-loop response shown in Figure 5.11.

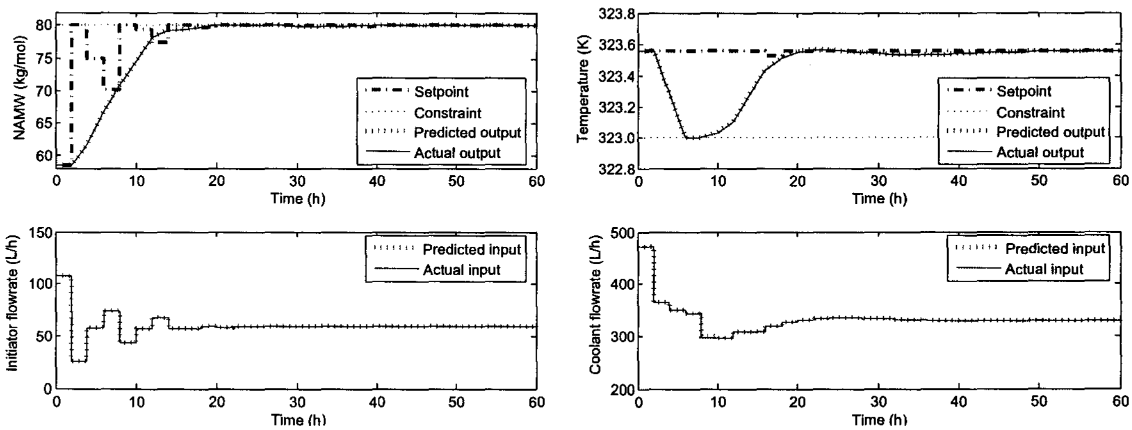


Figure 5.11: Optimal reference trajectory for perfect nonlinear model

The two-tiered approach was implemented to reduce setpoint variability by solving a subsequent optimization, minimizing the squared deviation between the setpoint and target, subject to an additional constraint satisfying the previous objective function value of 0.1210×10^4 within a numerical tolerance of 1%. The optimal solution was obtained in 11258.6 CPU seconds, and the closed-loop response shown in Figure 5.12.

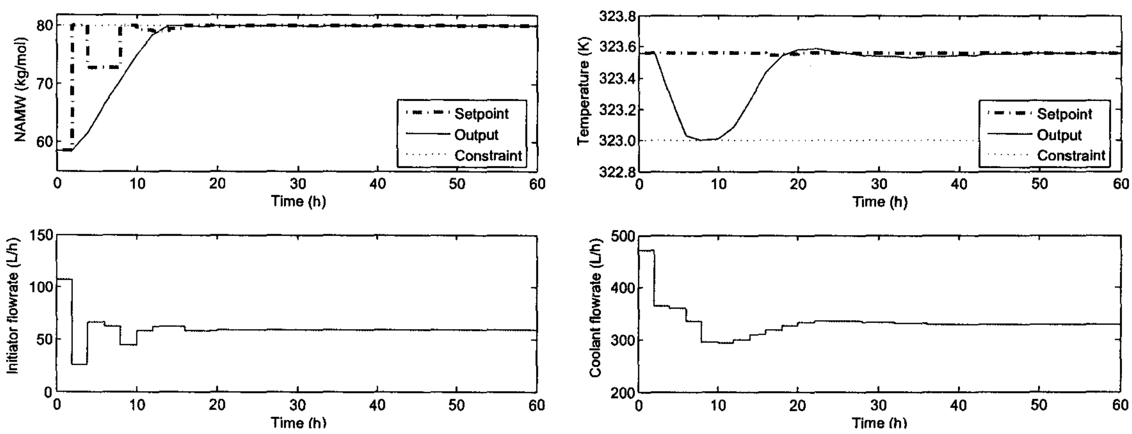


Figure 5.12: Optimal reference trajectory with minimal setpoint variability

Although input saturation was not encountered in the previous simulations, the general framework enables the capability of treating input constraints under constrained model predictive control. Thus the lower bound for the coolant flow rate was set at 280 L/h to demonstrate the effective handling of input saturation. The optimal solution was obtained in 1996.9 CPU seconds, and the closed-loop response shown in Figure 5.13.

However, the reduced input constraints required relaxation of the constraints on allowable setpoints to the region spanned between the lower and upper output constraints. Thus, in the presence of input saturation, additional flexibility may be required to satisfy strict performance bounds.

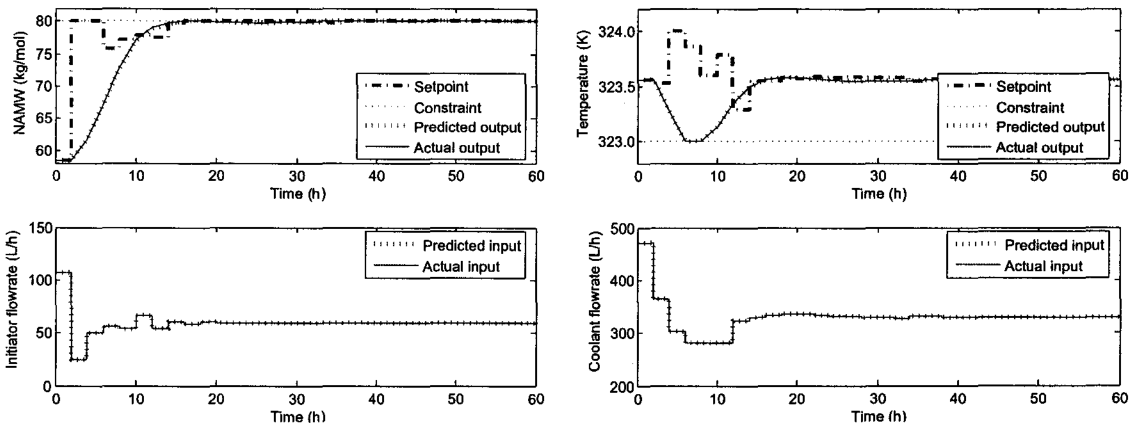


Figure 5.13: Optimal reference trajectory for perfect nonlinear model

The two-tiered approach was implemented to reduce the setpoint variability by solving a subsequent optimization, minimizing the squared deviation between the setpoint and target, subject to an additional constraint satisfying the previous objective function value of 0.1113×10^4 within a numerical tolerance of 1%. The optimal solution was obtained in 1285.1 CPU seconds, and the closed-loop response shown in Figure 5.14.

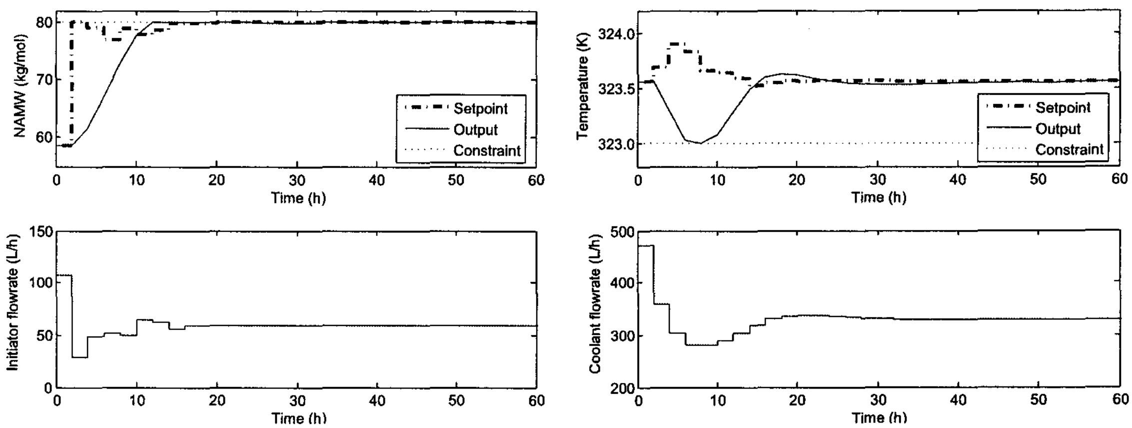


Figure 5.14: Optimal reference trajectory with minimal setpoint variability

The application of reference management based on minimizing the squared deviation between the setpoint and target was also investigated, resulting in a similar closed-loop response without the two-tiered approach, thus reducing computational expense.

Thus the methodology for reference management may similarly be applied to nonlinear models, but subject to the availability of such models for optimization and requiring significantly larger computational expense.

5.6 Reference Management with Dynamic Economics

In steady-state real time optimization, an improvement in profit is possible in the presence of excess optimization variables available for adjustment after satisfying safety, product quality, and production rate objectives (Marlin and Hrymak, 1997). However, economic improvement is possible even for square systems with the consideration of dynamic operation. Thus, Govatsmark and Skogestad (2005) differentiated between steady-state degrees of freedom, determined by subtracting the number of controlled variables from the number of manipulated variables, and dynamic degrees of freedom, determined by the number of manipulated variables.

In the development of economic objective functions, consideration of the current market opportunities is important in defining operational objectives to increase profit. Product quality control is particularly important for emerging industries where the production cost to selling price ratio is low (Kravaris et al., 1989), and the quantity of off-specification product must be reduced because product produced outside commercial product quality specifications must be sold at discount while product variability may eventually lead to loss of market share (McAuley and MacGregor, 1992). Furthermore, in periods of low demand improvement in profit is attained by the minimization of off-specification product at the expense of a longer transition time (McAuley, 1991), while minimizing the transition cost (Tousain, 2002; Bosgra et al., 2004; Tousain and Bosgra, 2006).

In contrast, yield optimization is particularly important in mature industries where the production cost to selling price ratio is high (Kravaris et al., 1989). Similarly, in periods of high demand, improvement in profit is attained by maximizing production and minimizing the transition time (McAuley and MacGregor, 1992; McAuley, 1991; Tousain, 2002; Bosgra et al., 2004; Tousain and Bosgra, 2006). In highly saturated markets such as the refinery process, throughput is maximized at the expense of conversion in the presence of large feed inventory (Caldwell and Dearwater, 1991).

Thus, market conditions define the appropriate operational response to increase profit, and must be considered in the formulation of appropriate economic objective functions. However, the explicit consideration of economic operation minimizes the distinction between the two market situations assuming adequate modelling of complex pricing schemes, and assuming that the resulting mathematical formulation is well-posed for optimization.

5.6.1 Process Description

The grade transition from an initial number average molecular weight of 80 kg/mol to a desired target of 58.481 kg/mol was considered to investigate competing objectives with the minimization of operating costs and maximization of product revenue. The initial conditions shown in Table 5.3 are determined by simulation of the nonlinear model in MatLab 7.0 using Simulink, and correspond with the final steady-state conditions in Sections 5.2-5.5.

Table 5.3: Styrene reactor initial conditions: Grade B

Variable	Initial Value	Units
$[I]$	3.6559x10^{-2}	mol/L
$[M]$	3.3635	mol/L
T_c	307.61	K
D_0	1.5069x10^{-4}	mol/L
D_1	12.055	g/L
Q_i	0.0164	L/s
Q_c	0.0916	L/s
$NAMW$	80.000	kg/mol
T	323.5558	K

The closed-loop response with a single setpoint change for grade transition on the linearized system is shown in Figure 5.15. Thus, the potential for economic improvement during transient operation using reference management based on an explicit economic objective function was investigated.

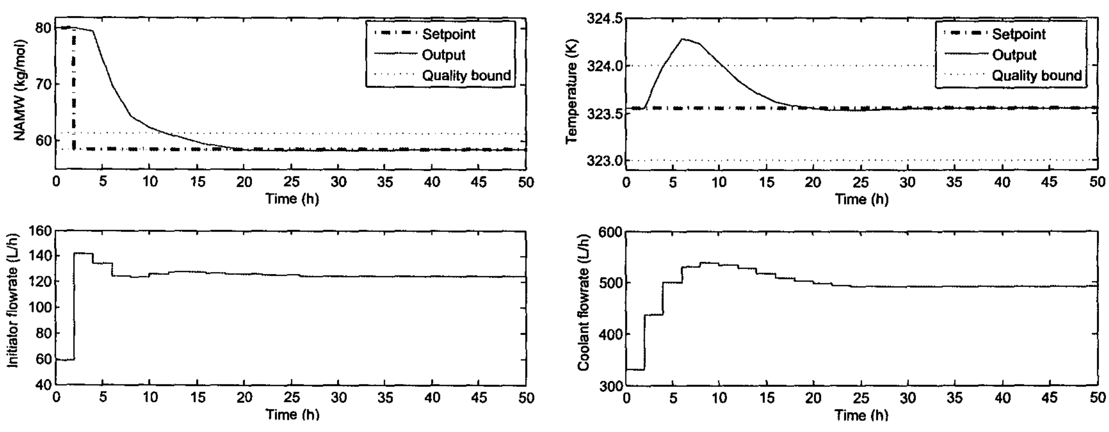


Figure 5.15: Grade transition on linearized system

The grade transition implemented on the actual nonlinear system with a single setpoint change resulted in more aggressive manipulation of the initiator flow rate with the given controller tuning as seen in Figure 5.16.

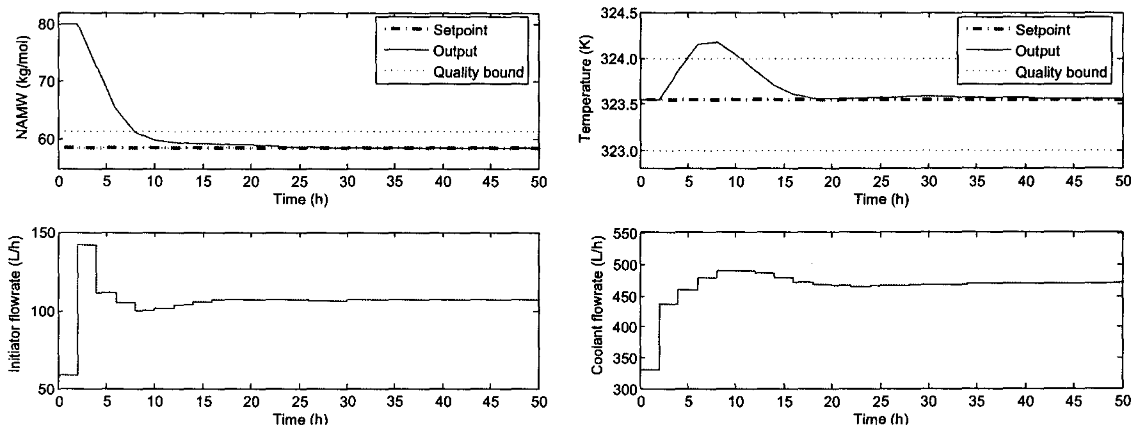


Figure 5.16: Grade transition on nonlinear system

5.6.2 Development of the Economic Objective Function

An economic objective function was proposed to take into account the loss in revenue for producing off-specification product outside the product quality tolerances around the desired targets as shown in Figure 5.17.

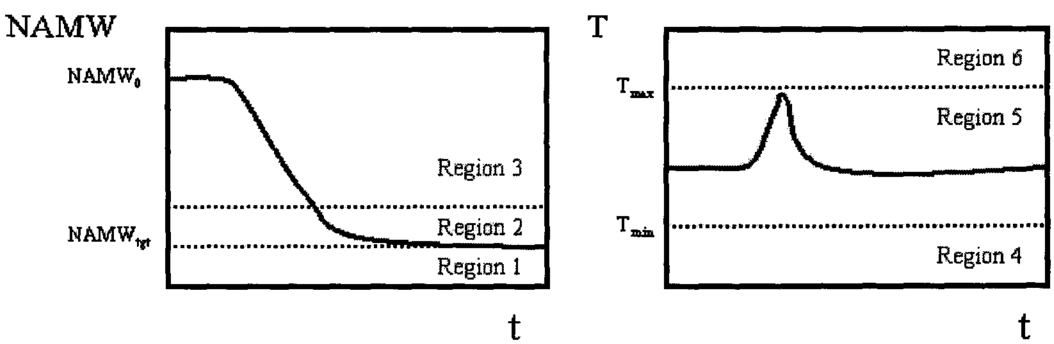
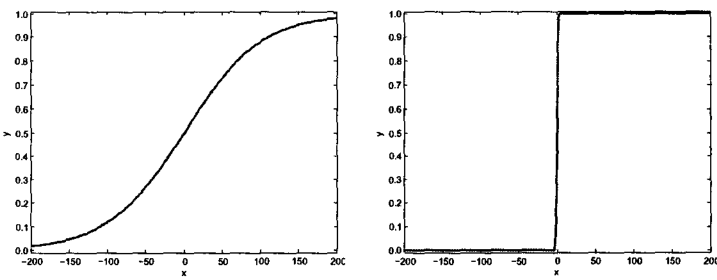


Figure 5.17: Polymerization univariate product quality specifications

The revenue from the initial steady-state was not taken into account, and market sales for off-specification product was assumed to be negligible. The hyperbolic tangent switching function with weighting parameter γ was used to identify product quality regimes without the introduction of integer variables, similar to the technique used by MacRosty (2005) to represent the activation of constraints. Tousain (2002) also considered using the hyperbolic tangent function to define product quality bands, as defined in Equation 5.18.

$$R_i = \frac{1}{2}\tanh(\gamma x) + \frac{1}{2} \approx \begin{cases} 0 & x < 0 \\ 1 & x > 0 \end{cases} \tag{5.18}$$

The effect of increasing the weighting parameter in the switching function is shown by comparing Figures 5.18(a) and 5.18(b).



(a) $\gamma = 0.01$ (b) $\gamma = 1.00$

Figure 5.18: Switching functions where $y = \frac{1}{2}\tanh\gamma x + \frac{1}{2}$

Thus, the given quality variable regime given in Figure 5.17 may be defined mathematically with a continuous objective function. The switching function R_1 given by

$$R_1 = \frac{1}{2}\tanh\left[\gamma\left(NAMW - NAMW_{tgt}\right)\right] + \frac{1}{2} \approx \begin{cases} 0 & NAMW < NAMW_{tgt} \\ 1 & NAMW > NAMW_{tgt} \end{cases} \tag{5.19}$$

is zero for operation in Region 1, resulting in lost revenue because product quality is outside the desired control region for product quality specifications for the number average molecular weight. Region 2 represents the product quality band at the desired steady-state where the upper bound is 5% of the steady-state value. The switching function R_2 given by

$$R_2 = \frac{1}{2}\tanh\left[\gamma\left(1.05NAMW_{tgt} - NAMW\right)\right] + \frac{1}{2} \approx \begin{cases} 0 & NAMW > 1.05NAMW_{tgt} \\ 1 & NAMW < 1.05NAMW_{tgt} \end{cases} \tag{5.20}$$

is zero for operation in Regions 3, resulting in lost revenue because product quality is outside the control region for product quality specifications for the number average molecular weight. The switching function R_3 given by

$$R_3 = \frac{1}{2}\tanh\left[\gamma\left(T - T_{min}\right)\right] + \frac{1}{2} \approx \begin{cases} 0 & T < T_{min} \\ 1 & T > T_{min} \end{cases} \tag{5.21}$$

is zero for operation in Region 4, resulting in lost revenue because product quality is outside the control region of product quality specifications resulting from temperature effects. The switching function R_4 given by

$$R_4 = \frac{1}{2}\tanh\left[\gamma\left(T_{max} - T\right)\right] + \frac{1}{2} \approx \begin{cases} 0 & T > T_{max} \\ 1 & T < T_{max} \end{cases} \tag{5.22}$$

is zero for operation in Region 6, resulting in lost revenue because product quality is outside the control region of product quality specifications resulting from temperature effects. The switching functions were used with a weighting parameter of $\gamma = 0.01$ to improve conditioning for gradient based optimization as discussed further in Subsection 5.6.4. Thus the revenue R obtained during transient operation is given by

$$R = Q\left[F\right]PR_1R_2R_3R_4 \tag{5.23}$$

consisting of the amount of product produced within the product quality specifications at the desired steady-state sold at a market price of P=\$0.1355/mol based on commodity marginal spot market prices obtained from ICIS-LOR (2005), Q is the total product flowrate, and $[F]$ is given by

$$[F] = [P] + [M] + [I] \tag{5.24}$$

representing the concentration of the product effluent without solvent recovery, and may be approximated by an average of 232 mol/L within the product band. In this work, a constant pricing scheme was assumed with the effluent treated as the final product stream. This simplification, however, results in complications in industry as discussed by Bailey et al. (1993), where multiple pricing is based on contract and spot market sales, and the determination of inter-process stream pricing requires estimates of value added and potential worth at each stage of the process. Dynamic pricing with lower initial pricing to establish demand, followed with subsequent increases in pricing to yield an increase in cumulative profit as discussed by Fan et al. (2005) was not considered.

Furthermore, the use of univariate specifications on instantaneous properties was assumed to adequately reflect the cumulative end-use product quality. In reality, additional measurements would be required to classify quality based on the breadth and shape of the molecular weight and composition distributions (McAuley and MacGregor, 1992), and product properties should be considered simultaneously due to the multivariate nature of product quality (Kourti and MacGregor, 1996). In fact, individual specification of desired target specifications without accounting for the correlation structure among quality variables may result in infeasibility (Jaeckle and MacGregor, 1998).

The switching functions used to represent production within product quality bands were squared,

$$R = Q\left[F\right]PR_1^2R_2^2R_3^2R_4^2 \tag{5.25}$$

to improve numerical conditioning arising from small but negative solutions. An equivalent formulation of Equation 5.23 used by Tousain (2002) is given by

$$R = Q\left[F\right]P\left(R_1 + R_2 - 1\right)\left(R_3 + R_4 - 1\right) \tag{5.26}$$

However, consideration of numerical conditioning of Equation 5.26 would result in increased inaccuracy, and was not considered further. The revenue obtained from off-specification product was assumed to be negligible and the opportunity cost of producing high quality product was not taken into account. The operating cost C is given by

$$C = C_1Q_m\left[M_f\right] + C_2Q_i\left[I_f\right] + C_3Q_c \tag{5.27}$$

where C_1=\$0.1123/mol based on commodity marginal spot market prices obtained from ICIS-LOR (2005), C_2=\$0.1200/mol for initiator costs and C_3=\$0.0400/L for cooling water. The cost function is based on raw material feed and utility costs, assuming monomer in the effluent is not recovered and cooling water purchased and discharged. Thus there are economic incentives to operate at a low initiator flow rate due to high initiator costs as discussed by Lewin and Bogle (1996). Thus the economic objective function is given by

$$\min_{y_{sp}} \Phi = \sum_{t_0}^{t_N}\{C\left(t\right) - R\left(t\right)\}\Delta t \tag{5.28}$$

assuming static incremental prices and utility costs integrated over a simulation horizon $[t_0, t_N]$. Tousain and Bosgra (2000) proposed a similar economic cost function based on minimizing raw material costs and maximizing production, where different prices were assigned at fixed points in time based on the expected closed-loop response during transitions, but was extended to include the use of product quality bands by Tousain (2002) and Bosgra et al. (2004).

However, the economic objective function based on product quality specification bands did not result in a well-posed optimization problem due to the possibility of indeterminacy within acceptable bands. Thus the objective function used for optimization was modified, and given by

$$\Phi = \sum_{t_0}^{t_N} \{C(t) - R(t)\left[1 - (NAMW(t) - NAMW_{tgt})^2 - 100\,(T(t) - T_{tgt})^2\right]\}\Delta t \quad (5.29)$$

which includes a control penalty term to ensure the desired steady-state target is reached once product specifications are within acceptable product quality bands, where cost considerations are no longer as important. This improves convergence to the desired steady-state target without enforcing end point constraints at an arbitrary point in time. Furthermore, the end point constraints may not necessarily result in a smooth closed-loop response since there is no penalty on deviation from target once within product quality bands.

Thus the objective function is based explicitly on economics while a control performance objective dominates once product quality is within acceptable product quality bands. Note that the control performance objective does not contribute to the objective function value when outside the desired product quality specifications, since revenue is not generated. Furthermore, the constant term within the control performance term may be increased to a larger value than unity, but at the expense of increased variability within the product quality specification band.

Tousain (2002) also investigated the use of an explicit economic objective function with consideration of a control performance objective function to optimize grade transitions for polyethylene polymerization. However, the proposed objective function was based on an arbitrary weighting between the two objectives. Similarly, Becerra et al. (1998) and Zanin et al. (2002) proposed combining online optimization of economics with control objectives, using a single scalar objective function combining the linear and quadratic objective functions with arbitrary weightings. Bosgra et al. (2004) avoided indeterminacy and convergence difficulties by enforcing end point conditions to the desired grade, solved using mixed integer linear programming (MILP).

In contrast, the formulation presented in this work avoided the use of integer variables by using a smooth approximation of the economic objective function. The resulting objective minimizes operational costs during transient operation, and minimizes product variability once within product quality specifications when control performance objectives dominate economic considerations.

5.6.3 Improvement in Profit in the Linear System

The simultaneous optimization of transient operation was based on the developed economic objective function without hard output constraints, and considering a perfect linear model. The optimal solution was obtained in 48.5 CPU seconds, and the closed-loop response shown in Figure 5.19. Comparison of Figure 5.19 to nominal operation in Figure 5.15, the supervisory controller based on an economic objective function minimized the amount of initiator used by transferring variability to the coolant flow rate, while the transition time was minimized to reduce the amount of off-specification product produced during transient operation. The economic improvement resulted in a profit of $\$ 1.2788 \times 10^6$ (US) compared to $\$ 0.5215 \times 10^6$ (US) for the single setpoint change on the linear system, based on Equation 5.28 evaluated every 2 hours over 100 hours.

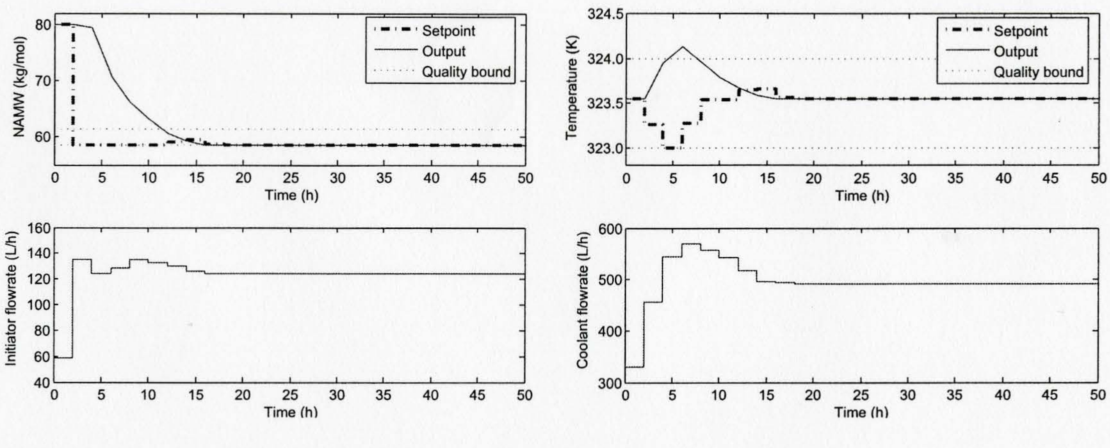


Figure 5.19: Optimal economic operation for perfect linear model

5.6.4 The Effect of the Weighting Parameter in Switching Functions

Increasing the weighting parameter in Equations 5.19-5.22 to $\gamma = 0.05$ from $\gamma = 0.01$ resulted in a suboptimal solution with an oscillatory setpoint trajectory that did not reach steady-state. Increasing the weighting parameter to $\gamma = 1$ resulted in a suboptimal solution where the desired steady-state was not obtained as seen in Figure 5.20.

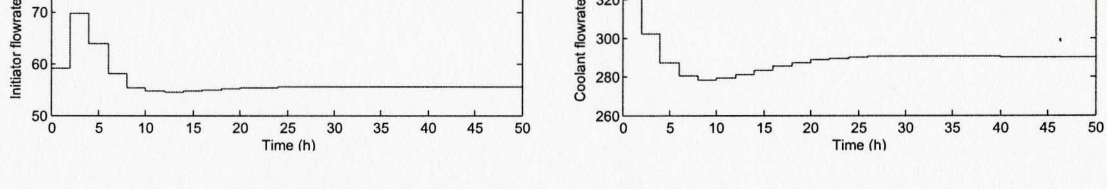


Figure 5.20: Suboptimal solution resulting with $\gamma = 1.00$

The inclusion of an end point constraint at an arbitrary point in time, introduced half way into the simulation horizon, may improve the step length in the descent direction of the true objective function. The optimal solution for a weighting parameter in the switching function of $\gamma = 0.05$ was obtained in 63.7 CPU seconds, and the closed-loop response shown in Figure 5.21. However, the solver terminated prematurely when the weighting parameter was increased to $\gamma = 1$ after 476.7 CPU seconds.

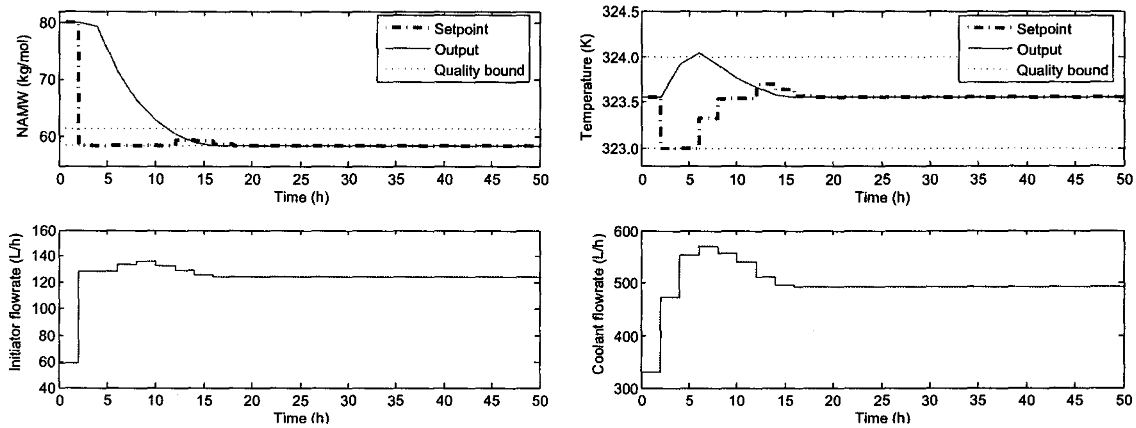


Figure 5.21: Optimal solution obtained with $\gamma = 0.05$ using end point constraints

The effect of increasing the weighting parameter in the switching function is shown in Figures 5.18(a)-5.18(b). It is believed that increasing the weighting parameter introduced numerical problems with near-derivative discontinuities into the objective function causing difficulties in gradient based optimization, possibly resulting in suboptimal solutions. Schot et al. (1999) similarly considered product specification bands for grade transitions in a high density polyethylene plant and noted strong nonlinearity due to sharp edges in pricing between on and off-specification product, causing inefficient gradient based optimization requiring several iterations.

5.6.5 Alternative Objective Function Formulations

The use of the economic objective function without consideration of the control performance term as in Equation 5.28 does not guarantee transition to the desired steady-state, as seen in the closed-loop response shown in Figure 5.22. The solution was obtained in 75.3 CPU seconds with a weighting parameter of $\gamma = 0.01$ used in Equations 5.19-5.22.

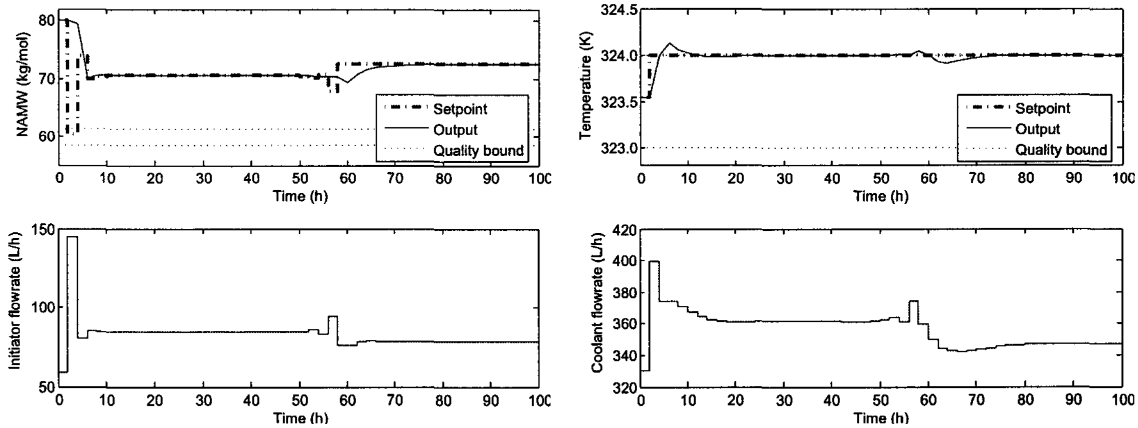


Figure 5.22: Suboptimal solution based on economics without conditioning

Furthermore, the use of the economic objective function shown in Equation 5.28 in addition to an end point constraint does not guarantee a smooth transition to the desired steady-state. The solution was obtained in 88.3 CPU seconds, and the closed-loop response is shown for a weighting parameter of $\gamma = 0.01$ in Figure 5.23.

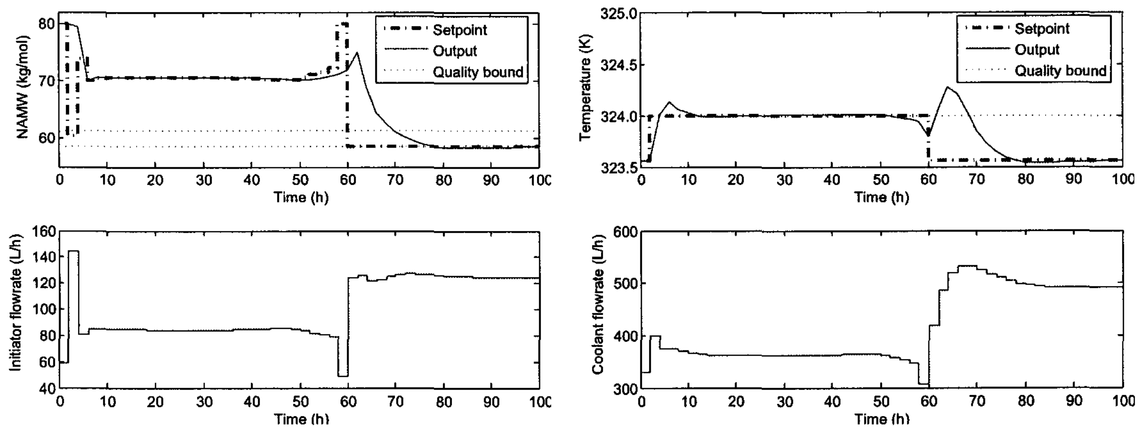


Figure 5.23: Suboptimal solution obtained with end point constraints

Thus the incorporation of the control performance objective function in addition to the relaxation of pricing discontinuity is important to improve smooth convergence to the desired steady-state target when using gradient based optimization. The discontinuous nature of the objective function must be conditioned by smooth approximation, and is particularly important when using IPOPT-C (Wächter, 2005).

Alternative solution strategies may be based on mixed integer programming (Bosgra et al., 2004) or derivative free optimization. Zyngier and Marlin (2006) used derivative free optimization for performance assessment of closed-loop real time optimization, solving a three-level optimization problem with derivative discontinuity introduced by an inner optimization problem.

5.6.6 Improvement in Profit in the Nonlinear System

The simultaneous approach to reference management for economic optimization was implemented on a perfect nonlinear model, with the closed-loop response shown in Figure 5.24. The optimal setpoint trajectory was determined in 1220.6 CPU seconds, with a weighting parameter of $\gamma = 0.05$ used in Equations 5.19-5.22. The economic improvement resulted in a profit of \$ 1.3166×10^6 (US) compared to \$ 0.9817×10^6 (US) for the single setpoint change on the nonlinear system, based on Equation 5.28 evaluated every 2 hours over 100 hours using average product properties within product specifications. The optimal transition minimized production of off-specification product to 10 hours compared to 12 hours for nominal operation based on a single setpoint change.

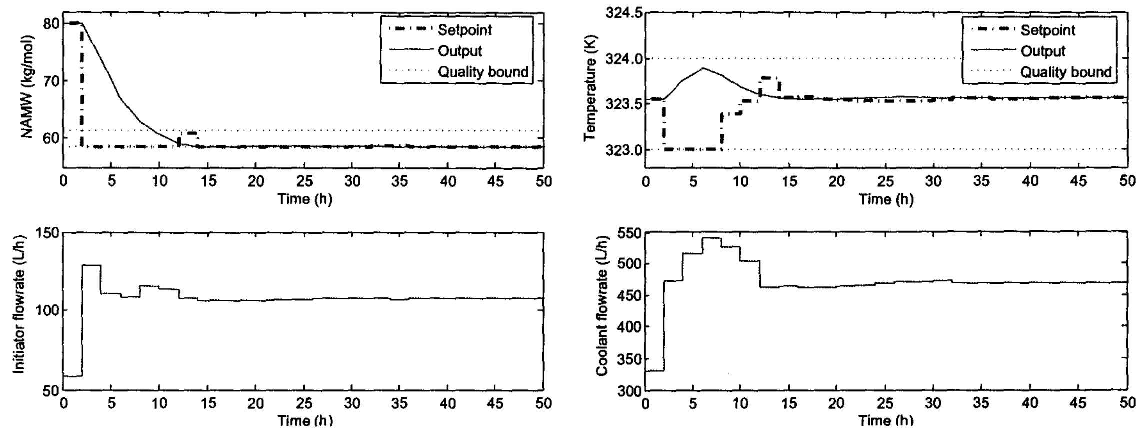


Figure 5.24: Optimal economic operation for perfect nonlinear model

5.6.7 Utilization of Additional Degrees of Freedom

Common heuristics used in industry to improve grade transitions were discussed by Debling et al. (1994), including de-inventorying reactor contents by 50% to reduce off-specification product by removal of on-specification product while minimizing the transition time. Similar proactive solutions were investigated by Bathazaar (2005) in response to unit shutdown failure in pulp and paper production.

However, in this work, the reactor bed level was not manipulated, but the production rate was adjusted as an additional degree of freedom to minimize the production of off-specification product by manipulating the monomer flow rate.

Thus the monomer flow rate was incorporated as an additional degree of freedom and allowed to vary between [300, 378] L/h, while the solvent flow rate was ratio controlled and the reactor level maintained by manipulating the product flow rate. Thus inclusion of the monomer flow rate as an additional degree of freedom available for optimization enabled the total flow rate to vary throughout the grade transition, and would result in minimizing the production of off-specification product. Increasing the monomer flow rate had the effect of increasing the operating cost during transient operation, but would result in a net profit once within product quality specification bands.

The objective function was based on Equation 5.29 with a switching function weighting parameter of $\gamma = 0.05$ used in Equations 5.19-5.22. Additional constraints forcing the setpoint to target were enforced approximately half way through the simulation time horizon of 100 hours to ensure the desired steady-state was reached.

The optimal setpoint trajectory was obtained in 996.8 CPU seconds, and the closed-loop response when implemented on a perfect nonlinear model is shown in Figure 5.25.

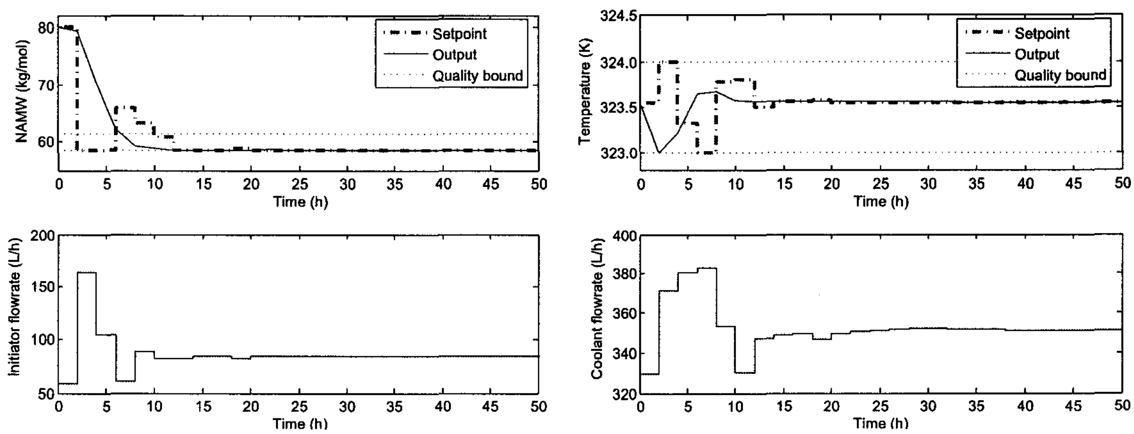


Figure 5.25: Closed-loop response minimizing transient variability

The production rate is shown in Figure 5.26, where a reduction in productivity was required to minimize cost and product variability during the transition. However, the reduction in productivity was sustained at the desired steady-state, thus resulting in suboptimal steady-state operation.

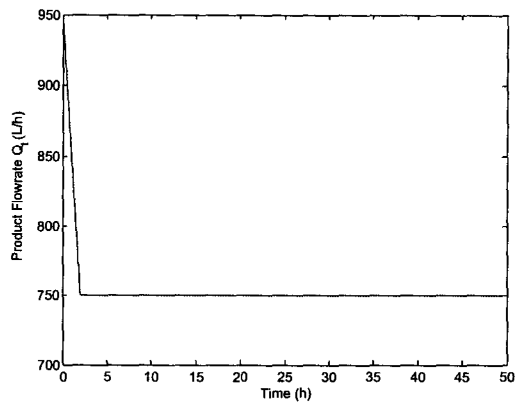


Figure 5.26: Productivity minimized to reduce costs

The suboptimal solution was obtained as a result of using a weighting parameter of $\gamma = 0.05$ in the switching functions causing ambiguity between the actual cost and revenue during the transition where the actual revenue was underestimated. To compensate for the effect of the weighting parameter on the objective function, the concentration of growing polymer contributing to the revenue term in Equations 5.23-5.24 was multiplied by a large scaling factor ($S = 10^{11}$) shifting the objective towards maximizing productivity. The objective function was modified as shown by

$$\Phi = \sum_{t_0}^{t_N}\{C - Q\,(S\,[P] + [M] + [I])\,PR_1^2R_2^2R_3^2R_4^2\,[100 - (NAMW - NAMW_{tgt})^2 - 100\,(T - T_{tgt})^2]\}\Delta t \qquad (5.30)$$

where the tolerance on control performance was relaxed, resulting in abrupt maximization of production at the expense of a slight increase in output variability. The optimal setpoint trajectory was obtained in 577.0 CPU seconds, and the closed-loop response when implemented on a perfect nonlinear model is shown in Figure 5.27.

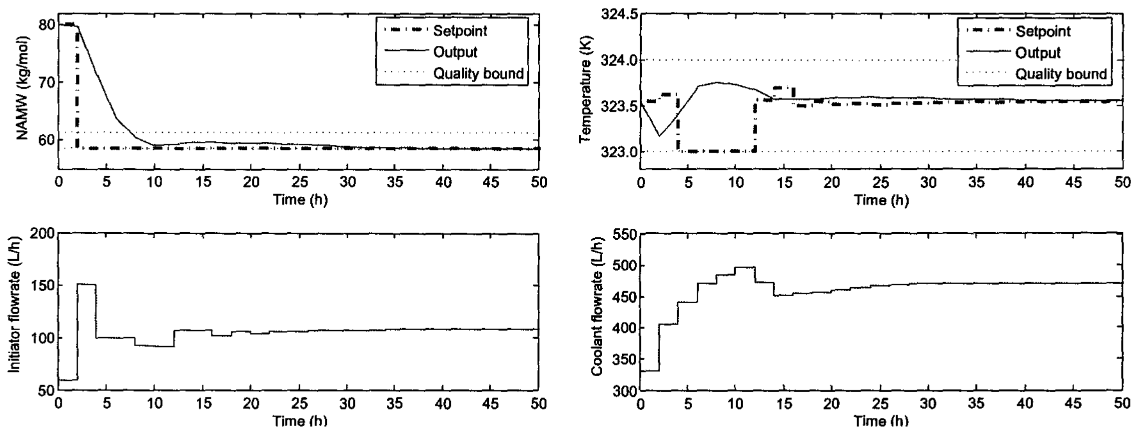


Figure 5.27: Optimal operation with productivity maximization

The product flow rate is shown in Figure 5.28, where optimal operation at the desired steady-state resulted in maximizing productivity. The decreased production rate during transient operation reduced the amount of monomer consumed, thus lowering operating costs, while reducing the amount of off-specification product produced thus reducing variability in the product properties of the cumulative polymer in storage.

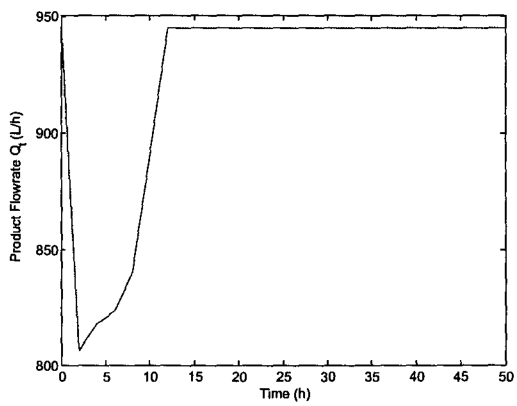


Figure 5.28: Maximizing productivity

A similar strategy to reduce the production of off-specification product during the initial transient operation for grade changes in polyethylene polymerization was proposed by McAuley and MacGregor (1992), however, by manipulating the reactor bed level. Chatzidoukas et al. (2003) demonstrated an additional reduction in transition time of 5% and a reduction in the amount of off-specification product produced by 7.7% by manipulating the bed height and production rate. Similarly, startup of a continuous polymerization reactor was shown to result in reduced transition times compared to grade transitions as a result of the absence of polymer in the reactor (Cozewith, 1988). Thus additional improvements in closed-loop performance may be possible by manipulating the setpoint of the reactor bed level.

Similar advantages utilizing available degrees of freedom were noted with Flender et al. (1996) demonstrating a 75% reduction in transition time for a distillation column operating under minimal reflux, thus resulting in near total removal of distillate during transient operation. A reduction in transition time for multi-effect batch distillation was also shown experimentally by (Noda et al., 2000) by allowing changes in holdup. Thus further improvement in economic operation may be realized by manipulating additional degrees of freedom.

5.6.8 Consideration of Initial Product Quality Bands

The revenue obtained from production within the initial grade specification was also considered, defined by a 5% band below the initial specifications of the number average molecular weight, and described using the switching functions given by

$$R_5 = \frac{1}{2}\tanh\left[\gamma\left(NAMW - 0.95NAMW_0\right)\right] + \frac{1}{2} = \begin{cases} 0 & NAMW < 0.95NAMW_0 \\ 1 & NAMW > 0.95NAMW_0 \end{cases} \quad (5.31)$$

$$R_6 = \frac{1}{2}\tanh\left[\gamma\left(NAMW_0 - NAMW\right)\right] + \frac{1}{2} = \begin{cases} 0 & NAMW > NAMW_0 \\ 1 & NAMW < NAMW_0 \end{cases} \tag{5.32}$$

The revenue B obtained from production within the initial product quality specifications before grade change is determined by

$$B = Q\left[F\right] P_B R_1^2 R_2^2 R_3^2 R_4^2 \tag{5.33}$$

where $P_B = \$0.131/\text{mol}$ based on commodity marginal spot market prices obtained from ICIS-LOR (2005). The switching functions were also squared to improve numerical conditioning arising from small but negative solutions and a weighting function consistent with previous simulations of $\gamma = 0.01$ was used.

The economic objective function, modified with consideration of control performance within the desired product quality specification bands was extended to

$$\Phi = \sum_{t_0}^{t_N} \{C\left(t\right) - B\left(t\right) - R\left(t\right)\left[1 - \left(NAMW\left(t\right) - NAMW_{tgt}\right)^2 - 100\left(T\left(t\right) - T_{tgt}\right)^2\right]\}\Delta t \tag{5.34}$$

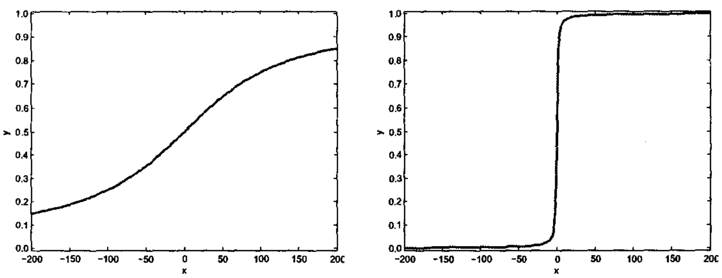
The optimal solution was obtained in 1030.3 CPU seconds, resulting in a similar closed-loop response as shown in Figure 5.24. However, the profit calculation was extended with the term given in Equation 5.33 and resulted in a profit of \$ 1.3913×10^6 (US). Similarly, utilizing the monomer flow rate as an additional degree of freedom resulted in a similar closed-loop response as shown in Figures 5.27-5.28, with an optimal solution obtained in 406.4 CPU seconds.

5.6.9 Alternative Switching Functions

An alternative switching function given by Tousain (2002) was used to represent product quality specification regions based on the arctangent function given by

$$R_i = \frac{1}{\pi}\arctan(\gamma x) + \frac{1}{2} = \frac{i}{2\pi}\log\left(\frac{i+\gamma x}{i-\gamma x}\right) + \frac{1}{2} = \begin{cases} 0 & x < 0 \\ 1 & x > 0 \end{cases} \tag{5.35}$$

This formulation introduces less discontinuity into the objective function in the limit as $\gamma \to \infty$ compared to the hyperbolic tangent function as seen in Figures 5.29(a)-5.29(b), but represents a less accurate description of the product quality specification bounds.



(a) $\gamma = 0.01$ (b) $\gamma = 1.00$

Figure 5.29: Arctangent switching functions where $y = \frac{1}{\Pi}\arctan\gamma x + \frac{1}{2}$

The objective function given in Equation 5.29 with revenue calculated according to Equation 5.25 using a weighting parameter of $\gamma = 0.01$ in Equations 5.19-5.22, was modified with the arctangent function given in Equation 5.35. The solution for a perfect nonlinear model was obtained in 1039.3 CPU seconds, and the closed-loop response shown in Figure 5.30.

A reduction in performance was demonstrated in comparison with Figure 5.24 with increased utilization of initiator and an aggressive setpoint trajectory. However, increasing the weighting parameter to $\gamma = 0.05$ was capable of yielding a solution driven to the desired steady-state without the inclusion of end point constraints. The solution was obtained in 1702.6 CPU seconds, and the closed-loop response shown in Figure 5.31.

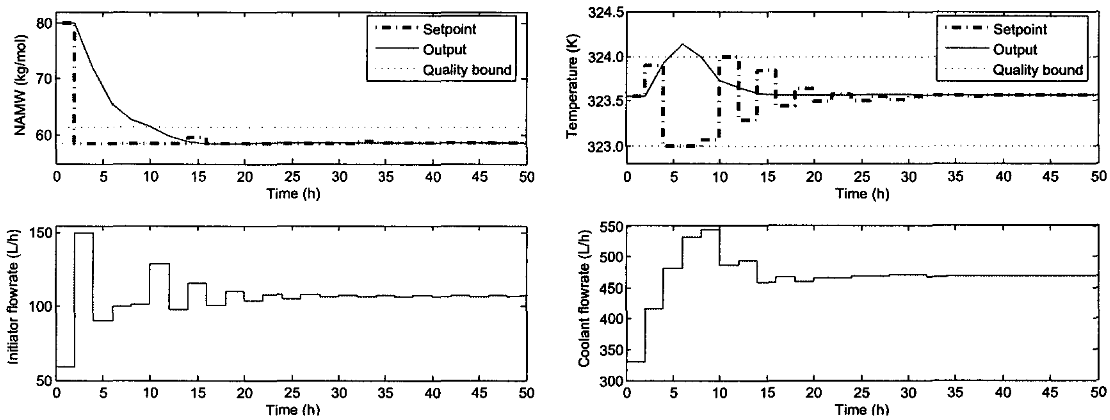


Figure 5.30: Use of arctangent switching functions with $\gamma = 0.01$

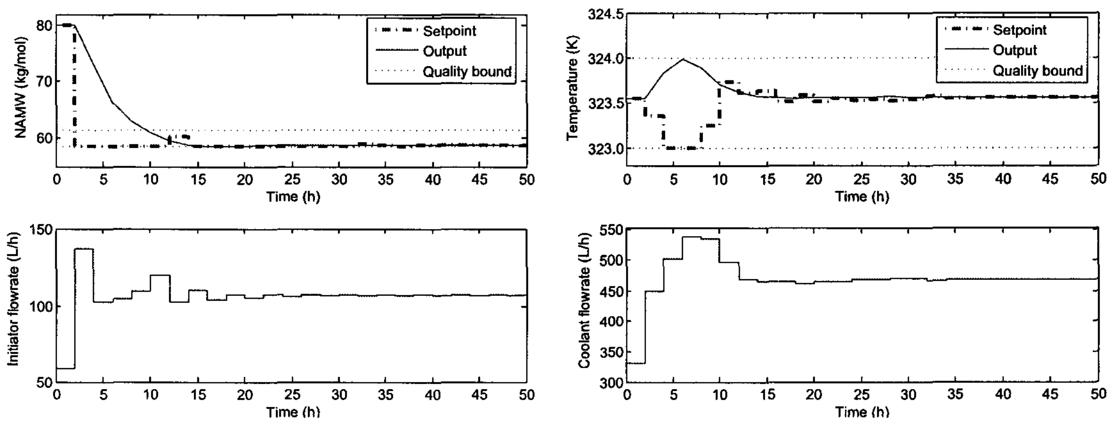


Figure 5.31: Use of arctangent switching functions with $\gamma = 0.05$

The weighting function was further increased to $\gamma = 1.00$, yielding a solution in 1045.9 CPU seconds, and the closed-loop response shown in Figure 5.32. The conflicting objectives for minimizing the transition cost and maximizing revenue at the desired steady-state is evident.

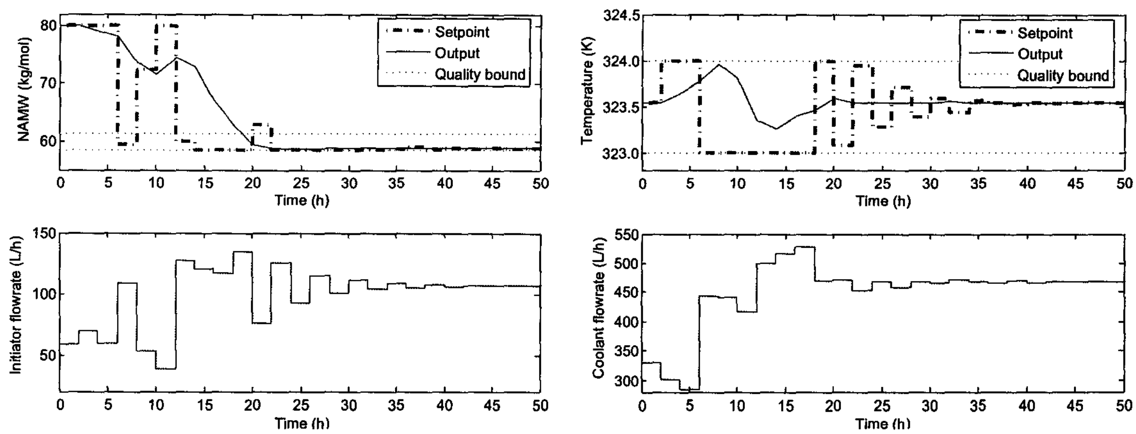


Figure 5.32: Use of arctangent switching functions with $\gamma = 1.00$

Another alternative switching function given by Flores-Cerrillo and MacGregor (2005) was used for data smoothing, based on the sigmoidal function given by

$$R_i = \frac{1}{1+\exp\left[-6.9068\left(\frac{a+b-2x}{b-a}\right)\right]} = \begin{cases} 0 & x > b \\ (0,1) & a < x < b \\ 1 & x < a \end{cases} \tag{5.36}$$

where the tuning parameters $a = 100, b = 300$ were chosen in Figure 5.33. This formulation would enable specification of the range allowed to be relaxed.

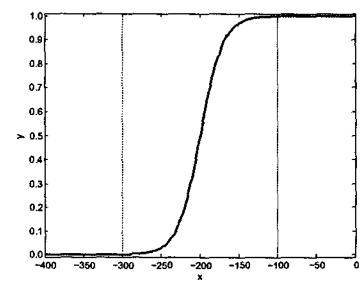


Figure 5.33: Sigmoidal switching functions where $y = \left\{1+\exp\left[-6.9068\left(\frac{a+b-2x}{b-a}\right)\right]\right\}^{-1}$

The objective function given in Equation 5.29 with revenue calculated according to Equation 5.25 was used where the hyperbolic tangent switching function in Equation 5.20 was replaced with the sigmoidal switching function given in Equation 5.36, with $a = 1.05y_{tgt}$ and $b = 1.07y_{tgt}$. The solution was obtained in 523.2 CPU seconds, and the closed-loop response shown in Figure 5.34.

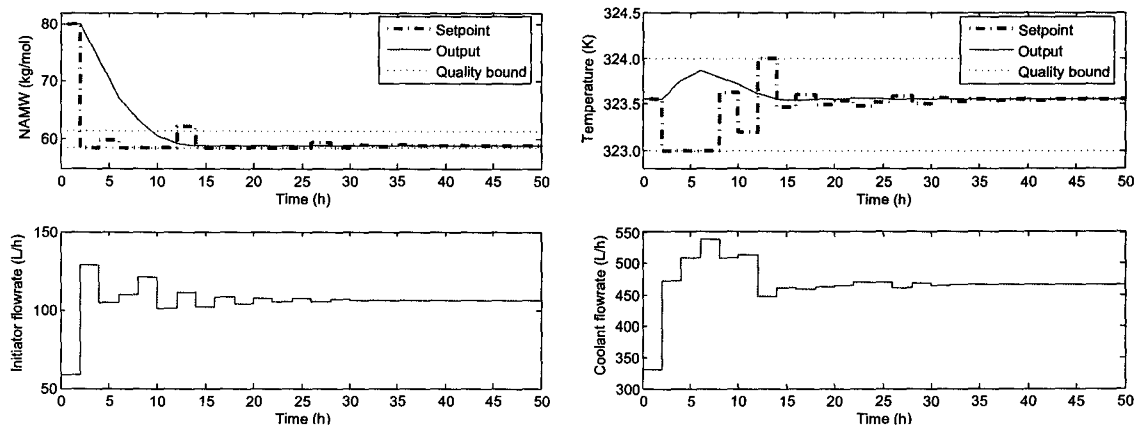


Figure 5.34: Use of the sigmoidal function with $a = 1.05NAMW_{tgt}$ $b = 1.07NAMW_{tgt}$

However, a solution was not obtained when the relaxation limits were decreased to $a = 1.05y_{tgt}$ and $b = 1.06y_{tgt}$ due to difficulties in convergence. Thus, the use of the sigmoidal function may enable investigation of the range of relaxation required for convergence of the gradient based algorithm to an optimal solution.

5.7 Summary of Results

This chapter detailed the application of the proposed methodology to nonlinear dynamic systems, and summarized optimal grade transitions investigated in literature. The multi-input multi-output control of styrene polymerization was described, and application of reference management to the linearized system demonstrated by minimizing the production of off-specification product with suitable hard output constraints defined based on economic considerations. The discrete reference filter was implemented and alternative objective function formulations investigated. The resulting offline optimal input trajectory was implemented on the nonlinear system to demonstrate the presence of steady-state offset due to model mismatch, which was eliminated by online tracking of the offline optimal setpoint trajectory.

Furthermore, the optimal setpoint trajectory was determined based on the nonlinear model discretized using orthogonal collocation on finite elements. An objective function was formulated with explicit consideration of economics using product quality specification bands, with control performance objectives once within product quality specifications. The optimal economic operation was determined for the linear and nonlinear systems during grade transitions, and the effect of weighting function parameters, switching functions and objective function formulations on the optimal solution were investigated. Also, the utilization of additional degrees of freedom was shown to be capable of yielding further economic improvements.

Chapter 6

Online Implementation

Within the standard automation and control hierarchy, low frequency disturbances are rejected by real time optimization while high frequency disturbances are handled by regulatory control. In this work, quadratic dynamic matrix control (QDMC) was used for regulatory control with the standard assumption of unmeasured step disturbances in the output. Thus, disturbances are handled through feedback with bias update, eliminating steady-state offset arising from model mismatch, although suboptimally. In this chapter, updating the reference trajectory was investigated using a bias update for disturbance estimation rather than online closed-loop model identification and estimation of stochastic states. The bias update is based on the difference between the actual output measured from the process and the output prediction within the supervisory controller at a given point in time.

A single-input single-output system was investigated in Section 6.1, with the performance of bias updating evaluated in the presence of step disturbances in the output, model mismatch and pulse disturbances in the output. The methodology implemented online was also demonstrated on a multi-input multi-output system in Section 6.2, corresponding to using the linear model to update the reference trajectory when applied to the nonlinear polymerization process.

Within the simulations conducted, the computational time required to determine the optimal trajectory was not taken into account. However, the methodology was investigated using linear models to reduce computational expense.

6.1 Single-Input Single-Output Systems

The following linear single-input single-output system given by

$$G_p(s) = \frac{-0.4191e^{-2s}}{6.1024s + 1} \tag{6.1}$$

was used as a case study for improvement of closed-loop performance by updating the reference trajectory. The constrained model predictive control tuning used an output to input move weighting ratio of 10:1, a prediction horizon of 20, and an input horizon of 5 at a sampling time of 2 time units. The setpoint target was $y = 80$ from an initial steady-state of $y = 58.481$ and the input was constrained to $[0, 500]$ from an initial steady-state value of $u = 108$.

The linear system was discretized at a sampling time of 2 time units resulting in the difference equation which was used to represent the process within the dynamic optimizer,

$$y(k+1) = 0.7206y(k) - 0.1171u(k-1) + d(k+1) \tag{6.2}$$

The optimal solution was obtained using simultaneous optimization in 3.4 CPU seconds. The optimal setpoint trajectory was based on minimizing the squared deviation between the output and target every 2 time units for 50 time units, and the closed-loop response when applied to the discrete linear process model without model mismatch is shown in Figure 6.1.

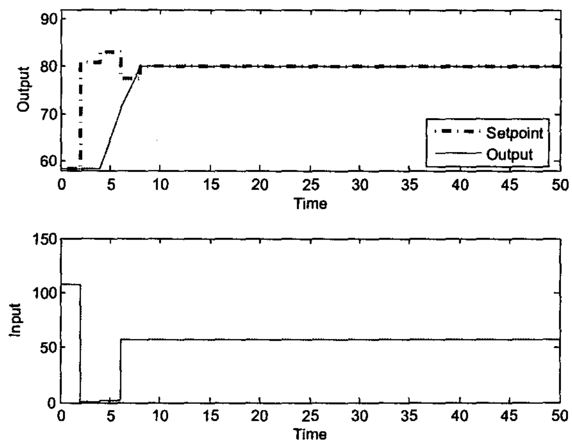


Figure 6.1: Optimal reference trajectory without model mismatch

6.1.1 Step Disturbances in the Output

The implementation of the nominal setpoint trajectory on the discrete linear process model with a step disturbance in the output of $d = 20$ at 4 time units is shown in Figure 6.2, resulting in a cost objective function value of 1129.5924 based on the squared deviation between the actual output and target every 2 time units for 50 time units.

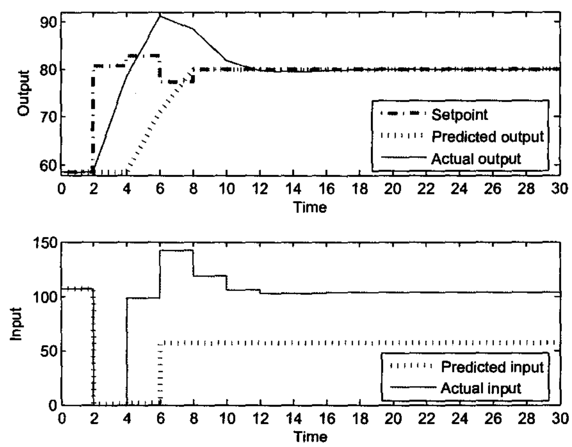


Figure 6.2: Implementation on the actual system with step disturbance

Assuming a perfect model with knowledge of the step disturbance, the optimal reference trajectory was determined and implemented on the actual continuous system. The closed-loop response is shown in Figure 6.3, representing the best achievable performance possible with a cost objective function value of 928.4421.

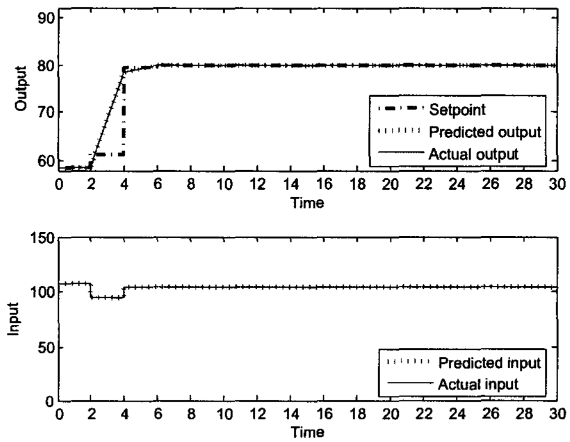


Figure 6.3: Optimal reference trajectory with perfect process and disturbance model

However, in the presence of the unmeasured step disturbances and using an online bias update to the system, the correct disturbance was estimated after implementing the first step change since the disturbance occurs at this point in time and no other disturbances were present. The disturbance was estimated as the difference between the actual measured output and the predicted output within the dynamic optimizer at the current time of 4 time units.

The updated setpoint trajectory was implemented on the actual continuous system and the closed-loop response shown in Figure 6.4, resulting in an improvement in the cost objective function value to 1052.2700 with no further changes in the setpoint trajectory required.

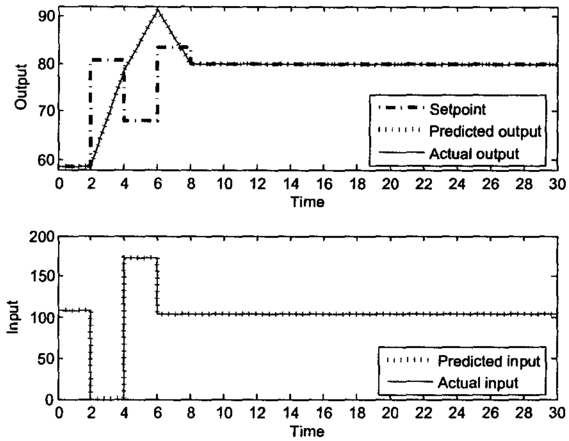


Figure 6.4: Reference trajectory update with step disturbance estimate

Thus updating the reference trajectory was capable of improving the cost performance objective function using a bias update on process model predictions for step disturbances in the measured output. An improvement of 38.44% of total benefits was realized as calculated by

$$IMPROVEMENT = \frac{Actual}{TotalPossible} = \frac{1129.5924 - 1052.2700}{1129.5924 - 928.4421} = 0.3844 \tag{6.3}$$

6.1.2 Model Mismatch

While the bias update may handle step disturbances in the output effectively, the performance of updating the reference trajectory may deteriorate in the presence of uncertainty in the form of input disturbances, structural model mismatch and parametric model mismatch. Thus, the effects of parametric model mismatch was investigated where the process model used within constrained model predictive control and for reference management was based on Equation 6.1, while the actual process may be described by

$$G_p(s) = \frac{-0.6191e^{-2s}}{6.1024s + 1} \tag{6.4}$$

The process gain was underestimated by approximately 47.72%, thus resulting in overshoot arising from a more aggressive closed-loop response. The implementation of the nominal setpoint trajectory on the actual system with model mismatch is shown in Figure 6.5, resulting in a cost objective function value of 1544.7404 based on the squared deviation between the actual output and target every 2 time units for 50 time units.

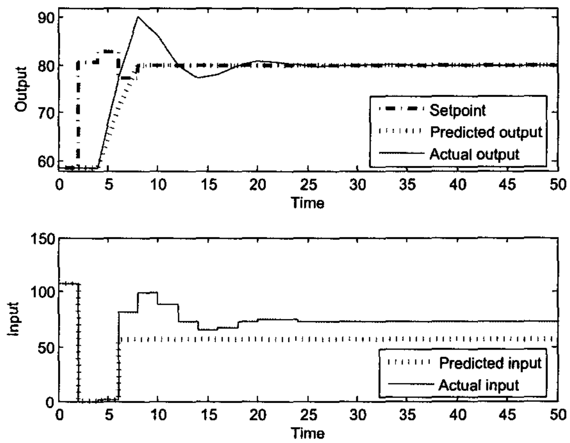


Figure 6.5: Implementation on the actual system with model mismatch

Assuming a perfect model was available, the best achievable performance possible resulted in a cost objective function value of 1397.2393 using the discretized process transfer function corresponding to Equation 6.4 within calculations for reference management:

$$y(k+1) = 0.7206y(k) - 0.173u(k-1) \tag{6.5}$$

Reference management without model mismatch resulted in the closed-loop response shown in Figure 6.6.

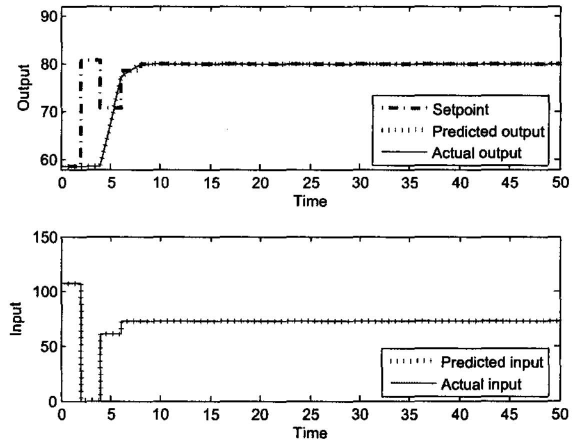


Figure 6.6: Optimal reference trajectory with perfect model

However, given model mismatch, the reference trajectory was subsequently updated online to account for gain mismatch by bias updating. The reference trajectory was updated after implementation of the first setpoint change, but coincided with the previous predicted trajectory since the disturbance estimate was zero as a result of process delay.

Note that the objective function was based on minimizing the squared deviation between the output and target using simultaneous optimization. Additional constraints were enforced to define previous setpoint changes, measured outputs and implemented inputs, while removing the corresponding process equations defining their relationships. This was required to prevent overspecification of constraints while reducing computational expense and enabling a consistent process model to be used throughout the simulation horizon within the supervisory controller. Conceptually, the degrees of freedom consist of the setpoint, input, output or disturbance vectors, only 2 of which are required to be specified for a unique solution to be defined. Additional specifications may result in infeasibility, and difficulty in convergence as a result of inconsistent constraints due to tolerances in numerical precision.

Subsequent to implementation of the first setpoint change, the disturbance estimate of $\hat{d} = 6.0353$ was assumed to be constant through the remaining simulation and represented a positive step disturbance. The closed-loop response is shown in Figure 6.7, assuming the entire remaining trajectory is implemented without further model updating. The optimal solution attempted to reduce the effect of a positive disturbance by reducing the setpoint, and resulted in a cost objective function value of 1514.0942.

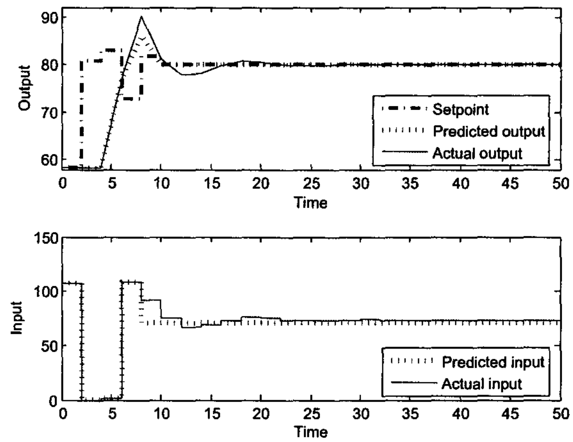


Figure 6.7: Second model update enforcing 2 setpoint changes

The third model update was performed after implementing the next setpoint change, and a cumulative positive disturbance was estimated at $\hat{d} = 10.2699$. Note that the current disturbance estimate was based on the difference between the predicted output within the supervisory controller and the actual measured output from the plant at the current time. However, the cumulative disturbance estimate would be required for the next model update since the current output prediction is based on the assumption of a constant step disturbance in the output using the previous disturbance estimate. The resulting closed-loop response is shown in Figure 6.8, assuming the entire remaining trajectory is implemented without further feedback for model updating. The implementation of the optimal solution resulted in a cost objective function value of 1538.1094.

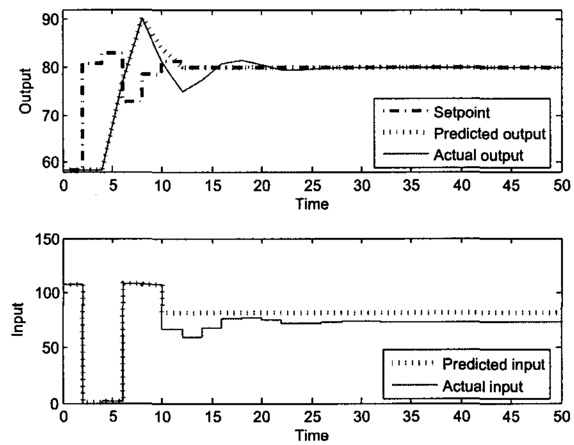


Figure 6.8: Third model update enforcing 3 setpoint changes

The benefit of successive model updates were progressively smaller, and the ninth model update resulted in near convergence as shown in Figure 6.9, assuming the entire remaining trajectory is implemented without further feedback for model updating.

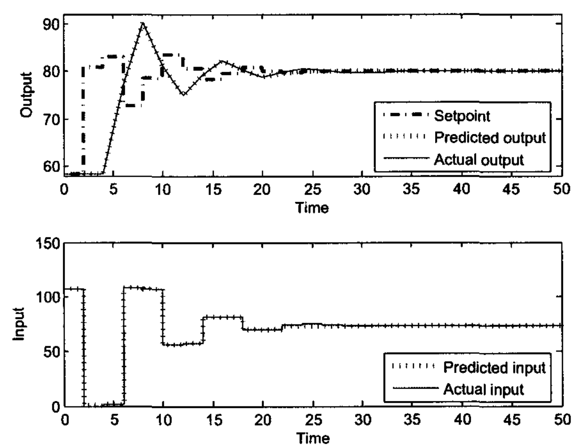


Figure 6.9: Ninth model update enforcing 9 setpoint changes

The implementation of the optimal solution resulted in a cost objective function value of 1536.1840, representing an improvement of 5.80% of total benefits being realized as calculated by

$$IMPROVEMENT = \frac{Actual}{TotalPossible} = \frac{1544.7404 - 1536.1840}{1544.7404 - 1397.2393} = 0.0580 \quad (6.6)$$

Thus the improvement realized by updating the reference trajectory through bias updating was less effective in the presence of model mismatch than for step disturbances. However both simulations indicated the possible advantages of online updating due to the presence of uncertainty arising from unmeasured disturbances and model mismatch, namely to improve performance towards the theoretical optimum during transient operation.

6.1.3 Pulse Disturbances

A large pulse disturbance $d = -25$ with a duration of 4 time units was simulated at time unit 4 causing temporary input saturation during the steady-state transition to $y_{tgt} = 80$. Implementation of the nominal setpoint trajectory on the actual system is shown in Figure 6.10, resulting in a cost objective function value of 4301.9270.

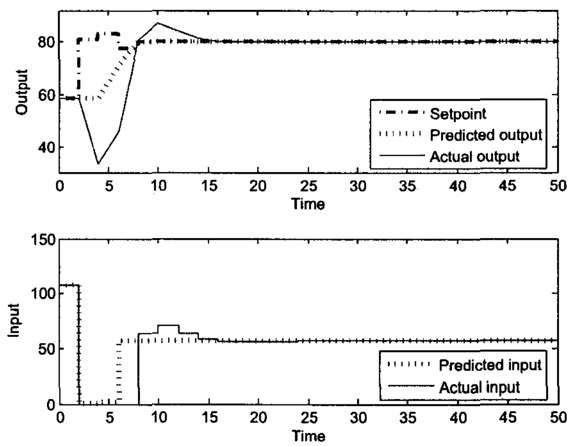


Figure 6.10: Implementation on actual system with pulse disturbance

The best achievable performance was determined with a cost objective function value of 4250.8433 assuming the disturbance realization is known in advance. The closed-loop response is shown in Figure 6.11.

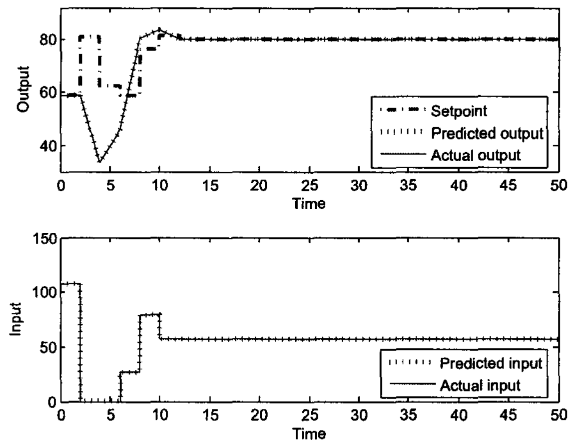


Figure 6.11: Reference trajectory with pulse disturbance under perfect model

However, in the presence of the unmeasured pulse disturbance, an online optimization after implementation of the first step change resulted in a large negative disturbance estimate of $\hat{d} = -25$, assumed to be constant in the future. Steady-state offset from target at $y_{sp} = 78.7479$ was required to ensure feasibility due to predicted input saturation as seen in Figure 6.12, assuming the entire remaining trajectory is implemented without further feedback for model updating. The implementation of the optimal solution resulted in an increase in the cost objective function value to 4576.0026, as a result of the predicted input saturation based on the disturbance estimate obtained using bias updating.

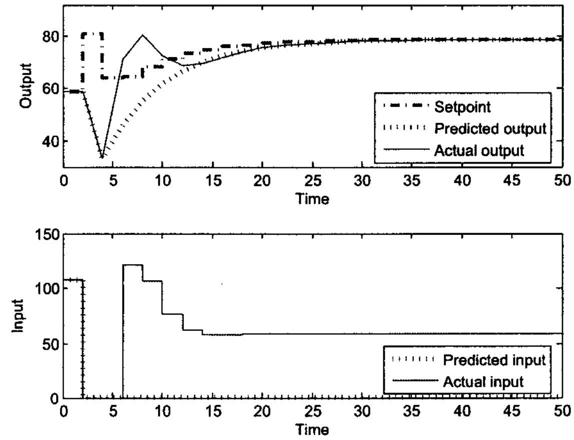


Figure 6.12: First model update enforcing 1 setpoint change to pulse disturbance

The second model update after implementing the first two step changes did not significantly alter the reference trajectory due to minimal changes in the disturbance estimate. However, within the next bias update, the system returned to target specifications since the cumulative disturbance estimate was reduced to $\hat{d} = -0.0026$, and the resulting closed-loop response shown in Figure 6.13.

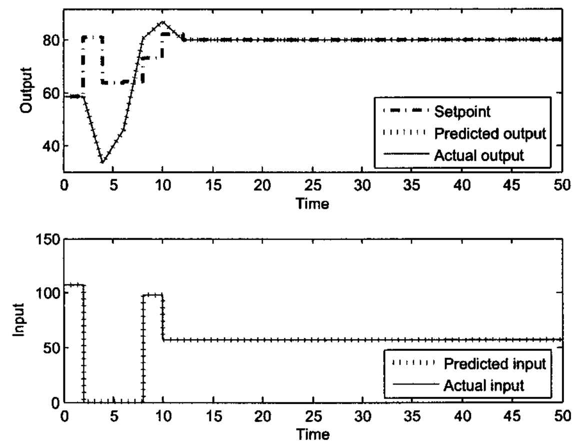


Figure 6.13: Third model update enforcing 3 setpoint changes to pulse disturbance

The implementation of the optimal solution resulted in a cost objective value of 4283.8866, and an overall improvement of 35.32% as calculated according to Equation 6.7.

$$IMPROVEMENT = \frac{Actual}{TotalPossible} = \frac{4301.9270 - 4283.8866}{4301.9270 - 4250.8433} = 0.3532 \quad (6.7)$$

6.2 Multi-Input Multi-Output Systems

The online adjustment of the reference trajectory was investigated to improve operation for the polymerization case study presented in Section 5.5. The optimal setpoint trajectory was determined based on minimizing the squared deviation between the outputs from target with suitable hard output constraints defined arising from economic considerations. The application of the offline optimal reference trajectory determined based on a linear process model on the nonlinear system resulted in model mismatch with undesirable characteristics in the closed-loop response, as shown in Figure 5.10.

The updating strategy at the current time was based on the measured outputs, and the assumption of independent step disturbances in the output. The additional constraints include the current measured output and the current input implemented, while the setpoint change implemented over the next sampling period was determined in addition to the remaining setpoint trajectory through reference management.

6.2.1 Online Reference Management

The reference trajectory was optimized online after implementation of the first two setpoint changes using a bias update and assuming a constant step disturbance in the number average molecular weight of $\hat{d}_1 = -1.8480$ kg/mol and in the reactor temperature of $\hat{d}_1 = 0.0462$ K over the simulation horizon. The implementation of the updated setpoint trajectory is shown in Figure 6.14, assuming no further updates.

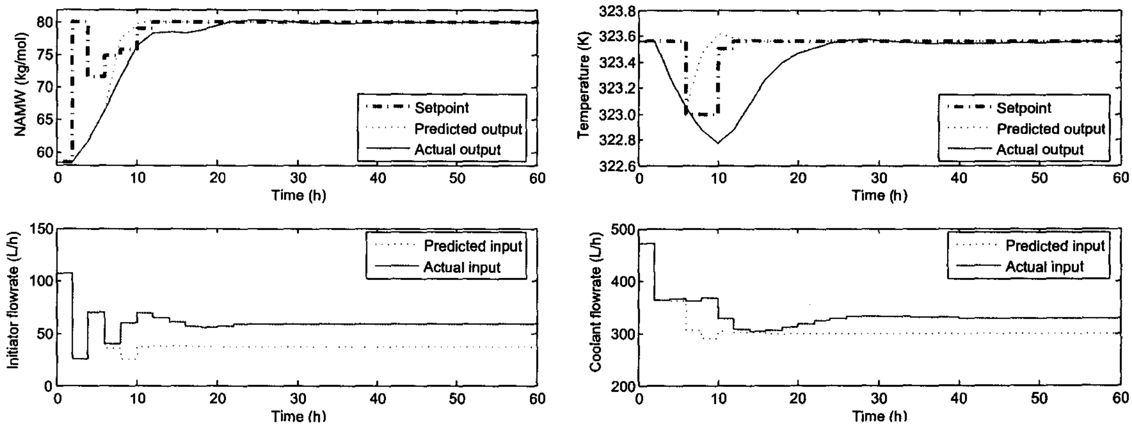


Figure 6.14: First model update enforcing two setpoint changes

However, online updating with aggressive setpoint manipulation in the presence of model mismatch may deteriorate the closed-loop performance as a result of poor predictions in the closed-loop response despite the use of a bias update. The closed-loop response shown for seven updates in Figure 6.15, may be compared to implementation of the offline optimal solution in Figure 5.10.

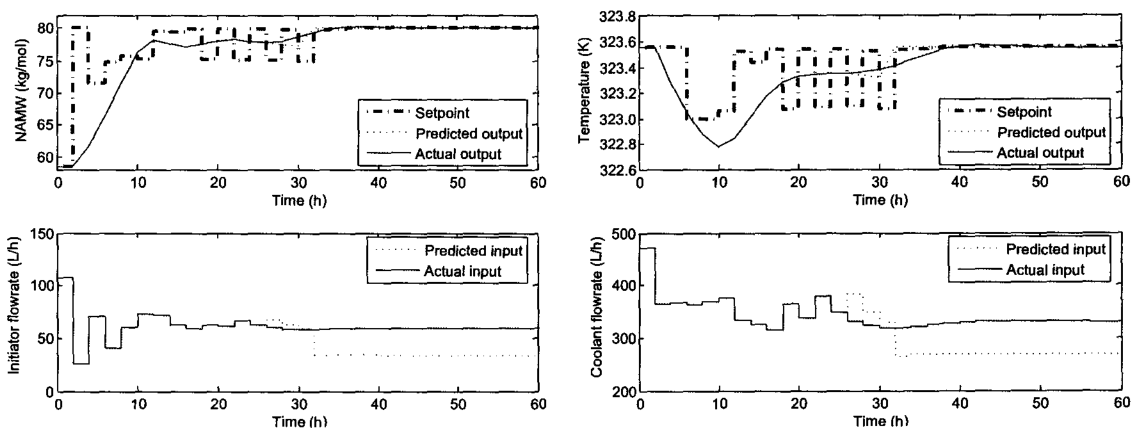


Figure 6.15: Seventh model update enforcing fourteen setpoint changes

6.2.2 Enforcing the Successive Setpoint Change

The online strategy was modified by implementing at each update, the setpoint as calculated in the previous re-optimization calculation. The update procedure was carried out every second sampling period.

The reference trajectory was optimized online after implementation of the first setpoint change using a bias update and assuming a constant step disturbance in the number average molecular weight of $\hat{d}_1 = 2.5436$ kg/mol and in the reactor temperature of $\hat{d}_1 = 0.1573$ K over the simulation horizon. The implementation of the updated setpoint trajectory is shown in Figure 6.16, assuming no further updates.

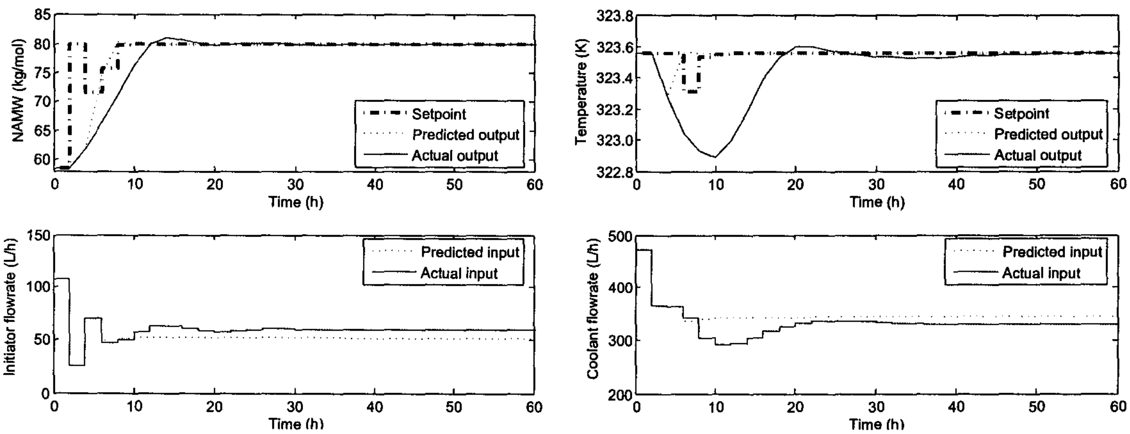


Figure 6.16: First model update enforcing two setpoint changes

Within the fifth model update, the disturbance estimate is negligible and the predicted and actual outputs converge. The implementation of the updated setpoint trajectory is shown in Figure 6.17, assuming no further updates.

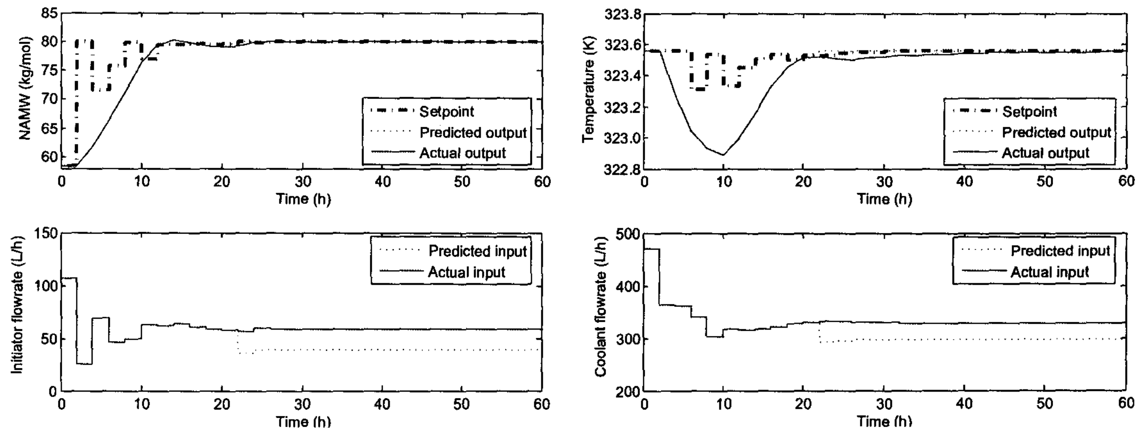


Figure 6.17: Fifth model update enforcing ten setpoint changes

There is only a slight improvement in the closed-loop response but the desired setpoint target was obtained. In contrast, the predicted and actual final steady-state input values did not correspond since uncertainty in the controlled variables arising from model mismatch was shifted to the manipulated variables. The predicted steady-state input values were determined within the supervisory controller based on a linear time-invariant model of the nonlinear system. Thus using the approximate linear closed-loop dynamic model with the given bias update strategy did not satisfy point-wise model adequacy (Forbes and Marlin, 1994; Forbes et al., 1994; Forbes, 1994), but the benefit of alternative disturbance estimation strategies such as closed-loop model identification and parameter estimation was not explored.

The enforcement of the following setpoint change based on the previous solution was capable of improving the closed-loop response by comparison of Figures 6.15 and 6.17. The additional constraint was believed to have reduced the sensitivity of the cascade control system by restricting aggressive manipulation of the setpoint trajectory in the presence of uncertainty.

6.2.3 Effect of Increasing Frequency of Re-optimization

Increasing the frequency of re-optimization may not necessarily result in an improvement in the closed-loop response despite a more frequent disturbance update. The update procedure was carried out every sampling period.

The setpoint trajectory was updated after implementation of the first setpoint change using a bias update and assuming a constant step disturbance in the number average molecular weight of $\hat{d}_1 = -2.8633$ kg/mol and in the reactor temperature of $\hat{d}_1 = 0.2250$ K over the simulation horizon. The implementation of the updated setpoint trajectory is shown in Figure 6.18, assuming no further updates.

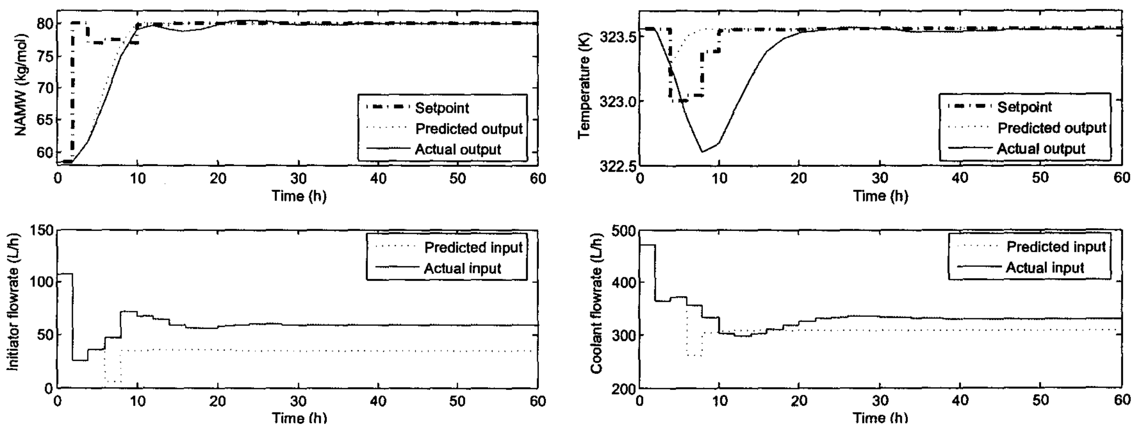


Figure 6.18: First model update enforcing one setpoint change

The closed-loop response after the tenth model update is shown in Figure 6.19, assuming no further updates. However, the performance has deteriorated in comparison to Figure 6.17. Thus, increasing the frequency of re-optimization may not necessarily result in an improvement in performance since the predicted optimal changes in the setpoint trajectory may actually introduce additional disturbances into the closed-loop system due to model mismatch.

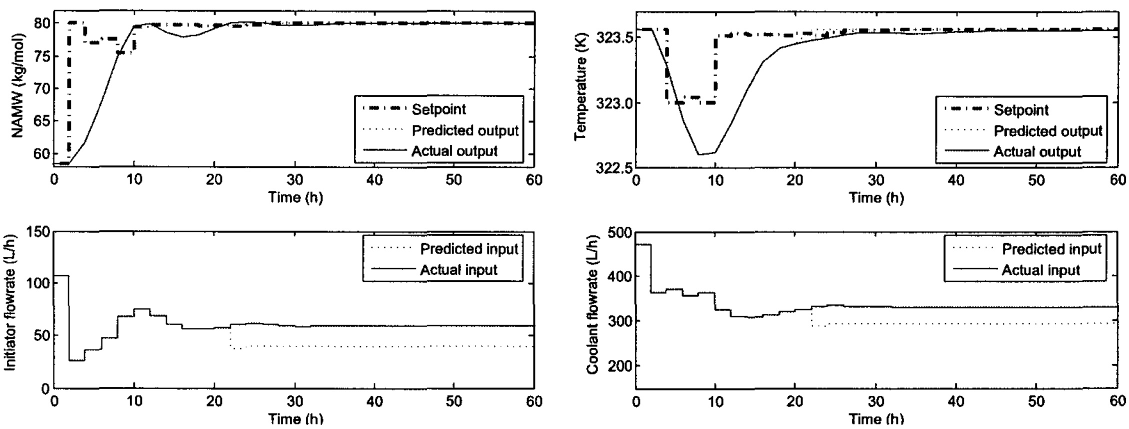


Figure 6.19: Tenth model update enforcing ten setpoint changes

6.3 Summary of Results

This chapter detailed the online implementation of the proposed methodology using a bias update for disturbance estimation. The bias update was based on the difference between the predicted and actual output, as used in steady-state economic optimization (Brosilow and Zhao, 1988; Yousfi and Tourier, 1991; Forbes, 1994). The efficiency of the scheme was demonstrated on a single-input single-output system under step disturbances, model mismatch and pulse disturbances. However, application to a nonlinear multi-input multi-output system using a linear model with bias updating, was shown to possibly worsen closed-loop performance.

The online implementation of the proposed methodology may not necessarily yield significant improvement in operation. Abel and Marquardt (2000) and Abel and Marquardt (2003) investigated the optimal operation of an industrial polymerization reactor in the presence of sudden changes in product pricing, but discovered online solutions were similar to offline solutions. Thus, the implementation of offline optimal solutions may be acceptable with minimal loss in performance.

Chapter 7

Conclusions and Recommendations

7.1 Conclusions

Reference management with consideration of constrained model predictive control was proposed to determine the setpoint trajectory required to achieve feasible and optimal operation during steady-state transitions. The supervisory controller required the solution of an optimization problem where an economic or dynamic performance objective function was considered at the upper level, and a series of control performance objective functions corresponding to the regulatory controller at the lower level. The mathematical formulation of the resulting multi-level optimization problem was described and a solution strategy developed based on a simultaneous approach using interior point methods. The benefits of the simultaneous compared to the sequential approach was demonstrated in terms of solution reliability and reduced computational expense, particularly in the presence of input saturation. The methodology was demonstrated on single-input single-output and multi-input multi-output systems with linear and non-linear dynamics in addition to a system with non-minimum phase characteristics.

One of the proposed formulations was based on a quadratic dynamic performance objective function minimizing the production of off-specification product. Minimizing the squared deviation between the *setpoint* and target resulted in a similar closed-loop response to that obtained by minimizing the squared deviation between the *output* and target, but without requiring a two-tiered approach to reduce setpoint variability arising from indeterminacy. The effect of various constraint formulations on the optimal solution was investigated, and the discrete reference filter shown to result with suitable constraints on the setpoint trajectory.

The second proposed formulation was based on the explicit consideration of economics during transient operation. Univariate product quality specification bands were modelled using switching functions and a control performance objective incorporated to improve solution convergence to the desired steady-state. Application to a polymerization system was capable of reducing the transition cost, and further improvement in economic operation was demonstrated with the manipulation of additional degrees of freedom.

Finally, a feedback mechanism was incorporated into the proposed methodology for updating the setpoint trajectory online in the presence of disturbances and model mismatch. The bias update scheme resulted in an improvement in performance compared to tracking the offline optimal setpoint trajectory, particularly for step output disturbances in a linear system.

7.2 Recommendations for Future Work

7.2.1 State-Space Model Predictive Control

The step response model may be formulated into state-space model predictive control (Ricker, 1991), and may result in reduced computational expense and improved performance arising from state-space identification techniques such as Kalman filtering (Li et al., 1989) and the extended Kalman filter (Lee and Ricker, 1994). A significant advantage of the state-space formulation is the capability to control open-loop unstable systems, and to improve closed-loop performance with flexibility in disturbance modelling. The sluggish performance, particularly in the presence of disturbances affecting the output through slow dynamics, is a direct result of the disturbance assumption in dynamic matrix control (Morari and Lee, 1991). Thus, reference management under state-space model predictive control may enable extensions to additional applications for improved dynamic performance.

7.2.2 Application to Startups and Shutdowns

Ensuring feasibility and optimality during startups and shutdowns is a particularly important, yet challenging area for the application of advanced process control in industry. Application of the methodology to startups and shutdowns is complicated by the need to consider plantwide dynamics (Verwijs et al., 1995) with material recycle, energy integration and inventory considerations (Luyben, 2004). Operation during startups and shutdowns are typically implemented open-loop and procedures followed carefully, particularly for polymerization systems characterized by exothermic reactions to prevent reactor runaway (Choi and Ray, 1985). However, significant improvement in performance may be possible if implemented successfully.

7.2.3 Application to Batch Processes

Multi-product batch processes are well-suited for flexible operation required to respond to short time to market constraints and rapid changes in demand (Rippin, 1983). However, modelling is rarely developed due to excessive costs and minimum time to market, and current operation of industrial batch processes is based on heuristics determined through trial and error (Terwiesch et al., 1994). Furthermore, advanced control may constitute 10% of process control and automation activities in the batch industry (Bonvin, 1998), and thus limiting applications of the proposed methodology in industry.

7.2.4 Multivariate Quality Specifications

According to MacGregor and Kourti (1998), product quality is a multivariate property and thus, multivariate specification regions are the ultimate objective function for multivariate control. However, according to Clarke-Pringle and MacGregor (1998) and Clarke-Pringle (1999), the indirect control of product quality by controlling a subset of quality variables is typical due to the high correlation between quality variables, particularly in polymerization, but may result in the inflation of the effect of disturbances onto the uncontrolled quality space. Thus the consideration of the multivariate nature of product quality is important to realize improvement in the control of end-use properties through optimization.

7.2.5 Integration of Optimization, Control and Design

While there are increasing benefits of reducing conservatism in competitive markets, significant investment in developing and maintaining advanced control may be required relative to the economic loss resulting from overdesign to provide margins of safe operation (Seider et al., 1990). Thus, the integration of control and design is important in evaluating the potential improvement in performance for various design configurations. For example, Chatzidoukas et al. (2003) investigated the optimal control structure pairing and operating policy for grade transitions in polymerization by solving a mixed integer dynamic optimization problem, reducing the transition time by 17.7% and the amount of off-specification product by 15%. Thus, to improve economic operation during transient operation, the proposed methodology may be extended to consider integrated control and design.

In addition to design considerations, improvement in dynamic operation is possible with integration into real time optimization and production scheduling, and particularly important in response to instantaneous demand. However, incorporation of the proposed methodology into higher level optimization is complicated by successive application of the first order optimality conditions. An alternative strategy was investigated by Tousain (2002), Bosgra et al. (2004) and Tousain and Bosgra (2006) to determine economic market oriented scheduling of high density linear polyethylene grade transitions considering market demand with long term and short term commitments, market opportunities, inventory and product storage control and internal supply chain management. The optimal operating policies for grade transitions were computed offline using dynamic optimization, and subsequently modelled as discontinuous events using binary decision variables at specified time intervals, resulting in a mixed integer linear programming problem. The resulting flexible schedule was found to improve performance by 16.8% relative to a fixed duration production slate.

The simplification of using fixed changeover times in scheduling (Méndez and Cerdá, 2000; Mendéz and Cerdá, 2002; Giannelos and Georgiadis, 2002; Munawar et al., 2003), however, may not necessarily reflect current plant operation and would otherwise require frequent updating of look-up tables. Similar strategies are used in parametric programming for flexibility analysis in the optimal design problem by Bansal et al. (2000) and Bansal et al. (2002), and multi-parametric quadratic programming by Pistikopoulos et al. (2000) and Bemporad et al. (2000). But while convenient, the dimension would increase with consideration under various operating conditions.

7.2.6 Incorporation of Feedback

The proposed methodology was implemented online but possible extensions include application to multi-input multi-output systems and investigation of the effect of input disturbances. Possible benefits of closed-loop model identification and parameter updating compared to the bias update may also be investigated. Furthermore, the introduction of feedback into the cascade control system, may affect closed-loop stability although improvement may be possible due to the consideration of the closed-loop system. Similarities with reference governors and two degrees of freedom internal model control, and LP/QP-MPC may provide insight in the analysis of nominal closed-loop stability. However, consideration of the effect of uncertainty on robust stability represents a challenging area for future research.

7.2.7 Explicit Consideration of Uncertainty

Uncertainty within the framework presented may be handled by conservative output constraints or reserving additional capacity for disturbance rejection through conservative input constraints to maintain feasibility. However, the explicit consideration of uncertainty may improve closed-loop performance by reducing arbitrary conservatism introduced into constraint formulations. More importantly, consideration of uncertainty may improve economics operation during dynamic transitions.

Hessem and Bosgra (2002) proposed closed-loop model predictive control in the presence of stochastic disturbances to determine the optimal input and state backoff required to prevent violation of linear inequality constraints. The solution strategy involved the solution of second order cone programming solved using interior point methods, but was computationally expensive. Similarly, robust linear model predictive control without consideration of input saturation was investigated by Warren and Marlin (2003) and Warren and Marlin (2004), to determine the optimal setpoint and input trajectories based on the expected performance subject to the closed-loop propagation of worst-case disturbances handled through probabilistic constraint satisfaction. Conservatism in future output uncertainty was reduced compared to conventional min-max control by considering control compensation in future inputs and outputs.

The use of explicit uncertainty descriptions may improve closed-loop performance and extend the proposed methodology by considering robust performance, while retaining the separation of economic and control performance objectives.

7.2.8 Suitable Model Development for Optimization

The development of suitable models for optimization and control must ensure accurate prediction of the optimum with reasonable computational expense. This may require model reduction for online implementation with increasing frequency of re-optimization. According to Roos et al. (1997), transparency in process modelling is important for model development but resulting in superfluous variables and redundant constraints, increasing memory storage and the number of arithmetic operations per iteration. An improvement in the sparsity structure may reduce the number of iterations required, while compact model formulation in a minimal representation may significantly affect the computational speed of interior point algorithms.

In addition, there may be a well defined solution but the optimization problem may be poorly posed (Gill et al., 2004), and the formulation of constraints may affect the local optimum obtained in nonlinear programming (Tenny et al., 2004). The constraint formulation may assist the determination of worthwhile solutions by steering the system to more attractive local optima. These considerations were required for the successful application of real time optimization to a hydrocracking fractionation plant at Sunoco by Bailey et al. (1993). Similarly, there are several considerations in model development based on ensuring accurate prediction of the true optimum and suitable for efficient optimization with minimal computational expense, necessary for the successful application of the proposed methodology. In particular, an efficient mathematical formulation for the explicit consideration of economics in the objective function requires further investigation.

Appendix A

KKT Conditions for QDMC

The mathematical algorithm for quadratic dynamic matrix control is derived for a single-input single-output system as detailed in Bequette (2003) and Soliman (2005), and extended to consider penalty on input deviation from ideal resting values. The control performance objective function is given by,

$$\min_{\Delta u_f} \left(y_{sp} - \hat{y}\right)^T \Gamma^T \Gamma \left(y_{sp} - \hat{y}\right) + \left(u_{tgt} - u_f\right)^T \Lambda_{ss}^T \Lambda_{ss} \left(u_{tgt} - u_f\right) + \Delta u_f^T \Lambda^T \Lambda \Delta u_f \tag{A.1}$$

where $Q = \Gamma^T \Gamma \in \Re^{P \times P}$, $S = \Lambda_{ss}^T \Lambda_{ss} \in \Re^{M \times M}$ and $R = \Lambda^T \Lambda \in \Re^{M \times M}$ are positive definite matrices defining the relative weighting for the vector of predicted outputs $\hat{y} \in \Re^P$, optimal future inputs $u_f \in \Re^M$ and input moves $\Delta u_f \in \Re^M$. The vector of setpoints $y_{sp} \in \Re^P$ and ideal input resting values $u_{tgt} \in \Re^M$ are given by

$$y_{sp} = \begin{bmatrix} y_{sp,k+1} & \cdots & y_{sp,k+P} \end{bmatrix}^T \tag{A.2}$$

$$u_{tgt} = \begin{bmatrix} u_{tgt,k+1} & \cdots & u_{tgt,k+P} \end{bmatrix}^T \tag{A.3}$$

where the subscript k refers to the current time step and indicates a scalar variable. The objective function in Equation A.1 is subject to the following,

$$\hat{y} = S_{past}\Delta u_p + s_N u_p + S_f \Delta u_f + \hat{d} \tag{A.4}$$

$$y_{\min} \leq \hat{y} \leq y_{\max} \tag{A.5}$$

$$u_{\min} \leq u_f \leq u_{\max} \tag{A.6}$$

$$\Delta u_{\min} \leq \Delta u_f \leq \Delta u_{\max} \tag{A.7}$$

where $y \in \Re^P$, $u \in \Re^M$ and $\Delta u \in \Re^M$ with subscripts min and max represent vectors of the minimum and maximum bounds for the output, input and change in inputs respectively:

$$y_{\min} = \begin{bmatrix} y_{\min,k} & \cdots & y_{\min,k} \end{bmatrix}^T \tag{A.8}$$

$$y_{\max} = \begin{bmatrix} y_{\max,k} & \cdots & y_{\max,k} \end{bmatrix}^T \tag{A.9}$$

$$u_{\min} = \begin{bmatrix} u_{\min,k} & \cdots & u_{\min,k} \end{bmatrix}^T \tag{A.10}$$

$$u_{\max} = \begin{bmatrix} u_{\max,k} & \cdots & u_{\max,k} \end{bmatrix}^T \tag{A.11}$$

$$\Delta u_{\min} = \begin{bmatrix} \Delta u_{\min,k} & \cdots & \Delta u_{\min,k} \end{bmatrix}^T \tag{A.12}$$

$$\Delta u_{\max} = \begin{bmatrix} \Delta u_{\max,k} & \cdots & \Delta u_{\max,k} \end{bmatrix}^T \tag{A.13}$$

In the following development, inequality constraints on outputs and input changes are not further considered. The change in inputs are partitioned into previous input moves and future input moves, defined by

$$\Delta u_p = \begin{bmatrix} u_{k-1} \\ \vdots \\ u_{k-N+2} \end{bmatrix} - \begin{bmatrix} u_{k-2} \\ \vdots \\ u_{k-N+1} \end{bmatrix} = \begin{bmatrix} \Delta u_{k-1} \\ \vdots \\ \Delta u_{k-N+2} \end{bmatrix} \quad (A.14)$$

$$\Delta u_f = \begin{bmatrix} u_{k} \\ \vdots \\ u_{k+M-1} \end{bmatrix} - \begin{bmatrix} u_{k-1} \\ \vdots \\ u_{k+M-2} \end{bmatrix} = \begin{bmatrix} \Delta u_{k} \\ \vdots \\ \Delta u_{k+M-1} \end{bmatrix} \quad (A.15)$$

The vectors of inputs $u_p \in \Re^P$ and $u_f \in \Re^M$ are defined by

$$u_f = \begin{bmatrix} u_k & \cdots & u_{k+M-1} \end{bmatrix}^T = I_L \Delta u_f + u_L \quad (A.16)$$

$$u_p = \begin{bmatrix} u_{k-N+1} & \cdots & u_{k-N+P} \end{bmatrix}^T \quad (A.17)$$

where k represents the current time step, $I_L \in \Re^{M \times M}$ is the lower triangular identity matrix and $u_L \in \Re^M$ given by

$$I_L = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 1 & 1 & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ 1 & 1 & \cdots & 1 \end{bmatrix} \quad (A.18)$$

$$u_L = \begin{bmatrix} u_{k-1} & \cdots & u_{k-1} \end{bmatrix}^T \quad (A.19)$$

The predicted output is given by

$$\hat{y} = \begin{bmatrix} \hat{y}_{k+1} & \cdots & \hat{y}_{k+P} \end{bmatrix}^T \quad (A.20)$$

The estimated disturbance, with the standard assumption of uncorrelated integrated random walk disturbances in the outputs (Morari and Lee, 1991), is given by

$$\hat{d} = \begin{bmatrix} \hat{d}_{k+1} \\ \vdots \\ \hat{d}_{k+P} \end{bmatrix} = \begin{bmatrix} d_k \\ \vdots \\ d_k \end{bmatrix} = \begin{bmatrix} y_k - \hat{y}_k \\ \vdots \\ y_k - \hat{y}_k \end{bmatrix} \tag{A.21}$$

where y and $\hat{y}$ denote the actual measured and predicted outputs at the current time step k respectively, and the predicted disturbance $\hat{d} \in \Re^P$ is assumed to be constant over the prediction horizon P (Bequette, 2003). The dynamic matrix consisting of step response coefficients s_i, is partitioned as shown below,

$$S_{past} = \begin{bmatrix} s_2 & s_3 & \cdots & s_{N-2} & s_{N-1} \\ s_3 & s_4 & \cdots & s_{N-1} & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ s_{P+1} & s_{P+2} & \cdots & 0 & 0 \end{bmatrix}_{P \times N-2} \tag{A.22}$$

$$S_f = \begin{bmatrix} s_1 & 0 & \cdots & 0 & 0 \\ s_2 & s_1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ s_P & s_{P-1} & \cdots & s_{P-M+2} & s_{P-M+1} \end{bmatrix}_{P \times M} \tag{A.23}$$

where $S_{past} \in \Re^{P \times (N-2)}$ and $S_f \in \Re^{P \times M}$ denote dynamic matrices of previous and future step response coefficients s_i respectively. Thus reformulation of the optimization problem such that the decision variable is explicit in the objective function results in the following simplifications as detailed by Bequette (2003).

Let the vector of unforced errors, the future errors without implementing control move changes, be defined by

$$E = y_{sp} - \left[S_{past} \Delta u_p + s_N u_p + \hat{d} \right] \tag{A.24}$$

Thus, the objective function may be written as follows:

$$\min_{\Delta u_f} \Big[(E - S_f \Delta u_f)^T \Gamma^T \Gamma (E - S_f \Delta u_f) + (u_{tgt} - I_L \Delta u_f - u_L)^T \Lambda_{ss}^T \Lambda_{ss} (u_{tgt} - I_L \Delta u_f - u_L) + \Delta u_f^T \Lambda^T \Lambda \Delta u_f \Big] \tag{A.25}$$

Expansion of Equation A.25 and multiplying through by $\frac{1}{2}$ yields

$$\min_{\Delta u_f} \Big[\frac{1}{2} E^T \Gamma^T \Gamma E - E^T \Gamma^T \Gamma S_f \Delta u_f + \frac{1}{2} \Delta u_f^T S_f^T \Gamma^T \Gamma S_f \Delta u_f + \frac{1}{2} (u_{tgt} - I_L \Delta u_f - u_L)^T \Lambda_{ss}^T \Lambda_{ss} (u_{tgt} - I_L \Delta u_f - u_L) + \frac{1}{2} \Delta u_f^T \Lambda^T \Lambda \Delta u_f \Big] \tag{A.26}$$

Omitting the constant terms and rearranging Equation A.26 yields

$$\min_{\Delta u_f} \Big[\frac{1}{2} \Delta u_f^T \left(S_f^T \Gamma^T \Gamma S_f + \Lambda^T \Lambda \right) \Delta u_f - E^T \Gamma^T \Gamma S_f \Delta u_f + \frac{1}{2} (u_{tgt} - I_L \Delta u_f - u_L)^T \Lambda_{ss}^T \Lambda_{ss} (u_{tgt} - I_L \Delta u_f - u_L) \Big] \tag{A.27}$$

The input constraints are given by

$$u_{\min} \leq u_f = I_L \Delta u_f + u_L \leq u_{\max} \tag{A.28}$$

Equation A.28 may be rearranged to the form given by

$$-I_L \Delta u_f \geq u_L - u_{\max} \tag{A.29}$$

$$I_L \Delta u_f \geq u_{\min} - u_L \tag{A.30}$$

Hence the objective function written in the form given by Equation A.27 in conjunction with Equations A.29-A.30 constitute a quadratic programming (QP) problem. However, the inequality constraints in Equations A.29-A.30 may be converted into equality constraints using slack variables $s_1, s_2 \geq 0 \in \Re^M$ as given below:

$$I_L \Delta u_f + u_L - u_{\max} + s_1 = 0 \in \Re^M \tag{A.31}$$

$$-I_L \Delta u_f + u_{\min} - u_L + s_2 = 0 \in \Re^M \tag{A.32}$$

$$\tag{A.33}$$

Thus the objective function in Equation A.27 subject to the process description given in Equations A.14-A.24 and constraints presented in Equations A.29-A.30 define input constrained model predictive control. The Lagrangian function L is subsequently defined by

$$\begin{aligned} L = \frac{1}{2}\Delta u_f^T \left(S_f^T \Gamma^T \Gamma S_f + \Lambda^T \Lambda\right) \Delta u_f - E^T \Gamma^T \Gamma S_f \Delta u_f \\ + \frac{1}{2}\left(u_{tgt} - I_L \Delta u_f - u_L\right)^T \Lambda_{ss}^T \Lambda_{ss} \left(u_{tgt} - I_L \Delta u_f - u_L\right) \\ + \lambda_1^T \left(I_L \Delta u_f + u_L - u_{\max} + s_1\right) \\ + \lambda_2^T \left(-I_L \Delta u_f + u_{\min} - u_L + s_2\right) - \lambda_3^T s_1 - \lambda_4^T s_2 \end{aligned} \tag{A.34}$$

with equality lagrange multipliers $\lambda_1, \lambda_2 \in \Re^M$ and inequality lagrange multipliers $\lambda_3, \lambda_4 \geq 0 \in \Re^M$. Thus, the optimization problem may be reformulated into a set of algebraic equations using the Karush-Kuhn-Tucker (KKT) conditions shown below,

$$JL\left(\Delta u_f, \lambda_1, \lambda_2, s_1, s_2\right) = \left[\begin{array}{ccccc} J_1^T & J_2^T & J_3^T & J_4^T & J_5^T \end{array}\right]^T = 0 \in \Re^{5 \times M} \tag{A.35}$$

$$J_1 = \Delta u_f^T \left(S_f^T \Gamma^T \Gamma S_f + \Lambda^T \Lambda\right) - E^T \Gamma^T \Gamma S_f \\ - \left(u_{tgt} - I_L \Delta u_f - u_L\right)^T \Lambda_{ss}^T \Lambda_{ss} I_L + \lambda_1^T I_L - \lambda_2^T I_L \tag{A.36}$$

$$J_2 = \left(I_L \Delta u_f + u_L - u_{\max} + s_1\right)^T \tag{A.37}$$

$$J_3 = \left(-I_L \Delta u_f + u_{\min} - u_L + s_2\right)^T \tag{A.38}$$

$$J_4 = \left(\lambda_1 - \lambda_3\right)^T \tag{A.39}$$

$$J_5 = \left(\lambda_2 - \lambda_4\right)^T \tag{A.40}$$

where JL refers to the Jacobian of the Lagrangian. Furthermore, from the above conditions, $\lambda_1 = \lambda_3$ and $\lambda_2 = \lambda_4$. The complementarity conditions are given by

$$\lambda_3^T s_1 = 0 \tag{A.41}$$

$$\lambda_4^T s_2 = 0 \tag{A.42}$$

$$(\lambda_3, \lambda_4, s_1, s_2) \geq 0 \in \Re^M \tag{A.43}$$

Thus the first order optimality conditions may be subsequently used to solve for the optimal input changes in constrained model predictive control.

List of References

Abel, O., Helbig, A., Marquardt, W., Zwick, H., and Daszkowski, T. (2000). Productivity optimization of an industrial semi-batch polymerization reactor under safety constraints. *Journal of Process Control*, 10:351–362.

Abel, O. and Marquardt, W. (2000). Scenario integrated modelling and optimization of dynamic systems. *AIChE Journal*, 46(4):803–823.

Abel, O. and Marquardt, W. (2003). Scenario-integrated online optimization of batch reactors. *Journal of Process Control*, 13(8):703–715.

Alhammadi, H. and Romagnoli, J. (2004). *The Integration of Process Design and Control*, volume 17 of *Computer Aided Chemical Engineering (CACE) Series*, chapter Process design and operation: Incorporating environmental, profitability, heat integration and controllability considerations, pages 264–305. Elsevier Inc., San Diego, CA.

Angeli, D., Casavola, A., and Mosca, E. (1998). Enforcing constraints in an industrial control systems: Command governor tools. In *Proceedings of the 1998 IEEE International Conference on Control Applications*, volume 2, pages 746–750, Trieste, Italy.

Angeli, D., Casavola, A., and Mosca, E. (1999). Command governors for constrained nonlinear systems: Direct nonlinear vs. linearization based strategies. *International Journal of Robust and Nonlinear Control*, 9(10):677–699.

Angeli, D., Casavola, A., and Mosca, E. (2000). *Nonlinear model predictive control*, chapter A predictive command governor for nonlinear systems under constraints, pages 115–128. Birkhauser Verlag.

Angeli, D., Casavola, A., and Mosca, E. (2001). On feasible set membership state estimators in constrained command governors. *Automatica*, 37(1):151–156.

Backx, T. (2002). Model requirements for the next generation integrated mpc and dynamic optimization. In Rawlings, J., Ogunnaike, B., and Eaton, J., editors, *Proceedings of the 6th International Conference on Chemical Process Control*, volume 98 of *AIChE Symposium Series*, pages 43–54.

Backx, T., Bosgra, O., and Marquardt, M. (1998). Towards intentional dynamics in supply chain conscious process operations. In *FOCAPO 98*.

Backx, T., Bosgra, O., and Marquardt, W. (2000). Integration of model predictive control and optimization of processes. In *IFAC Symposium Advanced Control of Chemical Processes ADCHEM Conference Proceedings*, volume 1, pages 249–260.

Bahri, P., Bandoni, J., Barton, G., and Romagnoli, J. (1995). Backoff calculations in optimizing control: A dynamic approach. *Computers and Chemical Engineering*, 19:S699–S708.

Bahri, P., Bandoni, J., and Romagnoli, J. (1996a). Effect of disturbance in optimizing control: Steady-state open loop backoff problem. *AIChE Journal*, 42(4):983–995.

Bahri, P., Bandoni, J., and Romagnoli, J. (1997). Integrated flexibility and controllability analysis in design of chemical processes. *AIChE Journal*, 43(4):997–1015.

Bahri, P., Bondoni, J., and Romagnoli, J. (1996b). Operability assessment in chemical plants. *Computers and Chemical Engineering*, 20:S787–S792.

Bailey, J., Hrymak, A., Treiber, S., and Hawkins, R. (1993). Nonlinear optimization of a hydrocracker fractionation plant. *Computers and Chemical Engineering*, 17(2):123–138.

Baker, R. (2004). Personal communication. McMaster University.

Baker, R. and Swartz, C. (2004a). Inclusion of actuator saturation as complementarity constraints in integrated design and control. In Shah, S. and MacGregor, J., editors, *7th Symposium on Dynamics and Control of Process Systems*, Cambridge.

Baker, R. and Swartz, C. (2004b). Simultaneous solution strategies for inclusion of input saturation in the optimal design of dynamically operable plants. *Optimization and Engineering*, 5(1):5–24.

Baker, R. and Swartz, C. (2005). Interior point solution of multi-level qp problems arising in embedded mpc formulations. In *AIChE Conference*, Cincinnati.

Bandoni, J., Romagnoli, J., and Barton, G. (1994). On optimizing control and the effect of disturbances: Calculation of the open-loop backoffs. *Computers and Chemical Engineering*, 18:S505–509.

Bansal, V., Perkins, J., and Pistikopoulos, E. (2000). Flexibility analysis and design of linear systems by parametric programming. *AIChE Journal*, 46(2):335–354.

Bansal, V., Perkins, J., and Pistikopoulos, E. (2002). Flexibility analysis and design using a parametric programming framework. *AIChE Journal*, 48(12):2851–2868.

Bathazaar, A. (2005). Dynamic optimization of multi-unit systems under failure conditions. Master's thesis, McMaster University, Hamilton, Canada.

Becerra, V., Roberts, P., and Griffiths, G. (1998). Novel developments in process optimization using predictive control. *Journal of Process Control*, 8(2):117–138.

Bell, M. and Sargent, R. (2000). Optimal control of inequality constrained dae systems. *Computers and Chemical Engineering*, 24(11):2385–2404.

Bemporad, A. (1998a). Reducing conservativeness in predictive control of constrained systems with disturbances. In *Proceedings of the IEEE Conference on Decision and Control*, pages 1384–1389.

Bemporad, A. (1998b). Reference governor for constrained nonlinear systems. *IEEE Transactions on Automatic Control*, 43(3):415–419.

Bemporad, A., Casavola, A., and Mosca, E. (1997). Nonlinear control of constrained linear systems via predictive reference management. *IEEE Transactions on Automatic Control*, 42(3):340–349.

Bemporad, A., Casavola, A., and Mosca, E. (1998). Predictive reference governor for constrained control systems. *Computers in Industry*, 36(1-2):55–64.

Bemporad, A., Morari, M., Dua, V., and Pistikopoulos, E. (2000). Explicit solution of model predictive control via multi-parametric quadratic programming. In *Proceedings of the American Control Conference*, pages 872–876.

Bemporad, A., Morari, M., and Ricker, N. (2004). *Model predictive control toolbox for use with MatLab: User's guide*. The MathWorks Inc., Natick, MA, second edition.

Bemporad, A. and Mosca, E. (1994a). Constraint fulfillment in control systems via predictive reference management. In *Proceedings of the 33rd IEEE Conference on Decision and Control*, pages 3017–3022.

Bemporad, A. and Mosca, E. (1994b). Constraint fulfillment in control systems via predictive reference management. In *Proceedings of the IEEE Conference on Control Applications*, pages 1909–1914.

Bemporad, A. and Mosca, E. (1995). Nonlinear predictive reference governor for constrained control systems. In *Proceedings of the IEEE Conference on Decision and Control*, pages 1205–1210.

Bemporad, A. and Mosca, E. (1998). Fulfilling hard constraints in uncertain linear systems by reference managing. *Automatica*, 34(3):451–461.

BenAmor, S., Doyle, F. I., and McFarlane, R. (2004). Polymer grade transition control using advanced real time optimization software. *Journal of Process Control*, 14:349–364.

Bequette, B. (2003). *Process control: Modelling, design and simulation*, chapter Model predictive control, pages 487–519. Prentice Hall, Upper Saddle River, NJ.

Bequette, B. W. (1991). Nonlinear control of chemical processes: A review. *Ind. Eng. Chem. Res.*, 30:1391–1413.

Besl, H., Kossman, W., Crowe, T., and Caracotsios, M. (1998). Non-traditional optimization for isom unit improves profits. *The Oil and Gas Journal*, 96(19):61–65.

Biegler, L. (1984). Solution of dynamic optimization problems by successive quadratic programming and orthogonal collocation. *Computers and Chemical Engineering*, 8(3-4):243–248.

Biegler, L. (1998). Advances in nonlinear programming concepts for process control. *Journal of Process Control*, 8(5-6):301–311.

Biegler, L. (2000). *Nonlinear model predictive control*, chapter Efficient solution of dynamic optimization and NMPC problems, pages 219–242. Birkhauser Verlag, Boston.

Biegler, L., Cervantes, A., and Wächter, A. (2002). Advances in simultaneous strategies for dynamic process optimization. *Chemical Engineering Science*, 57(4):575–593.

Bloss, K., Biegler, L., and Schiesser, W. (1999). Dynamic process optimization through adjoint formulations and constraint aggregation. *Ind. Eng. Chem. Res.*, 38(2):421–432.

Bonvin, D. (1998). Optimal operation of batch reactors- a personal view. *Journal of Process Control*, 8(5-6):355–368.

Bonvin, D., Srinivasan, B., and Ruppen, D. (2002). Dynamic optimization in the batch chemical industry. In Rawlings, J., Ogunnaike, B., and Eaton, J., editors, *Proceedings of the 6th International Conference on Chemical Process Control*, volume 98 of *AIChE Symposium Series*, pages 255–273.

Bosgra, O., Tousain, R., and Hessem, D. v. (2004). Market-oriented scheduling, economic optimization and stochastic control of continuous multi-grade chemical processes. In Shah, S. and MacGregor, J. F., editors, *The 7th International Conference on Dynamics and Control of Process Systems DYCOPS7-2004*.

Brempt, W., Backx, T., Ludlage, J., Overschee, P., Moor, B., and Tousain, R. (2001). A high performance model predictive controller: Application on a polyethylene gas phase reactor. *Control Engineering Practice*, 9(8):829–835.

Brempt, W., Overschee, P., Backx, T., Ludlage, J., Hayot, P., Oostvogels, L., and Rahman, S. (2003). Grade change using inca model predictive controller: Applications on a dow polystyrene process model. In *Proceedings of the American Control Conference*, pages 5411–5416.

Brempt, W., Overschee, P., Backx, T., Moen, O., Kiparissides, C., and Chatzidoukas, C. (2004). Plantwide economical dynamic optimization: Application on a borealis borstar process model. In *7th Symposium on Advanced Control of Chemical Processes*, pages 825–831.

Brengel, D. and Seider, W. (1992). Coordinated design and control optimization of nonlinear processes. *Computers and Chemical Engineering*, 16(9):861–886.

Brosilow, C. (1990). Modular multivariable control applied to the shell heavy oil fractionator problem. In Prett, D., García, C., and Ramaker, B., editors, *The second shell process control workshop: Solutions to the shell standard control problem*, pages 367–373. Butterworth Publishers, Boston.

Brosilow, C. and Joseph, B. (2002). *Techniques of model based control*. Prentice Hall, New Jersey.

Brosilow, C. and Zhao, G. (1988). A linear programming approach to constrained multivariable process control. *Control and Dynamic Systems*, 27(3):141–181.

Byrd, R., Marazzi, M., and Nocedal, J. (2004). On the convergence of newton iterations to non-stationary points. *Mathematical Programming*, 99(1):127–148.

Byrd, R., Nocedal, J., and Waltz, R. (2003). Feasible interior point methods using slacks for nonlinear optimization. *Computational Optimization and Applications*, 26(1):35–61.

Calamai, G., Casavola, A., and Mosca, E. (2000). Command governor strategies for constrained control of an inverted pendulum. In *Proceedings of the 2000 IEEE International Conference on Control Applications*, pages 886–891, Anchorage.

Caldwell, J. and Dearwater, J. (1991). Model predictive control applied to fcc units. In Arkun, Y. and Ray, W., editors, *Proceedings of the Fourth International Conference on Chemical Process Control*, pages 319–334, New York. CACHE.

Campbell, J. (1985). Emulsion polymerization of styrene. Master's thesis, McMaster University, Hamilton, Canada.

Casavola, A. and Mosca, E. (1996). Reference governor for constrained uncertain linear systems subject to bounded input disturbances. In *Proceedings of the 35th IEEE Conference on Decision and Control*, volume 3, pages 3531–3536, Japan.

Casavola, A., Mosca, E., and Angeli, D. (2000). Robust command governors for constrained linear systems. *IEEE Transactions on Automatic Control*, 45(11):2071–2077.

Casavola, A., Mosca, E., and Papini, M. (2004). Control under constraints: An application of the command governor approach to an inverted pendulum. *IEEE Transactions on Control Systems Technology*, 12(1):193–204.

Cervantes, A., Tonelli, S., Brandolin, A., Bandoni, A., and Biegler, L. (2000). Large scale dynamic optimization of a low density polyethylene plant. *Computers and Chemical Engineering*, 24(2):983–989.

Cervantes, A., Tonelli, S., Brandolin, A., Bandoni, A., and Biegler, L. (2002). Large scale dynamic optimization for grade transitions in a low density polyethylene plant. *Computers and Chemical Engineering*, 26(2):227–237.

Chatzidoukas, C., Perkins, J., Pistikopoulos, E., and Kiparissides, C. (2003). Optimal grade transition and selection of feedback control loops in a gas phase polyolefin fbr using a mixed integer dynamic optimization approach. *Chemical Engineering Science*, 58:3643–3685.

Chen, T. and Vassiliadis, V. (2005). Inequality path constraints in optimal control: A finite iteration ϵ convergent scheme based on pointwise discretization. *Journal of Process Control*, 15(4):353–362.

Choi, K. and Ray, W. (1985). The dynamic behaviour of fluidized bed reactors for solid catalyzed gas phase olefin polymerization. *Chemical Engineering Science*, 40(12):2261–2279.

Clark, P. and Westerberg, A. (1990). Bi-level programming for steady-state chemical process design i: Fundamentals and algorithms. *Computers and Chemical Engineering*, 14(1):87–97.

Clarke-Pringle, T. (1999). *Product quality control in reduced dimension spaces*. PhD thesis, McMaster University.

Clarke-Pringle, T. and MacGregor, J. (1997). Nonlinear adaptive temperature control of multi-product, semi-batch polymerization reactors. *Computers and Chemical Engineering*, 21(12):1395–1409.

Clarke-Pringle, T. and MacGregor, J. (1998). Product quality control in reduced dimension spaces. *Ind. Eng. Chem. Res.*, 37:3992–4002.

Congalidis, J., Richards, J., and Ray, W. (1989). Feedforward and feedback control of a solution copolymerization reactor. *AIChE Journal*, 35(6):891–907.

Contreras-Dordelly, J. (1999). Steady-state optimization under uncertainty. Master's thesis, McMaster University, Hamilton, Canada.

Contreras-Dordelly, J. and Marlin, T. (2000). Control design for increased profit. *Computers and Chemical Engineering*, 24(2-7):267–272.

Cozewith, C. (1988). Transient response of continuous flow stirred tank polymerization reactors. *Computers and Chemical Engineering*, 34(2):272–282.

Crowley, T. and Choi, K. (1996). Online monitoring and control of a batch polymerization reactor. *Journal of Process Control*, 6(2-3):119–127.

Cuthrell, J. and Biegler, L. (1987). On the optimization of differential algebraic process systems. *AIChE Journal*, 33(8):1257–1270.

Cutler, C. and Perry, R. (1983). Real time optimization with multivariable control is required to maximize profits. *Computers and Chemical Engineering*, 7(5):663–667.

Dadebo, S., Bell, M., McLellan, P., and McAuley, K. (1997). Temperature control of industrial gas phase polyethylene reactors. *Journal of Process Control*, 7(2):83–95.

Datta, K. and Mohan, B. (1995). *Orthogonal Functions in Systems and Control*, volume 9 of *Advanced Series in Electrical and Computing Engineering*. World Scientific Publishing Company, London.

Debling, J., Han, G., Kuijpers, F., VerBurg, J., Zacca, J., and Ray, W. (1994). Dynamic modelling of product grade transitions for olefin polymerization processes. *AIChE Journal*, 40(3):506–520.

Doyle, F., Ogunnaike, B., and Pearson, R. (1995). Nonlinear model based control using second order volterra models. *Automatica*, 31(5):697–714.

Duff, I. (2004). Harwell subroutine library (hsl) archives. Hyprotech UK Ltd.

Edgar, T. (2004). Control and operations: When does controllability equal profitability? *Computers and Chemical Engineering*, 29(1):41–49.

Edgar, T., Himmelblau, D., and Lasdon, L. (2001). *Optimization of chemical processes*. McGraw Hill Chemical Engineering Series, New York, second edition.

Emoto, G., Tsuda, A., Takeshita, T., Monical, M., Nakagawa, S., and Fujita, K. (1998). Integrated large scale multivariable control and real time optimization of a power plant. In *Proceedings of the 1998 IEEE International Conference and Control Applications*, pages 1368–1372, Trieste, Italy.

Fan, Y., Bhargava, H., and Natsuyama, H. (2005). Dynamic pricing via dynamic programming. *Journal of Optimization Theory and Applications*, 127(3):565–577.

Feehery, W. and Barton, P. (1996). Dynamic simulation and optimization with inequality path constraints. *Computers and Chemical Engineering*, 20(1):S707–S712.

Feehery, W. and Barton, P. (1998). Dynamic optimization with state variable path constraints. *Computers and Chemical Engineering*, 22(9):1241–1256.

Figueroa, J. (2000). Economic performance of variable structure control: A case study. *Computers and Chemical Engineering*, 24(8):1821–1827.

Figueroa, J., Bahri, J., Bandoni, J., and Romagnoli, J. (1996). Economic impact of disturbances and uncertain parameters in chemical processes: A dynamic backoff analysis. *Computers and Chemical Engineering*, 20(4):S453–S461.

Fikar, M., Latifi, M., and Creff, Y. (1999). Optimal changeover profiles for an industrial de-propanizer. *Chemical Engineering Science*, 54(13-14):2715–2720.

Findeisen, W., Brdyś, M., Malinowski, K., Tatjewski, P., and Woźniak, A. (1978). Online hierarchical control for steady-state systems. *IEEE Transactions on Automatic Control*, 23(2):189–209.

Flender, M., Fieg, G., and Wozny, G. (1996). Classification of new product changeover strategy (nps) for different application of distillation columns. *Computers and Chemical Engineering*, 20(2):S1131–S1136.

Flores-Cerrillo, J. and MacGregor, J. (2005). Latent variable mpc for trajectory tracking in batch processes. *Journal of Process Control*, 15(6):651–663.

Forbes, J. (1994). *Model structure and adjustable parameter selection for operations optimization*. PhD thesis, McMaster University, Hamilton, Canada.

Forbes, J. and Marlin, T. (1994). Model accuracy for economic optimizing controllers: The bias update case. *Ind. Eng. Chem. Res.*, 33(8):1919–1929.

Forbes, J., Marlin, T., and MacGregor, J. (1994). Model adequacy requirements for optimizing plant operations. *Computers and Chemical Engineering*, 18(6):497–510.

Forsgren, A., Gill, P., and Wright, M. (2002). Interior methods for nonlinear optimization. *Society for Industrial and Applied Mathematics*, 44(4):525–597.

Fourer, R., Gay, D., and Kernighan, B. (2002). *AMPL: A mathematical programming language*. Thomson Learning, Pacific Grove, California, 2nd edition.

Funaro, D. (1992). *Polynomial approximation of differential equations*. Springer-Verlag, Berlin, Germany.

García, C. and Morari, M. (1986). Quadratic programming solution of dynamic matrix control (qdmc). *Chemical Engineering Communications*, 46:73–87.

García, C. and Prett, D. (1986). Advances in industrial model predictive control. In Morari, M. and McAvoy, T., editors, *Proceedings of the Third International Conference on Chemical Process Control (CPC) III*, pages 249–294, Asilomar, California.

García, C., Prett, D., and Morari, M. (1989). Model predictive control: Theory and practice: A survey. *Automatica*, 25(3):335–348.

Georgiou, A., Sapre, A., Taylor, P., Galloway, R., and Casey, L. (1998). Etylene optimization system reaps operations and maintenance benefits. *The Oil and Gas Journal*, 96(10):46–50.

Giannelos, N. and Georgiadis, M. (2002). A novel event driven formulation for short term scheduling of multipurpose continuous processes. *Ind. Eng. Chem. Res.*, 41:2431–2439.

Gilbert, E. and Kolmanovsky, I. (1994). Setpoint control of nonlinear systems with state and control constraints: A lyapunov, reference governor approach. In *Proceedings of the 38th IEEE Conference on Decision and Control*, pages 2507–2512.

Gilbert, E. and Kolmanovsky, I. (1995). Discrete time reference governors for systems with state and control constraints and disturbance inputs. In *Proceedings of the 34th IEEE Conference on Decision and Control*, pages 1189–1194.

Gilbert, E. and Kolmanovsky, I. (1999). Fast reference governors for systems with state and control constraints and disturbance inputs. *International Journal of Robust and Nonlinear Control*, 9(15):1117–1141.

Gilbert, E. and Kolmanovsky, I. (2001). A generalized reference governor for nonlinear systems. In *Proceedings of the IEEE Conference on Decision and Control*, pages 4222–4227.

Gilbert, E. and Kolmanovsky, I. (2002). Nonlinear tracking control in the presence of state and control constraints: A generalized reference governor. *Automatica*, 38(12):2063–2073.

Gilbert, E., Kolmanovsky, I., and Tan, K. (1994). Nonlinear control of discrete time linear systems with state and control constraints: A reference governor with global convergence properties. In *Proceedings of the 33rd IEEE Conference on Decision and Control*, pages 144–149.

Gill, P., Murray, W., and Wright, M. (2004). *Practical Optimization*. Elsevier Ltd., New York.

Glemmestad, B., Skogestad, S., and Gundersen, T. (1997). Online optimization and choice of optimization variables for control of heat exchanger networks. *Computers and Chemical Engineering*, 21(1):S379–S384.

Govatsmark, M. and Skogestad, S. (2005). Selection of controlled variables and robust setpoints. *Ind. Eng. Chem. Res.*, 44(7):2207–2217.

Guovêa, M. and Odloak, D. (1998). One layer real time optimization of lpg production in the fcc unit: Procedure, advantages and disadvantages. *Computers and Chemical Engineering*, 22(1):S191–S198.

Harold, M. and Ogunnaike, B. (2000). Process engineering in the evolving chemical industry. *AIChE Journal*, 46(11):2123–2127.

Hatanaka, T. and Takaba, K. (2005). Reference management using state observers. *International Journal of Control*, 78(8):566–576.

Henson, M. (1998). Nonlinear model predictive control: Current status and future directions. *Computers and Chemical Engineering*, 23(2):187–202.

Hessem, D. and Bosgra, O. (2002). Closed-loop stochastic dynamic process optimization under input and state constraints. In *Proceedings of the American Control Conference*, pages 2023–2028.

Hessem, D. and Bosgra, O. (2004). Closed-loop stochastic model predictive control in a receding horizon implementation on a continuous polymerization reactor example. In *Proceedings of the American Control Conference*, pages 914–919, Boston.

Hidalgo, P. and Brosilow, C. (1990). Nonlinear model predictive control of styrene polymerization at unstable operating points. *Computers and Chemical Engineering*, 14(4-5):481–494.

Hirata, K. and Kogiso, K. (2001). A performance improving offline reference management for systems with state and control constraints. In *Proceedings of the 40th IEEE Conference on Decision and Control*, pages 4645–4650, Orlando.

Hirata, K. and Minemura, H. (2004). Experimental evaluations of reference governor control schemes with applications to constrained control of rc helicopters. In *Proceedings of the IEEE International Conference on Control Applications*, pages 855–859, Taipei.

ICIS-LOR (2005). Chemical price reports. www.icislor.com.

Jaeckle, J. and MacGregor, J. (1998). Product design through multivariate statistical analysis of process data. *AIChE Journal*, 44:1105–1118.

Jakhete, R., Rager, W., and Hoffman, D. (1999). Online implementation of composite lp optimizes fccu and gpu complex. *Hydrocarbon Processing*, pages 69–76.

Kadam, J. and Marquardt, W. (2004). Sensitivity based solution updates in closed-loop dynamic optimization. In Shah, S. and MacGregor, J., editors, *7th Symposium on Dynamics and Control of Process Systems*, Cambridge.

Kadam, J., Schlegel, M., Marquardt, W., Tousain, R., Hessem, D., Berg, J., and Bosgra, O. (2002). A two-level strategy of integrated dynamic optimization and control of industrial processes-a case study. In *European Symposium on Computer Aided Process Engineering-12*, pages 511–516.

Kapasouris, P. and Athans, M. (1990). Control systems with rate and magnitude saturation for neutrally stable open-loop systems. In *Proceedings of the 29th IEEE Conference on Decision and Control*, pages 3404–3409, Honolulu.

Kapasouris, P., Athans, M., and Stein, G. (1988). Design of feedback control systems for stable plants with saturating sensors. In *Proceedings of the 27th IEEE Conference on Decision and Control*, pages 469–479, Austin.

Kapasouris, P., Athans, M., and Stein, G. (1989). Design of feedback control systems for unstable plants with saturating sensors. In *Proceedings of the IFAC Symposium on Nonlinear Control Systems Design*, pages 302–307, Capri, Italy.

Kassmann, D. E. and Badgwell, T. A. (2000). Robust steady-state target calculation for model predictive control. *AIChE Journal*, 46(5):1007–1024.

Kleinschrodt, F. I. and Jones, J. (1996). Industrial vision for process optimization. *Computers and Chemical Engineering*, 20(1):S473–S483.

Kogiso, K. and Hirata, K. (2002). An offline reference management technique for linear constrained systems with time varying uncertainties. In *Proceedings of the 4th Asian Control Conference*, pages 77–82, Singapore.

Kogiso, K. and Hirata, K. (2003). A reference governor in a piecewise state affine function. In *Proceedings of the 42nd IEEE Conference on Decision and Control*, pages 1747–1752, Maui.

Kolmanovsky, I. and Gilbert, E. (2001). Landing reference governor. In *Proceedings of the American Control Conference*, pages 374–375.

Kolmanovsky, I., Gilbert, E., and Cook, J. (1997). Reference governors for supplemental torque source control in turbo charged diesel engines. In *Proceedings of the American Control Conference*, pages 652–656.

Kookos, I. and Perkins, J. (2004). *The Integration of Process Design and Control*, volume 17 of *Computer Aided Chemical Engineering (CACE) Series*, chapter The backoff approach to simultaneous design and control, pages 216–238. Elsevier Inc., San Diego, CA.

Kourti, T. and MacGregor, J. (1996). Multivariate spc methods for process and product monitoring. *Journal of Quality Technology*, 28(4):409–428.

Kozub, D. (1997). Controller performance monitoring and diagnosis: Industrial perspective. In Kantor, J., Carnhan, B., and García, C., editors, *Proceedings of the 5th International Conference on Chemical Process Control*, volume 93 of *AIChE Symposium Series*, pages 83–96.

Kozub, D. and MacGregor, J. (1992). Feedback control of polymer quality in semi-batch copolymerization reactors. *Chemical Engineering Science*, 47(4):929–942.

Kravaris, C., Wright, R., and Carrier, J. (1989). Nonlinear controllers for trajectory tracking in batch processes. *Computers and Chemical Engineering*, 13(1-2):73–82.

Kruse, C., Fieg, G., and Wozny, G. (1996). A new time optimal strategy for column startup and product changeover. *Journal of Process Control*, 6(2-3):187–193.

Lauks, U., Vasbinder, R., Valkenburg, P., and Leeuwen, C. (1992). Online optimization of an ethylene plant. *Computers and Chemical Engineering*, 16(1):S213–S220.

Lear, J., Barton, G., and Perkins, J. (1995). Interaction between process design and process control: Economic analysis of process dynamics. *Journal of Process Control*, 5(1):49–62.

Lee, J. and Ricker, N. (1994). Extended kalman filter based nonlinear model predictive control. *Ind. Eng. Chem. Res.*, 33(6):1530–1541.

Lee, J. and Xiao, J. (2000). Use of two stage optimization in model predictive control of stable integrating systems. *Computers and Chemical Engineering*, 24(2-7):1591–1596.

Lee, M., Han, C., and Chang, K. (1997). Hierarchical time optimal control of a continuous co-polymerization reactor during start-up or grade change operation using genetic algorithms. *Computers and Chemical Engineering*, 21(1):S1037–S.

Lee, M., Han, C., and Chang, K. (1999). Dynamic optimization of a continuous polymer reactor using a modified differential evolution algorithm. *Ind. Eng. Chem. Res.*, 38(12):4825–4831.

Leung, D. and Romagnoli, J. (2000). Real time mpc supervisory system. *Computers and Chemical Engineering*, 24(2):285–290.

Lewin, D. and Bogle, D. (1996). Controllability analysis of an industrial polymerization reactor. *Computers and Chemical Engineering*, 20(2):S871–S876.

Li, S., Lim, K., and Fisher, D. (1989). A state-space formulation for model predictive control. *AIChE Journal*, 35(2):241–249.

Loeblein, C. and Perkins, J. (1996). Economic analysis of different structures for online process optimization systems. *Computers and Chemical Engineering*, 20(1):S551–S556.

Loeblein, C. and Perkins, J. (1998). Economic analysis of different structures of online process optimization systems. *Computers and Chemical Engineering*, 22(9):1257–1269.

Loeblein, C. and Perkins, J. (1999a). Structural design for online process optimization i: Dynamic economics of mpc. *AIChE Journal*, 45(5):1018–1029.

Loeblein, C. and Perkins, J. (1999b). Structural design for online process optimization ii: Application to a simulated fcc. *AIChE Journal*, 45(5):1030–1040.

Loeblein, C., Perkins, J., Srinivasan, B., and Bonvin, D. (1997). Performance analysis of online batch optimization systems. *Computers and Chemical Engineering*, 21(6-7):S867–S872.

Loeblein, C., Perkins, J., Srinivasan, B., and Bonvin, D. (1999). Economic performance analysis in the design of online batch optimization systems. *Journal of Process Control*, 9(1):61–78.

Lu, Y. and Arkun, Y. (2002). A scheduling quasi-min-max model predictive control algorithm for nonlinear systems. *Journal of Process Control*, 12(5):589–604.

Luenberger, D. (1984). *Linear and nonlinear programming*. Addison-Wesley Publishing Company Inc., London, second edition.

Lundström, P., Lee, J., Morari, M., and Skogestad, S. (1995). Limitations of dynamic matrix control. *Computers and Chemical Engineering*, 19(4):409–421.

Luyben, M. (2004). *The Integration of Process Design and Control*, volume 17 of *Computer Aided Chemical Engineering (CACE) Series*, chapter design of industrial processes for dynamic operability, pages 352–374. Elsevier Inc., San Diego, CA.

MacGregor, J. and Kourti, T. (1998). Multivariate statistical treatment of historical data for productivity and quality improvements. In Pekny, J., Blau, G., and Carnahan, B., editors, *AIChE Symposium Series*, volume 94 of *Foundations of Computer Aided Process Operations*, pages 31–41.

Maciejowski, J. (2002). *Predictive control with constraints*. Pearson Education Limited, New York.

MacRosty, R. (2005). *Modelling, optimization and control of an electric arc furnace*. PhD thesis, McMaster University, Hamilton, Canada.

Maner, B., Doyle, F., Ogunnaike, B., and Pearson, R. (1996). Nonlinear model predictive control of a simulated multivariable polymerization reactor using second order volterra models. *Automatica*, 32(9):1285–1301.

Marlin, T. (2000). *Process control: Designing processes and control systems for dynamic performance*. McGraw-Hill Inc., New York, 2nd edition.

Marlin, T. and Hrymak, A. (1997). Real-time operations optimization of continuous processes. In Kantor, J., Carnahan, B., and García, C., editors, *Proceedings of the 5th International Conference on Chemical Process Control*, volume 93 of *AIChE Symposium Series*, pages 156–164. AIChE and CACHE.

Marroquin, G. and Luyben, W. (1972). Experimental evaluation of nonlinear cascade controllers for batch reactors. *Ind. Eng. Chem. Fundam.*, 11(4):552–556.

McAuley, K. (1991). *Modelling, estimation and control of product properties in a gas phase polyethylene reactor*. PhD thesis, McMaster University.

McAuley, K., MacDonald, D., and McLellan, P. (1995). Effects of operating conditions on stability of gas-phase polyethylene reactors. *AIChE Journal*, 41(4):868–879.

McAuley, K. and MacGregor, J. (1991). Online inference of polymer properties in an industrial polyethylene reactor. *AIChE Journal*, 37(6):825–835.

McAuley, K. and MacGregor, J. (1992). Optimal grade transitions in a gas phase polyethylene reactor. *AIChE Journal*, 38(10):1564–1576.

McAuley, K. and MacGregor, J. (1993). Nonlinear product property control in industrial gas phase polyethylene reactors. *AIChE Journal*, 39(5):855–866.

McAuley, K., MacGregor, J., and Hamielec, A. (1990). A kinetic model for industrial gas-phase ethylene copolymerization. *AIChE Journal*, 36(6):837–850.

McKenna, T. and Malone, M. (1990). Polymer process design i. continuous productions of chain growth homopolymers. *Computers and Chemical Engineering*, 14(10):1127–1149.

Meister, B. and Cummings, C. (2003). *Modern styrenic polymers*, chapter Commercial processes for the manufacture of polystyrene, pages 45–72. John Wiley and Sons Ltd., West Sussex, England.

Méndez, C. and Cerdá, J. (2000). Optimal scheduling of a resource constrained multiproduct batch plant supplying intermediates to nearby end product facilities. *Computers and Chemical Engineering*, 24(2-7):369–376.

Mendéz, C. and Cerdá, J. (2002). Continuous time formulation for short term scheduling of multi-product continuous facilities. *Computers and Chemical Engineering*, 26(4-5):687–695.

Miletic, I. and Marlin, T. (1996). Results analysis for real time optimization (rto): Deciding when to change the plant optimum. *Computers and Chemical Engineering*, 20(2):S1077–S1082.

Miletic, I. and Marlin, T. (1998). Online statistical results analysis in real time operations optimization. *Ind. Eng. Chem. Res.*, 37:3670–3684.

Miller, R., Kolmanovsky, I., Gilbert, E., and Washabaugh, P. (2000). Control of constrained nonlinear systems: A case study. *IEEE Control Systems Magazine*, 20(1):23–32.

Mizoguchi, A., Marlin, T., and Hrymak, A. (1995). Operations optimization and control design for a petroleum distillation process. *The Canadian Journal of Chemical Engineering*, 73:896–906.

Mohideen, M., Perkins, J., and Pistikopoulos, E. (1996). Optimal synthesis and design of dynamic systems under uncertainty. *Computers and Chemical Engineering*, 20(2):S895–S900.

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

Morari, M. and Lee, J. (1991). Model predictive control: The good, the bad and the ugly. In Arkun, Y. and Ray, W., editors, *Proceedings of the Fourth International Conference on Chemical Process Control*, pages 419–444, New York. CACHE.

Morari, M. and Lee, J. (1999). Model predictive control: past, present and future. *Computers and Chemical Engineering*, 23:667–682.

Moro, L. and Odloak, D. (1995). Constrained multivariable control of fluid catalytic cracking converters. *Journal of Process Control*, 5(1):29–39.

Munawar, S., Bhushan, M., Gudi, R., and Belliappa, A. (2003). Cyclic scheduling of continuous multiproduct plants in a hybrid flowshop facility. *Ind. Eng. Chem. Res.*, 42(23):5861–5882.

Narraway, L. and Perkins, J. (1993). Selection of process control structure based on linear dynamic economics. *Ind. Eng. Chem. Res.*, 32:2681–2692.

Narraway, L. and Perkins, J. (1994). Selection of process control structure based on economics. *Computers and Chemical Engineering*, 18:S511–S515.

Nash, S. and Sofer, A. (1996). *Linear and nonlinear programming*. McGraw-Hill Companies Inc., New York.

Nath, R., Alzein, Z., and Vasbinder, R. (2000). Robust online dynamic optimization of olefin plants. In *Proceedings of ADCHEM*, Pisa, Italy.

Niessner, N. and Gausepohl, H. (2003). *Modern styrenic polymers*, chapter Polystyrenes and styrene co-polymers: An overview, pages 25–42. John Wiley and Sons Ltd., West Sussex, England.

Nocedal, J. and Wright, S. (1999). *Numerical optimization*. Springer-Verlag New York Inc., New York.

Noda, M., Chida, T., Hasebe, S., and Hashimoto, I. (2000). Online optimization system of pilot scale multi-effect batch distillation system. *Computers and Chemical Engineering*, 24:1577–1583.

Oh-Hara, S. and Hirata, K. (2003). Experimental evaluation of online reference governors for constrained systems. In *Proceedings of the SICE 2003 Annual Conference*, pages 824–829, Fukui.

Ohshima, M. and Tanigaki, M. (2000). Quality control of polymer production processes. *Journal of Process Control*, 10:135–148.

Oliveira, N. and Biegler, L. (1994). Constraint handling and stability properties of model predictive control. *AIChE Journal*, 40(7):1138–1155.

Pistikopoulos, E., Dua, V., Bozinis, N., Bemporad, A., and Morari, M. (2000). Online optimization via offline parametric optimization tools. *Computers and Chemical Engineering*, 14(2-7):183–188.

Prett, D. and García, C. (1987). The shell standard control problem. In Prett, D. and Garcia, C., editors, *The shell process control workshop*. Butterworth Publishers, Boston.

Psarris, P. and Floudas, C. (1991). Dynamic operability of mimo systems with time delays and transmission zeroes ii: Enhancement. *Chemical Engineering Science*, 46(10):2709–2728.

Qin, S. and Badgwell, T. (2003). A survey of industrial model predictive control technology. *Control Engineering Practice*, 11:733–764.

Raghunathan, A. and Biegler, L. (2003). Mathematical programs with equilibrium constraints (mpecs) in process engineering. *Computers and Chemical Engineering*, 27(10):1381–1392.

Raghunathan, A. and Biegler, L. (2005). An interior point method for mathematical programs with complementarity constraints (mpccs). *SIAM Journal on Optimization*, 15(3):720–750.

Raghunathan, A., Diaz, S., Biegler, L., and Kelly, J. (2004). A mpec formulation for dynamic optimization of distillation operations. *Computers and Chemical Engineering*, 28(10):2037–2052.

Ramos, C., Senet, J., Blasco, X., and Sanchis, J. (2002). Lp-dmc control of a chemical plant with integral behaviour. In *IFAC 15th Triennial World Congress*, Barcelona, Spain.

Raspanti, C., Bandoni, J., and Biegler, L. (2000). New strategies for flexibility analysis and design of linear process systems. *Computers and Chemical Engineering*, 24(9):2193–2209.

Ricker, N. (1991). Model predictive control: State of the art. In Arkun, Y. and Ray, W., editors, *Proceedings of the Fourth International Conference on Chemical Process Control*, pages 271–296, New York. CACHE.

Rico-Ramírez, V. and Westerberg, A. (2002). Interior point methods for the solution of conditional models. *Computers and Chemical Engineering*, 26(3):375–383.

Rippin, D. (1983). Simulation of single and multi-product batch chemical plants for optimum design and operation. *Computers and Chemical Engineering*, 7(3):137–156.

Roos, C., Terlaky, T., and Vidal, J. (1997). *Theory and Algorithms for Linear Optimization*. John Wiley and Sons Ltd., New York.

Ross, R. (1997). *Dynamic operability assessment: A mathematical approach based on Q-parametrization*. PhD thesis, University of Cape Town.

Ross, R., Perkins, J., Pistikopoulos, E., Koot, G., and Schijndel, J. (2001). Optimal design and control of a high purity industrial distillation systems. *Computers and Chemical Engineering*, 25(1):141–150.

Ross, R. and Swartz, C. (1997). Inclusion of model uncertainty in a computational framework for dynamic operability assessment. *Computers and Chemical Engineering*, 21(1):S415–S420.

Rowe, D., Perkins, J., and Walsh, S. (1997). Integrated design of responsive chemical manufacturing facilities. *Computers and Chemical Engineering*, 21(1):S101–S106.

Sargent, R. and Sullivan, G. (1979). Development of feed changeover policies for refinery distillation units. *Ind. Eng. Chem. Process Des. Dev.*, 18(1):113–124.

Schot, J. v. d., Tousain, R., Backx, A., and Bosgra, O. (1999). Ssqp for the solution of large scale dynamic-economic optimization problems. In *ESCAPE 1999*, Budapest, Hungary.

Scokaert, P. and Rawlings, J. (1999). Feasibility issues in linear model predictive control. *AIChE Journal*, 45(8):1649–1659.

Seider, W., Brengel, D., Provost, A., and Widagdo, S. (1990). Nonlinear analysis in process design: Why overdesign to avoid complex nonlinearities. *Ind. Eng. Chem. Res.*, 29(5):805–818.

Seki, H., Ogawa, M., Ooyama, S., Akamtasu, K., Ohshima, M., and Yang, W. (2001). Industrial application of a nonlinear model predictive control to polymerization reactors. *Control Engineering Practice*, 9(8):819–828.

Shobrys, D. and White, D. (2000). Planning, scheduling and control systems: Why can they not work together. *Computers and Chemical Engineering*, 24(2-7):163–173.

Singh, A., Forbes, J., Vermeer, P., and Woo, S. (2000). Model based real time optimization of automotive gasoline blending operations. *Journal of Process Control*, 10:43–58.

Skogestad, S. (2004). *The Integration of Process Design and Control*, volume 17 of *Computer Aided Chemical Engineering (CACE) Series*, chapter Integration of optimal operation and control, pages 485–500. Elsevier Inc., San Diego, CA.

Soliman, M. (2005). A strategy for inclusion of closed-loop dynamics in real time optimization with application to an oxygen delignification reactor. Master's thesis, McMaster University, Hamilton, Canada.

Sorensen, R. and Cutler, C. (1998). Lp integrates economics into dynamic matrix control. *Hydrocarbon Processing*, 57-65.

Soroush, M. and Kravaris, C. (1993). Optimal design and operation of batch reactors 1: Theoretical framework. *Ind. Eng. Chem. Res.*, 32:866–881.

Sriniwas, G., Arkun, Y., and Schork, F. (1995). Estimation and control of an α-olefin polymerization reactor. *Journal of Process Control*, 5(5):303–313.

Subramanian, S., Uztürk, D., and Georgakis, C. (2001). An optimization based approach for the operability analysis of continuously stirred tank reactors. *Ind. Eng. Chem. Res.*, 40:4238–4252.

Sugie, T. and Yamamoto, H. (2001). Reference management for closed loop systems with state and control constraints. *Proceedings of the American Control Conference*, pages 1426–1431.

Swartz, C. (1995). An algorithm for hierarchical supervisory control. *Computers and Chemical Engineering*, 19(11):1173–1180.

Takeda, M. and Ray, W. (1999). Optimal grade transition strategies for multistage polyolefin reactors. *AIChE Journal*, 45:1776–1793.

Tenny, M., Rawlings, J., and Wright, S. (2004). Closed-loop behaviour of nonlinear model predictive control. *AIChE Journal*, 50(9):2142–2154.

Terlaky, T. and Boggs, P. (2000). *Encyclopedia of Operations Research and Management Science*, chapter Interior point methods, pages 402–411. Kluwer Academic Publishers, 2 edition.

Terwiesch, P., Agarwal, M., and Rippin, D. (1994). Batch unit optimization with imperfect modelling: A survey. *Journal of Process Control*, 4(4):238–258.

Tjoa, I. and Biegler, L. (1991). Simultaneous solution and optimization strategies for parameter estimation of differential-algebraic equation systems. *Ind. Eng. Chem. Res.*, 30:376–385.

Tosukhowong, T., Lee, J., Lee, J., and Lu, J. (2004). Introduction to a dynamic plant-wide optimization strategy for an integrated plant. *Computers and Chemical Engineering*, 29(1):199–208.

Tousain, R. (2002). *Dynamic optimization in business wide process control*. PhD thesis, Delft University, Delft, The Netherlands.

Tousain, R. and Bosgra, O. (2000). Efficient dynamic optimization for nonlinear model predictive control: Application to a high density polyethylene grade change problem. In *Proceedings of the 39th IEEE Conference on Decision and Control*, volume 1, pages 760–765, Sydney, Australia.

Tousain, R. and Bosgra, O. (2006). Market oriented scheduling and economic optimization of continuous multi-grade chemical processes. *Journal of Process Control*, 16(3):291–301.

Tsoukas, A., Tirrell, M., and Stephanopoulos, G. (1982). Multi-objective dynamic optimization of semi-batch co-polymerization reactors. *Chemical Engineering Science*, 37(12):1785–1795.

Vanderbei, R. and Shanno, D. (1999). An interior point algorithm for non-convex nonlinear programming. *Computational Optimization and Applications*, 13(1-3):231–252.

Vasantharajan, S. and Biegler, L. (1990). Simultaneous strategies for optimization of differential algebraic systems with enforcement of error criteria. *Computers and Chemical Engineering*, 14(10):1083–1100.

Vassiliadis, V., Sargent, R., and Pantelides, C. (1994). Solution of a class of multistage dynamic optimization problems 1: Problems without path constraints. *Ind. Eng. Chem. Res.*, 33(9):2111–2122.

Vermeer, P., Pederson, C., Canney, W., and Ayala, J. (1997). Blend control system all but eliminates re-blends for canadian refiner. *The Oil and Gas Journal*, 95(30):73–79.

Verne, T., Jerrit, B., and Bester, P. (1999). Unique approach to real-time optimization. *Hydrocarbon Processing*, 53(92).

Verwijs, J., Kösters, P., Berg, H., and Westerterp, K. (1995). Reactor operating procedures for startup of continuously operated chemical plants. *AIChE Journal*, 41(1):148–158.

Villadsen, J. (1970). *Selected approximation methods for chemical engineering problems*. Reproset, Copenhagen, Denmark.

Villadsen, J. and Michelsen, M. (1978). *Solution of differential equation models by polynomial approximation*. Prentice-Hall Inc., Englewood Cliffs, New Jersey.

Villadsen, J. and Stewart, W. (1967). Solution of boundary value problems by orthogonal collocation. *Chemical Engineering Science*, 22:1483–1501.

Vu, T., Bahri, P., and Romagnoli, J. (1997). Operability considerations in chemical processes: A switchability analysis. *Computers and Chemical Engineering*, 21:S143–S148.

Wächter, A. (2002). *An interior point algorithm for large scale nonlinear optimization with applications in process engineering*. PhD thesis, Carnegie Mellon University, Pittsburgh.

Wächter, A. (2005). Personal communication.

Wächter, A. and Biegler, L. (2000). Failure of global convergence for a class of interior point methods for nonlinear programming. *Mathematical Programming*, 88(3):565–587.

Wächter, A. and Biegler, L. (2004). On the implementation of an interior point filter line search algorithm for large scale nonlinear programming. Technical report, AMPL.

Wang, Y., Seki, H., Ohyama, S., Akamatsu, K., Ogawa, M., and Ohshima, M. (2000). Optimal grade transition control for polymerization reactors. *Computers and Chemical Engineering*, 24(2-7):1555–1561.

Warren, A. and Marlin, T. (2003). Improved output constraint handling for mpc with disturbance uncertainty. *Proceedings of the American Control Conference*, pages 4573–4578.

Warren, A. and Marlin, T. (2004). Improved performance of robust mpc with feedback model uncertainty. In *7th Symposium of Advanced Control of Chemical Processes*, pages 980–986.

Weitz, O. and Lewin, D. (1996). Dynamic controllability and resiliency diagnosis using steady state process flowsheet data. *Computers and Chemical Engineering*, 20(4):325–335.

White, V., Perkins, J., and Espie, D. (1996). Switchability analysis. *Computers and Chemical Engineering*, 20(4):469–474.

Wright, M. (1998). The interior point revolution in constrained optimization. Technical report, Computing Sciences Research Center Bell Laboratories.

Wright, M. (2004). The interior point revolution in optimization: History, recent developments and lasting consequences. *The American Mathematical Society*, 42(1):39–56.

Xie, T., McAuley, K., Hsu, J., and Bacon, D. (1994). Gas phase ethylene polymerization: Production processes, polymer properties and reactor modelling. *Ind. Eng. Chem. Res.*, 33:449–479.

Yi, H., Kim, J., Han, C., Lee, J., and Na, S. (2003). Plantwide optimal grade transitions for an industrial high density polyethylene plant. *Ind. Eng. Chem. Res.*, 42:91–98.

Ying, C. and Joseph, B. (1999). Performance and stability analysis of lp-mpc and qp-mpc cascade control systems. *AIChE Journal*, 45(7):1521–1534.

Ying, C., Voorakaranam, S., and Joseph, B. (1998). Analysis and performance of the lp-mpc and qp-mpc cascade control system. In *Proceedings of the American Control Conference*, pages 806–810, Philadelphia, Pennsylvania.

Yoon, S., Dasgupta, S., and Mijares, G. (1996). Real time optimization boosts capacity of korean olefins plant. *The Oil and Gas Journal*, 94(25):36–41.

Young, J., Swartz, C., and Ross, R. (1996). On the effect of constraints, economics and uncertain disturbances on dynamic operability assessment. *Computers and Chemical Engineering*, 20(1):S677–S682.

Yousfí, C. and Tourier, R. (1991). Steady-state optimization inside model predictive control. *ACC 1991 Boston Massachusetts TP8.*

Zafiriou, E. (1990a). An operator control theory approach to the shell standard control problem. In Prett, D., García, C., and Ramaker, B., editors, *The second shell process control workshop: Solutions to the shell standard control problem*, pages 59–85. Butterworth Publishers, Boston.

Zafiriou, E. (1990b). Robust model predictive control of processes with hard constraints. *Computers and Chemical Engineering*, 14(4-5):359–371.

Zafiriou, E. (1991). On the effect of tuning parameters and constraints on the robustness of model predictive controllers. In Arkun, Y. and Ray, W., editors, *Proceedings of the Fourth International Conference on Chemical Process Control*, pages 363–393, New York. CACHE.

Zanin, A., Guovêa, M., and Odloak, D. (2000). Industrial implementation of a real time optimization strategy for maximizing production of lpg in a fcc unit. *Computers and Chemical Engineering*, 24:525–531.

Zanin, A., Guovêa, M., and Odloak, D. (2002). Integrating real-time optimization into the model predictive controller of the fcc system. *Control Engineering Practice*, 10(8):819–831.

Zhang, Y., Nadler, D., and Forbes, J. (2001). Results analysis for trust constrained real time optimization. *Journal of Process Control*, 11:329–341.

Zyngier, D. and Marlin, T. (2006). Monitoring and improving lp optimization with uncertain parameters. In *Proceedings of Process Systems Engineering*. Submitted.