Modeling and Model Updating in the Real-Time Optimization of Gasoline Blending

by

Aseema Singh

A thesis submitted in conformity with the requirements for the degree of Master of Applied Science
Department of Chemical Engineering and Applied Chemistry
University of Toronto

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MODELING AND MODEL UPDATING IN THE REAL-TIME OPTIMIZATION OF GASOLINE BLENDING

Master of Applied Science, 1997, by Aseema Singh,
Graduate Department of Chemical Engineering and Applied Chemistry,
University of Toronto

Abstract

This thesis provides a new approach to gasoline blender control that can out-perform conventional blend controllers. The proposed blend controller includes appropriate nonlinear blending models and adopts concepts from model predictive control theory in order to allow it to handle stochastic disturbances in feedstock qualities. The resulting Real-Time Optimization (RTO) system is similar to model predictive control in that it predicts disturbances over one time horizon and optimizes the blender control problem over another. It then implements control action for the current time-step and repeats the process in a receding horizon fashion.

Another important contribution is that of parameter observability for steady-state RTO systems. The currently available method provides only a necessary but not sufficient condition. A new approach has been presented which uses fundamental statistical principles and is applicable to any steady-state system where secondary measurements are used to estimate unmeasured quantities. Observability is then extended to a measure of degree of observability.
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# Contents

Abstract ........................................ ii

Acknowledgements ................................ iii

List of Figures .................................... vii

List of Tables ....................................... viii

1 INTRODUCTION .................................. 1

1.1 RTO STRUCTURE ........................................ 2

1.2 RTO DESIGN ........................................... 3

1.3 GASOLINE BLENDING ................................... 5

1.3.1 BLEND CONTROLLERS ................................. 9

1.4 THESIS OBJECTIVES & SCOPE ......................... 13

1.5 THESIS CONVENTIONS ............................... 14

2 GASOLINE BLENDING MODELS ........................ 15

2.1 OCTANE NUMBER ..................................... 15

2.1.1 BLENDING OCTANE NUMBER METHOD ................ 16

2.1.2 ETHYL RT-70 METHOD ............................... 16

2.1.3 STEWART METHOD .................................. 17

2.1.4 INTERACTION METHOD ............................. 18

2.1.5 TRANSFORMATION METHOD ......................... 20

2.1.6 EXCESS METHOD .................................. 23

2.1.7 ZAHED METHOD .................................. 24
2.1.8 SUMMARY OF OCTANE BLENDING MODELS ........................................... 25
2.2 REID VAPOUR PRESSURE ........................................................................ 26
  2.2.1 THEORETICAL APPROACHES ............................................................. 26
  2.2.2 INTERACTION METHOD .................................................................... 30
  2.2.3 BLENDING INDEX METHOD ................................................................ 30
  2.2.4 OTHER METHODS ............................................................................. 31
  2.2.5 SUMMARY OF RVP BLENDING MODELS .......................................... 31
2.3 ASTM DISTILLATION .............................................................................. 32
  2.3.1 INTERACTION METHOD .................................................................... 32
  2.3.2 EMPIRICAL MODELS ......................................................................... 32
2.4 BLENDING SIMULATION .......................................................................... 33
3 PARAMETER OBSERVABILITY IN RTO SYSTEMS ........................................ 35
  3.1 BACKGROUND ....................................................................................... 35
  3.2 PARAMETER OBSERVABILITY ............................................................... 41
    3.2.1 DEGREE OF OBSERVABILITY .......................................................... 47
  3.3 COVARIANCE MATRIX APPROXIMATION .............................................. 50
    3.3.1 ESTIMATION EXAMPLES ................................................................. 51
  3.4 DISCUSSION ......................................................................................... 58
4 BLENDING CONTROL TECHNOLOGY ............................................................. 61
  4.1 INTRODUCTION .................................................................................... 61
  4.2 GASOLINE BLENDING BENCHMARK PROBLEM ..................................... 62
    4.2.1 BLENDING PROBLEM .................................................................... 62
    4.2.2 STOCHASTIC DISTURBANCES ......................................................... 64
    4.2.3 CONTROLLER PERFORMANCE ....................................................... 65
  4.3 IDEAL BLEND CONTROLLER ................................................................. 67
    4.3.1 OPTIMAL BLEND TRAJECTORY FOR BENCHMARK PROBLEM .... 68
  4.4 CONVENTIONAL CONTROLLER ............................................................. 69
    4.4.1 CONVENTIONAL CONTROLLER PERFORMANCE STUDY .......... 71
  4.5 PARAMETRIC MISMATCH CASE ............................................................ 74
    4.5.1 PARAMETRIC MISMATCH PERFORMANCE STUDY ....................... 74
List of Figures

1-1 RTO Structure ................................................................. 3
1-2 Refinery Flow Diagram (blender feedstocks indicated in bold) .......... 6
1-3 Gasoline Blending Process .................................................. 7
1-4 Blending Control Hierarchy .................................................. 10

3-1 Steady-State System and Estimator Considered by Stanley and Mah [1981] ... 38
3-2 Parameter Updating .......................................................... 41
3-3 Confidence Contours ....................................................... 44
3-4 Probability Contours for Example 3.2 .................................. 50

4-1 Blending Process .............................................................. 64
4-2 Reformate qualities during 24 hour blend. .................................. 66
4-3 Blended Octane using LP + Bias Controller ............................... 72
4-4 Blended RVP using LP + Bias Controller .................................. 73
4-5 Uncaptured Profit for 24 hour Blend ...................................... 83
List of Tables

2.1 Comparison of Octane Blending Models ........................................... 26
2.2 Predictive Accuracy of Octane Blending Models ............................... 27
2.3 Predictive Accuracy of RVP Blending Models .................................. 31

4.1 Production Requirements ............................................................... 63
4.2 Feedstock Economic Data ............................................................... 63
4.3 Feedstock Qualities ................................................................. 63
4.4 Feedstock Sensitivity ................................................................. 65
4.5 Deviation from Specification at End of Blend ................................. 75
4.6 Comparison of Time-Horizon Controllers ..................................... 82
Chapter 1

INTRODUCTION

The economic benefits of process control are well recognized in the chemical and petrochemical industries. These benefits have led to the widespread use of advanced automation technologies in such plants. The control systems in these plants are designed to operate the process using some pre-determined policy, which may or may not be optimal. Additional benefits, which can be crucial in providing a competitive edge, can be realized by operating the process in an economically optimal manner. This is usually achieved by the optimization of steady-state operations policy [Forbes, 1994].

The major categories of steady-state optimization methods are direct search and model-based optimization methods. Direct search methods [e.g. McFarlane and Bacon, 1989] work on the actual process and involve plant experimentation to obtain new steady-state operations. The direction in which process economics are improved can be deduced from the experimental results and the process optimum is found by iteratively moving the process in this direction after each plant experiment. However, the amount of experimentation required, especially for large dimensional problems, can be prohibitive. Moreover, for complex and integrated plants with slow dynamics, it can take a long time for the process to reach steady-state after each perturbation. Using direct search methods on such plants would require the process to operate outside the normal region of operation for long periods of time, which may not be acceptable.

Model-based optimization methods, on the other hand, work on mathematical models that represent the plant, rather than the process itself. Optimization algorithms are used to find the optimum of the model, the results of which, after verification, are implemented on the plant.
A Real-Time Optimization (RTO) system is considered to be any closed-loop control system that is used to determine the optimal process operations and to implement this policy on the plant through the underlying control system. On-line optimization is required when plants are subject to disturbances which cause the process behaviour and the optimal process operation to vary substantially with time. In such situations, the economic optimum process operation is not a point but rather a trajectory in time and the objective of the RTO system is to cause the process to track this optimal trajectory.

One of the key petroleum refining processes which has long benefitted from RTO technology is gasoline blending [Leung, 1985]. This thesis considers RTO systems for gasoline blender control and offers solutions for improving blender efficiency. In doing so, observability issues in conventional steady-state RTO systems are also addressed.

1.1 RTO STRUCTURE

The structure of a typical RTO system is shown schematically in Figure 1-1 [Seferlis, 1995]. The constituent subsystems are briefly described below:

1. Process measurement: relevant measurements are taken which are used for updating models in the optimizer.

2. Data validation: at this stage, process measurements are examined to ensure that the process has indeed reached steady-state. Also, Gross Error Detection and Data Reconciliation are carried out. Gross Error Detection involves detecting errors in measurements resulting from sensor failures, leaks, etc., so as to eliminate erroneous data from being used in model updating. Data Reconciliation tries to adjust the data such that the material and energy balances are satisfied [Seferlis, 1995].

3. Model updating: validated data is used to update the model in some way. Model updating involves obtaining new estimates of some of the model parameters using estimation techniques such as regression analysis.

4. Optimization: model-based, steady-state optimization is used to calculate controller set-points. The optimization algorithm can be a linear program (LP) or a nonlinear program
Validation

Controllen

Sensors

Process

Model Update

Command Conditioning

Controllers

Figure 1-1: RTO Structure

(NLP) and, may require mixed integer programming (MIP) depending on the nature of the model equations.

5. Command conditioning (also called post-optimality or results analysis): at this stage, the outputs from the optimizer are examined in order to ensure that only acceptable setpoints which will result in a significantly improved plant operation, are passed to the controllers [Seferlis, 1995].

6. Control: the acceptable setpoints are used by the controllers to implement the operations policy on the plant. The controller structure can range from simple PID loops to advanced control schemes such as model predictive control (MPC).

More detailed treatments of the RTO structure can be found in Seferlis [1995] and Forbes [1994].

1.2 RTO DESIGN

The performance of any RTO system will depend on the characteristics of each of the constituent subsystems and their interactions with each other [Forbes, 1994]. All the components in the RTO system depicted in Figure 1-1 have been studied to some extent by various researchers.
Krishnan [1990] has studied the problem of selecting appropriate measurements for model updating. A measurement selection strategy based on minimizing error in estimated parameters has been provided. Issues in Gross Error Detection and Data Reconciliation have been addressed by Crowe [1988], Rosenberg et al. [1987], and Tjoa and Biegler [1990].

Crucial to the success of the RTO system is the quality of models used on the optimizer. Biegler et al. [1985] have found that a model is adequate for use in RTO if model parameter values can be found such that the gradients of the model with respect to the decision variables can be forced to match those of the plant. Model selection has also been studied by Forbes et al. [1994] who have defined model adequacy in terms of the model's ability to possess an optimum at the true plant optimum. That is, a model is defined to be point-wise adequate if there exist a set of values for the adjustable model parameters such that the model-based optimization possesses an optimum at the true plant optimum.

The model adequacy approach taken by Forbes et al. [1994] allows for the selection of adjustable model parameters. That is, model adequacy can be used as a criterion for selecting adjustable model parameters. Similarly, Roberts [1979], [1995] has stated that models and parameter estimation strategies should not be selected in isolation; the characteristics of the process model should be taken into account in order to allow the system to effectively handle plant-model mismatch. Krishnan [1990] has also looked at the problem of selecting the adjustable parameters in the model to be updated on-line and has suggested updating those parameters that have the most effect on the optimal value of the objective function or alter the active constraint set. Observability of the adjustable parameters from the available measurements has been studied by Krishnan [1990].

Optimization algorithms have been developed for several classes of optimization problems such as LP, NLP, and MIP, and are being continually improved for increased computational efficiency. Optimization theory and algorithms can be found in Fletcher [1987], Avriel [1976], Balakrishnan and Boyd [1992], Duran and Grossman [1986], and Edgar and Himmelblau [1988]. Post optimality analysis has been studied by Seferlis [1995] and Miletic [1996]. Tests have been provided to determine whether or not setpoints generated by the optimizer are to be passed to the controllers.
While most of the work has focused on individual components of the RTO system, the interactions among the subsystems and their effect on the whole structure have received little attention. Forbes and Marlin [1996] have provided the first approach to making RTO decisions based on the whole system. The approach is based on designing RTO components such that the loss of RTO performance is minimized. The measure of RTO performance used by Forbes and Marlin [1996], the Design Cost Criteria, looks at the loss of economic opportunity resulting from a given RTO design. This measure considers the deviation of the manipulated variables from the true plant optimum. An alternate approach due to Loeblin and Perkins [1996] uses the average deviation of the objective function rather than the setpoints.

The past sections have focused on RTO systems without application to any particular process. Since this thesis is concerned with RTO of gasoline blending, gasoline blending will be discussed next.

1.3 GASOLINE BLENDING

Gasoline is one of the most important refinery products since it can yield 60 to 70 percent of a typical refinery’s total revenue [DeWitt et al., 1989]. Fractional distillation of crude oil produces several “cuts”. Only a small portion of the distillation products, the light virgin naphtha or light straight run (LSR) naphtha, is suitable for blending directly into gasoline. Other fractions have to be further processed. A simplified flow diagram of the refinery processes is given in Figure 1-2. The flow diagram shows the main units and the refinery processes required for producing gasoline feedstocks in a typical refinery. Some of the refining processes are briefly described below [Givens, 1985]:

1. Catalytic Reforming: this is an upgrading process that increases the octane number of the heavy virgin naphtha by catalytically converting low octane hydrocarbons into high octane ones. The most important reactions taking place include the conversion of methyl cyclohexane (research octane number of 75) and n-heptane (zero octane by definition) to toluene which has a research octane of 120.

2. Catalytic Cracking: this is a conversion process that breaks large, low volatility molecules into smaller, more volatile ones. The product is then sent to the fractionator, a
distillation column, that separates the stream according to boiling range. About 50% of the catalytically cracked stream can be blended into gasoline without further upgrading. Another 20% contains light gases from which n-butane and iso-butane are separated and used later for blending in gasoline.

3. Alkylation: down stream from the catalytic cracker, the alkylation unit further processes light olefins produced during catalytic cracking. Although the light olefin stream has high octane quality, its boiling range is too low for gasoline. Alkylation involves catalytically reacting these olefins with iso-butane to form high quality hydrocarbons such as iso-octane.

4. Hydrotreating: feedstocks (including straight run naphtha from the crude distillation unit) are treated with hydrogen in the presence of catalysts to reduce the amount of sulphur, nitrogen, and oxygen.

Some of these refinery products are further separated into light and heavy fractions in order to provide more flexibility in blending. A large refinery can have more than 20 blender feedstocks
that are blended into several grades of gasoline [Givens, 1985]. Gasoline blending is the process of combining these blender feedstocks, together with small amounts of additives (such as antioxidants, corrosion inhibitors, metal deactivators, detergents, and dyes), to make a mixture meeting certain quality specifications. Specifications on gasoline qualities such as octane number, volatility, sulphur content, aromatics content, and viscosity are placed in order to ensure acceptable engine performance as well as for environmental reasons. Feedstocks can be blended out of storage tanks, intermediate tanks into which upstream processes are being fed, or directly from upstream processes [Agrawal, 1995]. The gasoline blending process of blending feedstocks from storage tanks, is shown in Figure 1-3.

![Gasoline Blending Process Diagram](image)

**Figure 1-3: Gasoline Blending Process**

Octane numbers are measures of a fuel’s antiknock properties. Knocking occurs when a fuel/air mixture ignites prematurely in the cylinder, producing a "knocking" sound in the engine. Knocking not only reduces the engine’s power by working against the piston, but it also exerts mechanical stress on the engine parts. The octane number of a fuel is defined as the percent of iso-octane (2,2,4-trimethyl pentane) in a blend with n-heptane that exhibits the same resistance to knocking as the test fuel under standard conditions in a standard engine [Palmer and Smith, 1985]. On the octane scale, iso-octane is assigned an octane number of 100 and n-heptane a
number of 0. Two standard test procedures are used to characterize the antiknock properties of fuels for spark engines - the ASTM D-908 test gives the research octane number (RON) and the ASTM D-357 gives the motor octane number (MON). The RON represents antiknock properties under conditions of low speed and frequent accelerations while the MON represents engine performance under more severe high speed conditions. The octane number posted at gasoline stations is the arithmetic mean of the RON and MON ($\frac{RON+MON}{2}$) [Gary and Handwerk, 1994]. The main difference between automotive gasoline grades is their antiknock properties. For example, regular and premium gasolines are specified to have posted octane numbers of 87 and 92, respectively.

Other important properties that affect engine performance are volatility and boiling range. A vapour pressure which is too high for the given ambient temperature will result in vapour stalling and motor locking, while a vapour pressure which is too low will lead to difficulties in engine startup [Palmer and Smith, 1985]. The boiling range also affects the engine during startup and driving, and is particularly important for good performance during quick acceleration and high speed operations. Like vapour pressure, the boiling range has to be tailored for a given geographical region and season. There should be a fairly reasonable distribution of light (more volatile), intermediate, and heavy (relatively non-volatile) components; however, gasolines blended for use in cold climates need more light components (front end volatility) than those intended for use in warmer climates [Palmer and Smith, 1985]. In addition, government regulations place maximum restrictions on the vapour pressure to limit the emission of volatile organic compounds into the atmosphere [Lo, 1994]. Other environmental restrictions include maximum compositions of aromatics, olefin, sulphur, and oxygenates.

The gasoline blending challenge is to produce blends in such a way as to maximize profit while meeting all quality specifications on all blends, in addition to satisfying any product demands and feedstock availability limits. Thus the blending problem is naturally posed as a constrained optimization problem and the blender control is traditionally based on optimization technology [Leffler, 1985].
1.3.1 BLEND CONTROLLERS

Blend controllers are used for making gasolines that meet quality specifications while satisfying demand and availability limits. In addition, the controller should work to maximize profit by using the least expensive feedstocks to make the most valuable products, minimizing "quality giveaway", and minimizing reblends. "Quality giveaway" refers to making gasoline with qualities that either exceed the minimum required or fall below the maximum allowed, thus reducing the profit margin. It is estimated that consistent octane giveaway of 0.1 can cost a refinery several millions of dollars a year [Givens, 1985]. Reblending can also lead to significant costs to a refinery by taking up valuable tank space and blending time, reducing overall capacity. Thus, the controller should be able to blend the products optimally and get the blends on specification the first time.

There is a wide range of sophistication in blending control technology presently employed by refiners. The typical state-of-the-art blending technology is built on three levels: off-line optimizer or scheduler, on-line optimizer, and regulatory control [Sullivan, 1990], [Agrawal, 1995]. The levels of control strategy are shown schematically in Figure 1-4.

At the top of the hierarchy lies the planner or scheduler which uses off-line optimization to plan refinery operations for the long range (months), intermediate range (weeks), and short range (days). Long-range planning can be performed at either the refinery or corporate level. Long range forecasts of product demands, crude oil prices, and process unit performances are used to plan refinery operations several months to a few years into the future [Sullivan, 1990], [Agrawal, 1995]. Medium-range planning provides scheduling of refinery operations on a shorter time frame (a few weeks) and is used to improve on the long-range plan. In addition to economic forecasts, forecasts of refinery feedstock qualities and quantities, and tank availability are used to check feasibility of the long range plan and to revise production targets set by the long-range planner. Here, the refinery schedule is also adjusted for major unit upsets and unscheduled shutdowns. Significant changes in expected crude quality and changes in operating flexibility (such as additional constraints) are used at this stage to revise refinery plans as well [Sullivan, 1990]. Short-range planning works at the unit level, rather than at the refinery level, and plans blender operations over a shorter time frame (1 to 2 days) [Agrawal, 1995]. At this stage, assumed feedstock qualities (or measured qualities, if available) are used to produce blend
recipes which are then downloaded to the on-line optimizer. Usually, all levels of planning using an off-line optimizer are conducted using linear programming [Sullivan, 1990], [Ramsey Jr. and Truesdale, 1990], [DeWitt et al., 1989].

The on-line optimizer uses on-line blended quality information to modify the initial recipe during the blend and provides final blend recipes to be executed by the controller. On-line optimizers are designed to minimize deviation from the initial blend recipe or optimize some economic performance (such as profit maximization) while satisfying all constraints [Michalek et al., 1994]. However, the move has been towards optimizing steady-state process economics. Thus the on-line optimizer is usually a conventional RTO system. Vermeer et al. [1996] have expanded on the conventional steady-state RTO to perform dynamic blend optimization. This is achieved by including blending dynamics into the controller to calculate expected blended qualities and using these expected qualities as feedback to the LP based on-line optimizer. Incorporating blending dynamics in such a way allows the RTO layer to operate at a higher frequency.
The blend recipes generated by the on-line optimizer are then implemented at the control level. Final blend control is achieved through conventional distributed control systems (DCS). The DCS-resident controller (usually PID loops) maintains flow ratio to match the recipe, maintains a target flowrate for the sum of all feedstock flows, and stops when the required amount of product has been blended [Agrawal, 1995]. The control layer is also used to ensure that quality specifications are met. It uses analyzer feedback and can deviate from the blend recipe determined by the on-line optimizer in order to keep the products on specification.

The different subsystems in Figure 1-4 have to be integrated to provide information flow (such as tank and feedstock inventory) necessary for the success of the whole system. Databases are used to keep track of feedstock inventory, tank availability, feedstock qualities, and blended qualities. The subsystems write to and/or retrieve information from these databases, thus linking the subsystems into an integrated network [Agrawal, 1995], [Ramsey Jr. and Truesdale, 1990], [Palmer et al., 1995], [Michalek et al., 1994].

At the heart of the entire blending control system shown in Figure 1-4 is the RTO layer which determines the final blend recipe and so the performance of the RTO system is crucial to the performance of the whole gasoline blender control effort. The design and performance of the gasoline blender RTO system is the focus of this thesis.

The on-line optimizer is usually based on linear programming (e.g. Benefield and Broadway, [1985], Diaz and Barsamian, [1996], White and Hall, [1992], McDonald et al., [1992], Serpemen et al., [1992], Michalek et al., [1994]) even though most important gasoline properties have been shown to blend in a nonlinear fashion [Rusin, 1975]. As a result, blender control systems must deal with structural mismatch. Some refiners have tried addressing this problem by using nonlinear models and employing nonlinear programming (NLP) in the on-line optimizer (e.g. Ramsey Jr. and Truesdale, [1990]); however, linear programming remains as the predominant technology, owing its popularity to reliability and ease of use [Magoulas et al., 1988]. Another approach that has been employed is to linearize the nonlinear models and use sequential linear programming (SLP) (e.g. Diaz and Barsamian, [1996]).

In an attempt to maintain accuracy of the models in the optimizer, the feedback employed is usually "bias updating" (e.g. Diaz and Barsamian, [1996], Bain et al., [1993]). Bias updating
involves comparing measured blended qualities with those predicted by the models in the on-line optimizer; the difference between the two is then added as an error term to the appropriate blending models. Thus the RTO system is most often formulated as linear programming with bias updating.

This approach of linear programming with bias updating has proven quite successful in practice and is the basis of most commercially available blend control systems. Its success was largely due to the practice of blending from well-mixed storage tanks. The current trends of in-line blending and blending from “running” tanks presents a problem that such a control structure cannot adequately address. This is because upstream process variations resulting from catalyst deactivation, heat exchanger fouling, etc., will cause variations in the feedstock qualities. The LP (or NLP) plus bias update formulation assumes constant feedstock qualities and so cannot adequately handle such time varying feedstock qualities. Forbes and Marlin [1994] have shown that this traditional blend controller approach can lead to a substantial loss in blender profitability given even a small variation in feedstock qualities.

Note that in the case of time-varying feedstocks, the bias updating approach can still be used to make products because the lower level feedback controllers in the RTO system will deviate from the blend recipe determined by the on-line optimizer in order to meet specifications as discussed above. Although products can be made in this manner to meet specifications, the resulting blend will not necessarily be optimal in that the best combination of feedstocks may not have been used.

Some refiners have tried addressing this problem by feedback of laboratory analyses of feedstock qualities and then using multiperiod optimization (e.g. McDonald et al., [1992] and Rigby et al., [1995]). The interval between optimizations is usually a day and feedstock qualities are assumed to remain unchanged during these periods. Thus this approach cannot effectively deal with higher frequency disturbances arising from upstream process operation changes. Vermeer et al. [1996] have used blended quality measurements to predict disturbances in these qualities. The disturbances, however, are assumed to be step disturbances that remain constant during the optimization interval. Therefore, this approach suffers from the same drawback as the multiperiod optimization strategy.
This thesis will address the problems associated with structural mismatch and inability of the bias update approach to adequately handle fluctuations in feedstock qualities. A new control approach that can incorporate nonlinear blending models and can deal with time-varying qualities will be developed.

1.4 THESIS OBJECTIVES & SCOPE

This thesis is concerned with the design of the blend controller shown in Figure 1-4, and the RTO layer in particular. As has been discussed in the previous section, the RTO layer is most often formulated as linear programming with bias updating. The LP plus bias updating formulation suffers from plant/model mismatch since most important gasoline qualities blend nonlinearly. Generally, the controller is not capable of adequately handling disturbances in feedstock qualities [Forbes and Marlin. 1994]. The objective of this thesis is to provide a blend controller that incorporates models which capture the inherent nonlinearities of the blending process, and one that can effectively deal with predictable variations in feedstock qualities.

Gasoline blending models are examined in Chapter 2 with respect to predictive accuracy and their ability to be implemented for control purposes. Once suitable models have been selected, it is crucial that their predictive accuracy be maintained by updating some parameters on-line. Therefore it is important to ensure that the adjustable parameters in these models be observable from the process measurements and the updating scheme. Chapter 3 looks at parameter observability for steady-state systems. A measure of observability for steady-state systems is developed and the concept is extended to degree of observability. The observability measure is based on fundamental statistical principles and can be applied to the blending models. The observability measure presented in Chapter 3 is not limited to the blending process or to RTO systems, but is applicable to any steady-state system where unmeasured quantities are to be estimated using available measurements.

Chapter 4 presents a new approach to blender control that can incorporate nonlinear models and can effectively deal with feedstock quality variations. The control approach is analogous to MPC in that a time-horizon approach is taken. A gasoline blending case-study is used to demonstrate the problems associated with the conventional bias updating approach and the benefits of adopting the new blending strategy.
Although the time-horizon strategy has been applied to the RTO layer in this thesis, it could also be adopted into the off-line optimization layer and used to improve the effectiveness of the planning and scheduling layer. Moreover, it could be applied to on-line or off-line optimization of other processes that are subject to stochastic disturbances.

1.5 THESIS CONVENTIONS

In accordance with the petroleum industry terminology, light and heavy components refer to relatively volatile and nonvolatile components, respectively. All terms are defined on first use and used thereafter. The Nomenclature section lists all symbols employed in this thesis while the acronyms used are summarized in the Glossary of Terms section.
Chapter 2

GASOLINE BLENDING MODELS

There are several properties that are important in characterizing automotive gasoline such as octane number (ON), Reid vapour pressure (RVP), ASTM distillation points, viscosity, flash point, and aniline point. Ideal mixing refers to a quality blending as its volumetric average [Barrow, 1961]; however, most gasoline properties blend in a non-ideal and nonlinear fashion, necessitating the use of more complex blending models to predict these properties [Rusin, 1975]. In this section, blending models for key properties - octane, RVP, and ASTM distillation points - are presented and examined. Blending models for other qualities can be found in Gary and Handwerk [1994] or McLellan [1981] and will not be discussed here.

There are several characteristics that are desirable in a blending model. In this thesis the most important of these characteristics are predictive accuracy and parsimony. Also, since feedstock qualities are dependent on upstream processes operations, they change over time. Therefore, blending models should remain accurate over a range of qualities beyond the data where the parameters are evaluated.

2.1 OCTANE NUMBER

Octane numbers indicate the antiknock characteristics of gasoline or the ability of the gasoline to resist detonation during combustion in the combustion chamber. The two most common types of octane numbers for spark engines are the research octane number (RON) and the motor octane number (MON). The RON, defined by the American Society for Testing and Materials under the designation ASTM D-908, represents the engine performance under city
driving conditions (frequent acceleration) while the MON (ASTM D-357) represents engine performance on the highway [Gary and Handwerk, 1994]. Since RON and MON of a gasoline blend in nonlinear fashion, complex blending models are needed for accurate prediction of blended octanes [Rusin, 1975].

2.1.1 BLENDING OCTANE NUMBER METHOD

In this method, fictitious blending octane numbers (BON's) are used for RON and MON. The BON's blend linearly on a volumetric basis to give the octane number of the blend [Gary and Handwerk, 1994]:

\[
(ON)_{\text{blend}} = \sum_{i=1}^{n} u_i (BON)_i
\]

where: \( u_i \) is the volume fraction of component \( i \), \((ON)_{\text{blend}}\) is the octane number (RON or MON) of the blend, \((BON)_i\) is the blending octane number (RON or MON) of the component. \( n \) is the number of components in the blend.

Blending octane numbers are usually obtained from regression analysis on small data sets and may be user-tuned. Thus their application is often based on user experience and judgment [Rusin et al., 1981]. BON's for some typical components can be found in Gary and Handwerk [1994]. The limitations of using BON's has long being recognized which has lead to the development of more reliable methods that do not depend so heavily on user judgment [Rusin et al., 1981].

2.1.2 ETHYL RT-70 METHOD

The Ethyl method is one of the oldest models available in literature. This method has been used as a benchmark against which newer models have been compared. Here, blending nonlinearity is modeled explicitly as a function of the component sensitivity (RON - MON), olefin content, and the aromatic content of the components as given below [Healy et al., 1959]:

\[
RON_{\text{blend}} = \bar{\tau} + a_1(\bar{\tau} \bar{s} - \bar{\tau} \bar{s}) + a_2(\bar{O}^2 - \bar{O}^2) + a_3(\bar{A}^2 - \bar{A}^2)
\]

\[
MON_{\text{blend}} = \bar{m} + a_4(\bar{m} \bar{s} - \bar{m} \bar{s}) + a_5(\bar{O}^2 - \bar{O}^2) + a_6 \left[ \frac{(\bar{A}^2 - \bar{A}^2)}{100} \right]^2
\]
where: \( r \) is \( RON \), \( m \) is \( MON \), \( s \) is sensitivity \( (RON - MON) \), \( O \) is olefin content (% by volume), \( A \) is aromatic content (% by volume), and \( a_1, a_2, a_3, a_4, a_5, a_6 \) are correlation coefficients. Quantities accented with an overbar represent volumetric averages.

Equations (2.2) and (2.3) contain a total of six parameters \( (a_1,a_2,a_3,a_4,a_5,a_6) \) for \( RON \) and \( MON \) blending. In order to estimate these parameters, the following data would be needed:

- \( RON \), \( MON \), olefin content, and aromatics content of each pure feedstock,
- \( RON \) and \( MON \) of each blend.

One of the advantages of using the Ethyl method is that it can be readily expanded to include the effects of other factors (such as sulphur content) on octane blending. These factors can be included in the model in a way similar to olefin and aromatics content by using additional nonlinear terms [Morris, 1975]. Blending characteristics can change considerably with changes in octane level and other feedstock qualities. Therefore, as properties of feedstocks change over time with changes in upstream process operations, blending model parameters may change as well [Morris, 1986]. In the Ethyl models, the parameters may be estimated on-line using historical blend data. Thus, the model can be made adaptive so that its accuracy does not decrease over time. However, the models require knowledge of the olefin and aromatics content which may not be readily available.

Some indication of the predictive accuracy of the models has been provided by Healy et al. [1959]. The standard deviations of prediction errors for unleaded blends similar to the ones the coefficients were determined from are reported to be 0.66 and 0.85 octane numbers for \( RON \) and \( MON \), respectively. For independent blends, the standard deviations of prediction errors were found to be 0.92 for \( RON \) and 0.61 for \( MON \).

### 2.1.3 STEWART METHOD

This method was proposed by Stewart [1959a] about the same time as the Ethyl method was published and is similar to the Ethyl method in that blending nonlinearity is attributed to the olefin content of the components. The blending models are:

\[
RON_{blend} = \frac{\sum_{i=1}^{n} V_i D_i [RON_i + \bar{e}(O_i - O_{blend})]}{\sum_{i=1}^{n} V_i D_i} \tag{2.4}
\]
\[ MON_{\text{blend}} = \sum_{i=1}^{n} \frac{V_i D_i [RON_i + \bar{C}(O_i - O_{\text{blend}})]}{\sum_{i=1}^{n} V_i D_i}, \]

where: \( V_i \) is the volume of component \( i \) in the blend, \( D_i = \frac{\bar{O}_i(O_{\text{blend}} - O_i)}{1 - \exp(\bar{O}_i(O_{\text{blend}} - O_i))} \), \( O_{\text{blend}} \) is the percent olefin content of the blend and is the volumetric average of the component olefin contents, and \( \bar{C} \) and \( \bar{a} \) are constants.

Stewart [1959a] has determined the constants \( \bar{a} \) and \( \bar{C} \) using least-squares analysis on 102 blends; the value of \( \bar{a} \) was determined to be 0.01414 for \( RON \) and 0.01994 for \( MON \), the value of \( \bar{C} \) was determined to be 0.130 for \( RON \) and 0.097 for \( MON \). However, only 10 of the blends used were multicomponent; the rest were binary blends.

The standard deviation of prediction error reported by Stewart [1959a] is 0.77 octane numbers for \( RON \) and 0.64 numbers for \( MON \). However, this prediction error reported is for prediction within the data set used for evaluating the correlation constants. No indication of the predictive accuracy outside the development data set is provided. Also, any indication of the level of industrial acceptance of this method could not be found.

### 2.1.4 INTERACTION METHOD

This method is based on the two-factor models where the overall effect is attributed to the main effects of each of the two factors and the nonlinearity is captured by an interaction term. The interaction term accounts for the effect of one factor on the other and can be determined using the design of experiments [Montgomery, 1991]. Similarly, in the Interaction method, octane blending nonlinearity is attributed to the two-factor interactions among the components in the blend and is accounted for by adding an interaction term to the volumetric average octane number. Only the two-way interactions between pairs of components are considered; the three-way and higher interaction terms are generally ignored [Morris, 1975], [Morris, 1986], [Morris et al., 1994]. For an \( n \) component system, the octane number (\( RON \) or \( MON \)) of the blend can be calculated as:

\[ (ON)_{\text{blend}} = \sum_{i=1}^{n} [u_i(ON)_i] + \sum_{i=1}^{n} \sum_{k=i+1}^{n} (u_i u_k I_{i,k}) \]

where: \( I_{i,k} \) is the interaction coefficient between components \( i \) and \( k \).
The interaction coefficient, $I_{i,k}$, between a pair of components is obtained by using the octane numbers of the pure components and that of a 50:50 blend of the two components as given below [Morris et al., 1994]:

$$I_{i,k} = 4(ON)_{i,k} - 2[(ON)_i + (ON)_k]$$

(2.7)

where $(ON)_{i,k}$ is the octane number of a 50:50 blend of $i$ and $k$.

For an $n$ component system, the number of two-way interaction coefficients are $\frac{n(n-1)}{2}$ for $RON$ and the same for $MON$, giving a total of $n(n-1)$ parameters to be determined. The experimental data required for estimating these parameters are:

- $RON$ and $MON$ for each pure component,
- $RON$ and $MON$ for 50:50 blend of all component combinations.

Thus, for either $MON$ or $RON$ in an $n$ component system, the total number of fuels to be tested are $n$ pure components plus $\frac{n(n-1)}{2}$ 50:50 blends giving a total of $\frac{n(n+1)}{2}$. The total number of tests required for $RON$ and $MON$ is $n(n+1)$.

Since octane blending characteristics may change with changes in octane level and other feedstock qualities, the interaction coefficients may become outdated if significant changes occur in the octane pool [Morris, 1986]. Thus the predictive accuracy of the Interaction model may decrease with time as the feedstock qualities change with changes in upstream operations or crude switches. However, unlike the Ethyl RT-70 method, the Interaction model cannot easily be made adaptive since the interaction coefficients $(I_{i,k})$ are not correlation coefficients but are determined experimentally. Instead of determining the interaction coefficients from binary blends, the interaction coefficients could be obtained using regression analysis on blend data (data on all feedstock qualities as well as blended qualities). The interaction coefficients could then be updated using historical blend data and made adaptive. However, Interaction model requires a large number of parameters to be determined. For example, a 7 component blend would require determination of 42 interaction coefficients while the Ethyl RT-70 method will require estimation of only 6 parameters. Therefore, a large amount of blend data would be
required to update the interaction coefficients. Also, all the model parameters would have to be re-evaluated as new feedstocks are entered into the blend.

Some indication of the predictive accuracy of the blending models have been provided in literature. Morris [1975] has studied the accuracy of the Interaction method and has compared it to the Ethyl RT-70 approach. It has been reported that while the Interaction models fit data more closely than the Ethyl models (this is to be expected since the interaction model has many more parameters that the Ethyl one), the predictive accuracy for a general untested data set using predetermined parameters is about the same for the two methods. The standard deviation of prediction error for both the methods were reported by Morris [1975] to be between 0.6 to 1.0 octane numbers.

While there has been some industrial acceptance of the Interaction models, they have not been widely used. This could be due to the large number of parameters that need to be determined.

2.1.5 TRANSFORMATION METHOD

The transformation method involves transforming the octane number, which blends nonlinearly, to a quality that does blend linearly and ideally. This new quantity is then blended ideally and the result is transformed back to octane number [Rusin et al., 1981]. This method is similar to the Blending Octane Number (BON) method in that transformed qualities are blended ideally; however, systematic methods of transforming the octane numbers to the transformed qualities and the blended transformed qualities back to blended octane numbers are provided. While the Transformation method is applicable to leaded as well as unleaded gasolines, only the unleaded case will be presented here. Discussions on the application of the transformation method to leaded gasolines can be found in Rusin et al. [1981]. For unleaded gasolines, this method takes into account the interaction of major classes of hydrocarbons and the change in conditions (severity levels) inside the engine when measuring different fuels. The effect of severity levels are accounted for by relating component octanes and sensitivities to reference levels. The steps required for unleaded gasoline are outlined below.
Step I: Transform properties for each component:

(a) evaluate sensitivity at reference engine severity levels,

\[ s_i = \frac{RON_i - MON_i}{1 - c_1(RON_i - RON_{ref}) + c_2(MON_i - MON_{ref})} \]

(b) adjust octanes to reference levels,

\[ RON_{\text{calc}_i} = RON_i + (c_1)(s_i)(RON_i - RON_{\text{ref}}) \]
\[ MON_{\text{calc}_i} = MON_i + (c_2)(s_i)(MON_i - MON_{\text{ref}}) \]

(c) determine hydrocarbon type adjustment,

\[ H_{RON_i} = \frac{c_3 O_i P_i}{1 + k_1 O_i} + \frac{c_5 A_i P_i}{1 + k_2 A_i} + c_7 A_i O_i \]
\[ H_{MON_i} = \frac{c_4 O_i P_i}{1 + k_1 O_i} + \frac{c_6 A_i P_i}{1 + k_2 A_i} + c_8 A_i O_i \]

(d) adjust octanes to "remove" hydrocarbon type interaction effects.

\[ RON_{\text{transf}_i} = RON_{\text{calc}_i} - H_{RON_i} \]
\[ MON_{\text{transf}_i} = MON_{\text{calc}_i} - H_{MON_i} \]

Step II: Blend transformed properties linearly:

\[ RON_{\text{transf,blend}} = \sum_{i=1}^{n} (u_i RON_{\text{transf}_i}) \]
\[ MON_{\text{transf,blend}} = \sum_{i=1}^{n} (u_i MON_{\text{transf}_i}) \]

\[ O_{\text{blend}} = \sum_{i=1}^{n} (u_i O_i) \]
\[ A_{\text{blend}} = \sum_{i=1}^{n} (u_i A_i) \]
Step III: transform the blended properties to blended octane numbers:

(a) hydrocarbon type adjustments,

\[ H_{RON \text{blend}} = \frac{c_3 O_{blend} P_{blend}}{1 + k_1 O_{blend}} + \frac{c_5 A_{blend} P_{blend}}{1 + k_2 A_{blend}} + c_7 A_{blend} O_{blend} \]

\[ H_{MON \text{blend}} = \frac{c_4 O_{blend} P_{blend}}{1 + k_1 O_{blend}} + \frac{c_6 A_{blend} P_{blend}}{1 + k_2 A_{blend}} + c_8 A_{blend} O_{blend} \]

(b) adjust transformed octanes to include effects of hydrocarbon type interactions,

\[ RON_{\text{calc\text{blend}}} = RON_{\text{transf\text{blend}}} - H_{RON\text{blend}} \]

\[ MON_{\text{calc\text{blend}}} = MON_{\text{transf\text{blend}}} - H_{MON\text{blend}} \]

(c) calculate sensitivity at reference octane severity levels.

\[ s_{\text{blend\text{ref}}} = RON_{\text{calc\text{blend}}} - MON_{\text{calc\text{blend}}} \]

(d) adjust from reference to actual severity levels.

\[ RON_{\text{blend}} = RON_{\text{calc\text{blend}}} - \frac{c_1 s_{\text{blend\text{ref}}} (RON_{\text{calc\text{blend}}} - RON_{\text{blend}})}{1 + c_1 s_{\text{blend\text{ref}}} \text{ MON}_{\text{calc\text{blend}}} - MON_{\text{calc\text{blend}}} - MON_{\text{blend}}} \]

\[ MON_{\text{blend}} = MON_{\text{calc\text{blend}}} - \frac{c_2 s_{\text{blend\text{ref}}} (MON_{\text{calc\text{blend}}} - MON_{\text{blend}})}{1 + c_2 s_{\text{blend\text{ref}}} \text{ MON}_{\text{calc\text{blend}}} - MON_{\text{calc\text{blend}}} - MON_{\text{blend}}} \]

where: \( c_1, c_2, c_3, c_4, c_5, c_6, c_7, c_8, k_1, \) and \( k_2 \) are constants to be determined, \( s \) is sensitivity \( (RON - MON) \), \( RON_{\text{ref}} \) and \( MON_{\text{ref}} \) are the reference \( RON \) and \( MON \) arbitrarily set at 90 [Rusin et al. 1981], \( H \) is effect of hydrocarbon type interaction, \( A_i, P_i, O_i \) are volume fractions of aromatics, paraffins, and olefins for component \( i \), respectively.

These blending models for \( RON \) and \( MON \) contain at least ten parameters \( (RON_{\text{ref}}, MON_{\text{ref}}, c_1, c_2, c_3, c_4, c_5, c_6, c_7, c_8, k_1, \) and \( k_2) \) which can be determined from the following experimental blending data:
- RON, MON, aromatics, paraffin, and olefin content of each component,
- RON and MON of each blend.

Predictive accuracy of the Transformation models was tested by Rusin et al. [1981] who used data from 564 gasolines of varying compositions from several independent blending studies. They split the data from each source roughly into halves and used the first half for determining the model parameters. The second half of the data set, together with data from two additional complete studies, was used to test the predictive accuracy of the models. The standard deviations of prediction errors were found to be around 0.4 to 0.5 of an octane number for both RON and MON blending.

As with the Ethyl method, the Transformation method requires RON, MON, olefin content, and aromatics content. The Transformation method also requires paraffin content. Moreover, the Transformation method requires the determination of ten regression coefficients compared to only six in the Ethyl models (three each for RON and MON). Furthermore, the Ethyl approach is much superior to the Transformation approach in terms of both model simplicity and ease of use.

2.1.6 EXCESS METHOD

This method deals with deviations from ideality by applying an “excess” term. These excess values are added to the volumetric average of the component octane numbers to predict the blended octane number (RON or MON) [Muller, 1992] as:

\[
(ON)_j = \sum_{i=1}^{n} u_{ij}(ON)_i + \sum_{i=1}^{n} u_{ij}(ON)_{ij}^E
\]

where: \((ON)_j\) is the octane number of blend \(j\), \((ON)_{ij}^E\) is the excess octane number associated with component \(i\) in blend \(j\), and \(u_{ij}\) is the volume fraction of component \(i\) in blend \(j\).

In this linear model, the excess octane number, \((ON)_{ij}^E\), gives an indication of the contribution to nonideality in blend \(j\) by component \(i\). These parameters for each blend are determined by preparing a series of “rest-blends”. The “rest-blends” are obtained by blending as many samples of the fuel as there are components but omitting one component after another. Note
that in preparing the “rest-blends” the volume of each component (except the omitted one) remains the same so the total volume and volumetric composition vary. Details of determining the excess numbers can be found in Muller [1992].

The number of \((ON)_{ij}^E\) values to be determined for each fuel grade (blend) is \(n\) and the experimental data needed to estimate these parameters are:

- octane number \((RON\text{ and } MON)\) of each component,
- octane number \((RON\text{ and } MON)\) of the blend,
- octane number \((RON\text{ and } MON)\) of the \(n\) “rest-blends”.

The number of fuels that need to be tested are \((n + d(n + 1))\). Thus, a total of \(2(n + d(n + 1))\) tests would be needed for \(MON\) and \(RON\) combined, where \(d\) is the number of gasoline grades.

The Excess method leads to linear blending models which has the advantage of allowing the use of linear programming (which is widely used in industry [Magoulas et al., 1988]) in determining the optimal blend recipe. However, the “excess” values are calculated for a given blend at its nominal composition. Therefore, the accuracy of this method will decrease as the composition deviates from this nominal point and new blending studies would have to be commissioned periodically to re-calculate “excess numbers”. Also, the parameters determined are specific to each blend. That is, “excess numbers” for different grades of gasoline (such as regular, premium, etc.) have to be determined separately whereas for other models, the same set of parameters is applicable to all gasoline grades.

No indication of the predictive accuracy or the level of industrial acceptance of this method could be found.

2.1.7 ZAHED METHOD

This method correlates feedstock octane numbers to predict the blended octane number. The parameters of the equation are estimated using regression analysis on experimental data [Zahed et al., 1993]. The blending model for \(RON\) is:

\[
(RON)_{\text{blend}} = M_0 + \sum_{i=1}^{n} M_i \left[u_i (RON)_i\right]^{k_3}
\]

(2.9)
An analogous method can be used for MON:

\[
(MON)_{\text{blend}} = Q_o + \sum_{i=1}^{n} Q_i [u_i (MON)]_{\text{blend}}
\]

(2.10)

where \(M_o, Q_o, M_1, Q_1, k_3, \) and \(k_4\) are constants, and \(n\) is the number of feedstocks in the blend.

Thus the parameters that need to be determined are \(M_o, M_1, ..., M_n,\) and \(k_3\) for RON, and \(Q_o, Q_1, ..., Q_n,\) and \(k_4\) for MON. The data needed for estimating these parameters are RON and MON of each blend and of the \(n\) components.

As with other models, the accuracy of this method is limited to the data set that is used in estimating the parameters since blending characteristics and therefore model parameters may change as feedstock qualities changes over time. The model parameters may be updated on-line using historical blend data. Zahed et al. [1993] have compared the predictive accuracy of the models in Equations (2.9) and (2.10) with that of the Stewart method and have shown it to be better at predicting blended RON for a set of experimental data. Standard deviations of prediction error were not provided.

### 2.1.8 SUMMARY OF OCTANE BLENDING MODELS

Table 2.1 summarizes blending models discussed above and Table 2.2 compares the predictive accuracy of the different models. Accuracy for interpolation (prediction within the development data set) as well as extrapolation (prediction outside the development data set) are provided. Surprisingly for the Transformation method, Rusin et al. [1981] have reported a higher prediction accuracy for extrapolation than for interpolation.

The Excess method, being linear, is valid only within the vicinity of the nominal blend. Also, there is little information available with regards to the predictive accuracy of the Excess, Stewart or Zahed methods. The Interaction method has been shown to be no more accurate than the Ethyl method in predicting blended octanes on general, untested data sets even though it has many more parameters than the Ethyl models. Although the Transformation models seem to provide slightly better predictive accuracy than the Ethyl models, they require more feedstock
quality data and contain more parameters (less parsimonious). Moreover, the Ethyl models are much more simple and easy to use than the Transformation models.

### 2.2 REID VAPOUR PRESSURE

The Reid Vapour Pressure (RVP), defined by the American Society for Testing and Materials under the designation ASTM D-323-56, gives an indication of the volatility of a gasoline blend and is approximately the vapour pressure of the gasoline at 100°F (38°C). The RVP of a gasoline blend affects the gasoline performance in terms of ease of starting, engine warm-up, and rate of acceleration [Gary and Handwerk, 1994]. RVP is also important because maximum specifications on RVP limit the amount of n-butane, a relatively cheap source of octane, that can be added to a blend.

#### 2.2.1 THEORETICAL APPROACHES

One of the first theoretical approaches available is that by Stewart [1959b] who presented a method for predicting blended RVP's by mathematically simulating the processes occurring during the Reid test (which measures the equilibrium pressure for a constant-volume partial vapourization of the fuel in air). The Stewart approach uses component data (such as feedstock

<table>
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<th>Model</th>
<th>Parameters</th>
<th># of Parameters</th>
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<tr>
<td></td>
<td>$a_4, a_5, a_6$</td>
<td></td>
</tr>
<tr>
<td>Stewart</td>
<td>$a, c$</td>
<td>2</td>
</tr>
<tr>
<td>Interaction</td>
<td>$I_{i,k}$</td>
<td>$\frac{n(n-1)}{2}$ for RON</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\frac{n(n-1)}{2}$ for MON</td>
</tr>
<tr>
<td>Transformation</td>
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<td>10</td>
</tr>
<tr>
<td></td>
<td>$c_5, c_6, c_7, c_8$</td>
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</tr>
<tr>
<td></td>
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<td></td>
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<td>Excess</td>
<td>$(ON)_{i,j}^E$</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>$n$ for MON</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$2n$ total for each grade</td>
</tr>
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<td>Zahed</td>
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</tr>
<tr>
<td></td>
<td>$Q_0, Q_i, k_4$</td>
<td>$n + 2$ for MON</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$2(n - 2)$ total</td>
</tr>
</tbody>
</table>

**Table 2.1: Comparison of Octane Blending Models**
Table 2.2: Predictive Accuracy of Octane Blending Models

composition and component volatility) and thermodynamic relationships in simulating the test. Several simplifying assumptions are made including: the presence of air and water vapour in the test chamber are ignored, the absolute pressure is taken as the RVP. volatile components are assumed to have the density of butanes, and the nonvolatile components are assumed to have the thermal expansion characteristics of n-octane [Stewart, 1959b].

The equations for estimating the blended RVP provided by Stewart [1959b] are:

$$(RV P)_{blend} = \frac{\sum_{i=1}^{k} \gamma_i \gamma_i (RV P)_i e^{0.0021(RVP)_i} e^{0.0021(RVP)_{blend}}}{\sum_{i=1}^{k} \gamma_i}$$

$$(RV P)_{blend} = \frac{u_i \rho_{M_i}}{\rho_{blend} - \frac{0.003632 e^{0.0021(RVP)_{blend}} \gamma_i e^{0.0021(RVP)_i}}{1 - e^{0.0021(RVP)_{blend} \gamma_i e^{0.0021(RVP)_i}}}}$$

where: $\gamma_i$ is the mole fraction of component $i$ in the liquid phase. $\gamma_i$ is the activity coefficient of component $i$. $u_i$ is the volume fraction of component $i$ in the blend (feed) at 1 atm and 60 °F. $\rho_{M_i}$ is the molar density of component $i$ (pound-moles per barrel as liquid at 1 atm and 60 °F). $\rho_{blend}$ is the density of the blend as saturated liquid at 60 °F (pound-moles per barrel). and $k$ is the number of components in the blend (components over all feedstocks).

The models given in Equation set (2.11) do not provide $(RV P)_{blend}$ explicitly as a function of component data; therefore, an iterative approach would have to be taken in solving for the blended RVP. The data required in using the Stewart method are RVP's of each feedstock, volume fractions of all components in each feedstock, molar densities of all components in each
feedstock, and estimates of activity coefficients of all components.

Vazques et al. [1992] have presented an algorithm for calculating the blended RVP's based on the work of Stewart [1959b]. The model assumes additivity of liquid and gas volumes and, as in the Stewart case, the algorithm is based on an air and water-free model. This approach differs from the Stewart method in the equation of state used and it requires that the molar composition of the feedstocks be known. An iterative procedure for calculating the vapour-liquid equilibrium for the flashing of the gasoline feed is provided. The steps required by this method are outlined below:

**Step 1:** Calculate the molecular weight of the blend:

\[
(MW)_{\text{blend}} = \sum_{i=1}^{m} \vartheta_i (MW)_i
\]

**Step 2:** Evaluate density of blend at 35 °F, 60 °F, and 100 °F. Compute liquid expansion of blend as:

\[
\nu_o = \rho_{60} \left[ \frac{5}{\rho_{35}} - \frac{1}{\rho_{100}} \right]
\]

**Step 3:** Perform "flash calculation" at 100 °F using the Gas Processors Association Soave-Redlich-Kwong equation of state [Vazques et al. 1992]. It is suggested that \( \frac{\bar{F}}{\bar{L}} \) of 0.97 be used initially.

**Step 4:** Calculate new \( \frac{\bar{F}}{\bar{L}} \) using:

\[
\frac{\bar{F}}{\bar{L}} = \frac{1}{1 + \left[ \frac{\rho_{60} (MW)_L (MW)_V}{\rho_L (MW)_L (MW)_V \frac{\nu_o}{1 - \frac{\rho_{60}}{\rho_L}}} \right]}
\]

**Step 5:** Use \( \frac{\bar{F}}{\bar{L}} \) from Step 4 to re-do the "flash calculation" in Step 3 and repeat until \( \frac{\bar{F}}{\bar{L}} \) converges to an acceptable degree.

**Step 6:** The pressure obtained from the equation of state in Step 3 using the converged \( \frac{\bar{F}}{\bar{L}} \) is the blended RVP.

where: \( F \) is the mass of the feed used in the Reid test, \( \bar{V} \) is the mass of the vapour phase obtained by flashing \( F \), and \( \bar{L} \) is the mass of the liquid phase; \((MW)_L\), \((MW)_V\), \((MW)_i\), and
\((MW)_{\text{blend}}\) are the molecular weights of the liquid phase, the vapour phase, component \(i\), and the blend, respectively; \(\rho_V\), \(\rho_L\), and \(\rho_{LF}\) are the densities of the liquid phase, vapour phase, and liquid feed (at 100 °F); \(\rho_{35}, \rho_{60}, \text{ and } \rho_{100}\) are the densities of the liquid blend at 35 °F, 60 °F, and 100 °F, respectively; \(\vartheta_i\) is the mole fraction of component \(i\), and \(u_o\) is the expanded liquid volume.

Details of how the blend densities at the different temperatures and the densities of the liquid and vapour phases can be obtained have not been provided. Also, it is not clear how values needed in Step 4 can be obtained from the equation of state in Step 3. The equation of state used is the Soave-Redlich-Kwong equation [Vazques et al. 1992]:

\[
\hat{P} = \frac{\hat{R}T}{v - \hat{b}} \left( v + \hat{b} \right)
\]

where: \(\hat{P}\) is the pressure, \(\hat{R}\) is the gas constant, \(v\) is gas volume, and \(\hat{a}\) and \(\hat{b}\) are constants.

The parameters \(\hat{a}\) and \(\hat{b}\) are determined according to the Gas Processors Association [Vazques et al. 1992] rules as:

\[
\hat{a} = \sum_{i=1}^{m} \sum_{j=i+1}^{m} \vartheta_i \vartheta_j \hat{a}_{ij} \\
\hat{b} = \sum_{i=1}^{m} \hat{b}_i \\
\hat{a}_{ij} = [\hat{a}_i \hat{a}_j]^{0.5} \left[ 1 - K_0 \hat{a}_{ij} - K_1 \hat{a}_{ij} \frac{T}{1000} \right]
\]

where: \(m\) is the number of components over all feedstocks, \(\hat{a}_i\) and \(\hat{a}_j\) are the Soave-Redlich-Kwong constants for the pure component \(i\) and \(j\), \(\hat{b}_i\) is the Soave-Redlich-Kwong constant for pure component \(i\), and \(K_0\) and \(K_1\) are the binary interaction parameters used to represent the vapour-liquid equilibria of binary mixtures.

This method requires that the molar composition of all the feedstocks be known which may not be readily available. Also, correlations for estimating densities would be required. In addition, experimental data may be needed to determine the parameters in the Soave-Redlich-Kwong [Vazques et al. 1992] equation of state.
The major drawback of the theoretical approaches is that they are not easy to use on-line in that they require complex calculations and iterative solutions. Also, they require data such as feedstock molar compositions and component activity coefficients which may not be available.

2.2.2 INTERACTION METHOD

The interaction approach has also been applied to \( RVP \) blending by Morris [1975]. The blending model is of the same form as in Equations (2.6) and (2.7) except \( RVP \) is blended instead of \( ON \) (octane numbers). Here also, only interactions between pairs of components is considered; the three-way and higher interaction terms are ignored. The Interaction model is:

\[
(RVP)_{\text{blend}} = \sum_{i=1}^{n} u_i (RVP)_i + \sum_{i=1}^{n} \sum_{k=i+1}^{n} (u_i u_k I_{i,k})
\]

\[
I_{i,k} = 4(RVP)_{i,k} - 2[(RVP)_i + (RVP)_k]
\]

where: \( n \) is the number of feedstocks, \( I_{i,k} \) is the interaction coefficient between feedstock \( i \) and \( k \), and \( (RVP)_{i,k} \) is the \( RVP \) of a 50:50 blend of \( i \) and \( k \).

The number of interaction coefficients required would be \( \frac{n(n-1)}{2} \). Some indication of the accuracy of the Interaction method can be found in Morris [1975] where the standard deviation of prediction error on an 8 component, 42 blend study is reported to be 0.18 psi.

2.2.3 BLENDING INDEX METHOD

An easy to use empirical method developed by the Chevron Research Company is the Blending Index method [Gary and Handwerk, 1994]. In this approach, blended \( RVP \)'s are predicted using the Reid Vapour Pressure Blending Indices \( (RVPBI) \) which blend linearly. The \( RVPBI \)'s are given in Gary and Handwerk [1994] and are of the form shown below [Gary and Handwerk, 1994]:

\[
RVPBI = (RVP)^{1.25}
\]

(2.12)

\[
(RVPBI)_{\text{blend}} = \sum_{i=1}^{n} (RVPBI)_i
\]

(2.13)
<table>
<thead>
<tr>
<th>Method</th>
<th>Standard Deviation (psi)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stewart</td>
<td>0.76</td>
</tr>
<tr>
<td>Ideal blending *</td>
<td>1.30</td>
</tr>
<tr>
<td>Haskel and Beavon [1942]</td>
<td>1.01</td>
</tr>
<tr>
<td>Molar average</td>
<td>1.17</td>
</tr>
</tbody>
</table>

*Ideal blending is volumetric average $RVP$

All data from Stewart [1959b]

Table 2.3: Predictive Accuracy of RVP Blending Models

2.2.4 OTHER METHODS

Haskell and Beavon [1942] presented a method which involves the volumetric averaging of the component $RVP$'s except those of butanes which were treated differently; the butanes are assigned variable “blending pressure values” which were calculated based on the $RVP$ of the butane and that of the debutanized blend (blend with all components except the butanes). Another simple approach that has been used involves molar averaging (not volumetric) of the component $RVP$'s based on the blend composition [Stewart, 1959b]. However, molar composition of feedstocks may not be readily available.

2.2.5 SUMMARY OF $RVP$ BLENDING MODELS

Comparisons of predictive accuracy of some of the methods can be found in Stewart [1959b] who looked at the standard deviation of prediction error for 67 blends using different models. The reported standard deviations are presented in Table 2.3. It is not surprising that the method based on modeling the actual process provides more accurate predictions. However, the theoretical methods by Stewart [1959b] and Vazques et al. [1992] are not suitable for use in on-line control systems due to their computational requirements. The interaction method is also not suitable for on-line implementation since it requires that a lot of parameters be updated on-line as discussed in the octane blending case. Although not as accurate as the theoretical methods, simpler methods such as the Blending Index method can easily be incorporated in on-line controllers.
2.3 ASTM DISTILLATION

Gasolines, since they are mixtures of hydrocarbons with different boiling points, vapourize over temperature ranges. For example, the light virgin naphtha stream vapourizes throughout a temperature range of 30°C - 90 °C. The volatility characteristics of gasoline is measured by the ASTM D-86 distillation which is a standardized laboratory batch distillation that is carried out at atmospheric pressure without fractionation. It gives amount (percent volume) distilled to a given temperature. Several temperatures along the distillation curve are used as reference points in comparing the volatility properties of gasolines. Equivalently, distillation properties can be specified as temperatures at a given percent evaporated. Some of the methods for predicting blended distillation points available in literature are briefly discussed next.

2.3.1 INTERACTION METHOD

The interaction method, as described for octane blending, can be used to predict the ASTM distillation points as percent evaporated at a given temperature [Morris, 1983], [Morris, 1975]. Again, only the two-way interactions are considered and the interaction coefficients between all the component pairs would have to be determined for each temperature on the distillation curve. As in the octane and RVP blending cases, determination of the interaction coefficients require the quality (percent evaporated at that temperature) of the individual components as well as those of the 50:50 blends and are calculated as described for the octane blending case. This method is only applicable to the intermediate points, not to end points of gasoline blends.

The biggest drawback to using the Interaction model is the large number of parameters that would have to be determined. For each temperature on the distillation curve, \( \frac{n(n-1)}{2} \) parameters are needed where \( n \) is the number of components. Thus for a 7 component blend with 5 points on the distillation curve, 105 interaction coefficients would be required.

2.3.2 EMPIRICAL MODELS

Empirical models are quite often used in predicting the ASTM distillation points of blends and owe their popularity to their ease of use. Stanley and Pingrey [1954] have developed correlations for predicting the end points of distillation curves when only the blend composition and component ASTM distillations are known. Correlation analysis on experimental data was
used (details of which were not provided) to produce tables of values that can be used for distillation end point estimation. This method does not provide estimates for intermediate points on the distillation curve.

Dhulesia [1984] has reported using models of the form:

\[
\tilde{v} = \left\{1 - e^{-\left(\frac{T}{\alpha_1}\right)^{\alpha_2}}\right\} 100
\]

\[
T^* = \frac{T_f - T_i}{T_f - T_i}
\]

where: \(\alpha_1\) and \(\alpha_2\) are constants, \(\tilde{v}\) is the percent volume evaporated, \(T_f\) and \(T_i\) are the final and initial boiling points, respectively, of the blend.

Another empirical model reported is of the form [DeWitt et al., 1989]:

\[
\tilde{v}_k = \alpha_3 + \alpha_4 \ln \left[ \sum_{i=1}^{n} (u_i \tilde{v}_{i,k}) \right]
\]

where: \(\alpha_3\) and \(\alpha_4\) are constants, \(\tilde{v}_k\) is the percent evaporated at temperature \(k\) for the blend, and \(\tilde{v}_{i,k}\) is the percent evaporated at temperature \(k\) for component \(i\) in the blend.

Indications of predictive accuracy of the models could not be found; thus sufficient information is not available to allow comparisons to be drawn among the different models.

### 2.4 BLENDING SIMULATION

In order to conduct blending control studies by simulation, models that can closely represent the blending process are required. Blending models are also needed for off-line blend optimization, as well as on-line blend optimization and control. For the purposes of the present research, only octane number (RON and MON) and RVP blending will be simulated. Other qualities will not be considered. The blending simulation has been restricted to the three most important gasoline properties so that the important results can be highlighted without adding unnecessary complications.

A good blending model should provide acceptable predictive accuracy, it should be parsimonious and easy to use, and it should not require a large data set to be trained on. Also, for on-line
optimization, a model that can be readily updated on-line would be desirable. This is because models are not perfect and their predictive accuracy usually degrades over time (as feedstock properties and thus blending characteristics change with time) unless they are appropriately updated periodically.

Octane blending models have been discussed and compared in Section 2.1. Among the models found in published literature, the Ethyl RT-70 [Healy et al., 1959] models were found to exhibit the best combination of predictive accuracy and parsimony. Also, the Ethyl models can readily be made adaptive for on-line implementation. Healy et al. [1959] have used data from 135 blends to determine the correlation coefficients. Thus the Ethyl correlations with the published coefficient values were chosen over the other octane blending models.

RVP blending models have been discussed in Section 2.2. Very little information is currently available in literature that can be used to choose the best RVP blending model. Also, blending data is not available that can allow the different models to be compared for predictive accuracy. Thus, based on ease of use and a high degree of industrial acceptance, the Blending Index method was chosen for modeling RVP blending. The selected models are presented again for completeness in the following equation set and will henceforth be used to model the gasoline blending process:

\[
\begin{align*}
RO_{Nblend} & = r + a_1(r\bar{s} - r\bar{\bar{s}}) + a_2(\bar{O}^2 - \bar{O}^2) + a_3(\bar{A}^2 - \bar{A}^2) \\
\text{MON}_{blend} & = \bar{m} + a_4(\bar{m}\bar{s} - \bar{m} \bar{s}) + a_5(\bar{O}^2 - \bar{O}^2) + a_6 \left[ \frac{(\bar{A}^2 - \bar{A}^2)}{100} \right]^2 \\
(RVP_{BII})_{blend} & = \frac{RVP_{BII}}{100} = \sum_{i=1}^{n} u_i(RVP)_{i}^{1.25}
\end{align*}
\]

The parameters used for octane number blending are [Healy et al., 1959]: \(a_1 = 0.03224\), \(a_2 = 0.00101\), \(a_3 = 0\), \(a_4 = 0.04450\), \(a_5 = 0.00081\), and \(a_6 = -0.00645\).

These equations and parameters will be considered to adequately represent the actual blending process for the purposes of the studies contained in this thesis.
Chapter 3

PARAMETER OBSERVABILITY IN RTO SYSTEMS

In Chapter 2, gasoline blending models were examined for use in the gasoline blending RTO system shown in Figure 1-4. Since the selected blending models are to be used on-line, the adjustable parameters in the models would have to be updated on-line in order to maintain model accuracy. Therefore, it is important that all adjustable models parameters be observable for the available measurements. That is, the measurements should allow unique estimates of the adjustable parameters to be obtained through some estimator. The success of any RTO system is dependent on all the adjustable parameters being observable from the process measurements and given estimation scheme.

This chapter investigates parameter observability and begins with a survey of the currently available methods of determining observability. A new measure of parameter observability is then developed based on fundamental statistical principles and the observability concept is extended to degree of observability. The chapter concludes with examples to illustrate how the new observability measure can be applied to different estimation schemes.

3.1 BACKGROUND

Observability was originally defined and studied for linear dynamic systems by Kalman [1960] as a dual to controllability. Kalman observability is used to determine whether a given set
of measurements contain sufficient information from which the states of the system can be
determined (Brogan [1991], Friedland, [1986]). It will only be briefly discussed here since the
focus of the present work is RTO of steady-state operations policy. Consider the standard
state-space representation of a dynamic linear process:
\begin{align}
\dot{y} &= A(t)y + B(t)u + \xi(t) \\
z &= C(t)y + \nu(t) \\
y(0) &= y_0 + \xi_0
\end{align}

where: $y$ is a vector of state variables, $u$ is a vector of control moves, $z$ is a vector of measure-
ments or outputs, and $\xi(t)$ and $\nu(t)$ are noise terms.

The system given in Equation set (3.1) is said to be completely observable if every initial state
$y(t_0)$ can be determined through knowledge of the system control, $u(t)$, and output, $y(t)$, over
some finite time interval $t_0 \leq t \leq t_1$ [Ray, 1981]. For systems where the matrices $A$ and $C$ do
not vary with time, observability can be checked by constructing the observability matrix $M:

$$M = \begin{bmatrix}
C \\
AC \\
A^2C \\
\vdots \\
A^{q-1}C
\end{bmatrix}$$

where: $q$ is the number of state variables.

The linear dynamic system with constant matrices $A$ and $C$ is completely observable if and
only if the rank of the observability matrix $M$ is $q$, where $q$ is the number of state variables
[Ray, 1981]. Here complete observability means that every state variable is observable. If only
a subset of the state variables are observable, the system is said to be partially observable.
Conditions for other classes of dynamic systems can be found in Bryson and Ho [1976] and
Aström [1970].

Note that checking for observability by testing the rank of the observability matrix can yield only
two possible outcomes - observable or unobservable. No indication of degree of observability is
provided by the test. Gudi [1995] has looked at the singular values of the observability matrix
to characterize degree of observability. Gudi [1995] has used the condition number, the ratio
of the largest singular value of $M$ to the smallest, as a measure of degree of observability.
A small condition number indicates that the state variables are "strongly observable" while a large condition number indicates "weak observability". Since condition numbers are scale dependent [Golub and Van Loan, 1989], such a measure of degree of observability will also be scale dependent.

The concept of observability was extended from linear dynamic systems to nonlinear steady-state systems by Stanley and Mah [1981] while retaining the fundamental idea behind observability. That is, it is used to check if changes in all the state variables can be determined through knowledge of the process outputs (measurements) and the steady-state models that describe the process. Stanley and Mah [1981] considered a steady-state system of dimension $q$ with $m$ measurements shown in Figure 3-1. They defined the system as the triplet $(S, \zeta, V)$ where $S$ is the feasible set of states that always satisfy equality, inequality and strict inequality constraints, $\zeta$ is the vector of equations that relate the measurements to the state variables, and $V$ is the set from which measurement noise realizations are obtained.

The measurements are given by the measurement functions as:

$$z = \zeta(y) + v, \quad v \in V, \ y \in S'$$

where: $y$ is a vector of state variables, $v$ is the noise vector, $z$ is the measurement vector, and $S'$ is the closure of set $S$ consisting of $S$ and all its limit points. In the case of perfect measurements, $V = \{0\}$, $v = 0$, and $z = \zeta(y)$.

The authors define the steady-state system $(S, \zeta, V)$ as being in "standard form" if $S = \{y : \omega(y) = 0, \ y \in N\}$ where vector $\omega$ contains plant model equations such as material and energy balances, thermodynamic relations, etc., $N$ is the union of a finite number of convex sets, $N_i \subset \mathbb{R}^q$, that defines the plant operating region. Since equations in vectors $\zeta$ and/or $\omega$ may be nonlinear, observability is defined as a local property.

Stanley and Mah [1981] have provided some definitions regarding observability that are useful for the present work. These are given below.

**Definition 1 Local Unobservability:** in a system $(S, \zeta, V)$ let $y_o \in S'$ and $I$ be an index
Figure 3-1: Steady-State System and Estimator Considered by Stanley and Mah [1981].

set. $y^f$ is locally unobservable at $y_o$ if there exists a sequence $\{y_k\}^\infty_{k=1}$ such that:

$$y_k \to y_o, \text{ as } k \to \infty$$

$$\begin{cases} y_k \in S \\ \zeta(y_k) = \zeta(y_o) \\ \delta y_k^f = y_k^f - y_o^f \neq 0 \end{cases} \text{ for all } k$$

That is, the states included in the index set $I$ are defined to be locally unobservable if there are changes within this set of states that do not result in a corresponding change in measurements. For the situation described in the definition of local unobservability, even though $y_k$ differs from $y_o$, they both result in the same measurement value. As a result, one cannot be distinguished from the other and the system is said to be locally unobservable at $y_o$. Observability is then defined by Stanley and Mah [1981] in terms of unobservability:

**Definition 2 Local Observability:** in a system $(S, \zeta, V)$ let $y_o \in S'$. $y^f$ is locally observable at $y_o$ if it is not unobservable.

Stanley and Mah [1981] have also provided a method of testing local observability which is
given in the following theorem:

**Theorem 3** For a system given in the standard form $S = \{ y : \omega(y) = 0, \ y \in \mathbb{N} \}, \ y_o \in S$, let $\omega$ and $\zeta$ be continuously differentiable in some neighbourhood of $\mathbb{R}^n$ containing $y_o$. The system is calculable on some set $S_o \subset S$ containing $y_o$ if rank

$$\begin{bmatrix}
\nabla_y \omega(y_o) \\
\nabla_y \zeta(y_o)
\end{bmatrix} = q$$

where $q$ is the number of states in the steady-state system, $\nabla_y \omega(y_o)$ and $\nabla_y \zeta(y_o)$ are the Jacobian matrices of $\omega$ and $\zeta$, respectively, evaluated at $y_o$.

Thus, instead of checking the rank of the observability matrix $M$, as in the case of linear dynamic systems, the rank of the augmented Jacobian matrix

$$\begin{bmatrix}
\nabla_y \omega(y_o) \\
\nabla_y \zeta(y_o)
\end{bmatrix}$$

should be checked. As in the linear dynamic case, if the rank is found to be less than $q$, the state variables are not completely observable. The rationale behind the rank requirement for local observability can be illustrated using first-order Taylor series approximation [Corwin and Szczarba, 1995] to the process model, $\omega(y)$, and measurement equations, $z = \zeta(y)$, about $y_o$:

$$\nabla_y \omega(y_o) \Delta y \approx 0$$

$$\Delta z - \nabla_y \zeta(y_o) \Delta y \approx 0$$

which can be written as:

$$\begin{bmatrix}
\nabla_y \zeta(y_o) \\
\nabla_y \omega(y_o)
\end{bmatrix} \Delta y = \begin{bmatrix} \Delta z \\ 0 \end{bmatrix}$$

In order to ensure that changes in states ($\Delta y$) are uniquely observable from the changes in the measurements ($\Delta z$), the matrix

$$\begin{bmatrix}
\nabla_y \zeta(y_o) \\
\nabla_y \omega(y_o)
\end{bmatrix}$$

must have rank $q$. That is, the augmented Jacobian matrix must not be column rank deficient.

The concepts of state observability for steady-state systems was extended to parameter observability by Krishnan [1990] who considered a general nonlinear system where the steady-state model of the process and the measurement equations are defined as:

$$\omega(y, \beta) = 0$$

$$z = \zeta(y)$$
where: $\beta \in \mathbb{R}^p$ is the adjustable parameter vector to be determined.

As an extension of the rank condition in Theorem 3 for local state observability, for all the parameters and states of the systems to be observable at $y_o$, the observability criterion presented by Krishnan [1990] requires that:

$$\text{rank} \begin{bmatrix} \nabla_y \omega(y_o) & \nabla_\beta \omega(y_o) \\ \nabla_y \zeta(y_o) & 0 \end{bmatrix} = q + p \tag{3.2}$$

where: $q$ is the number of state variables and $p$ is the number of parameters to be determined.

The need for the above rank requirement can be illustrated using the Implicit Function Theorem [Corwin and Szczarba, 1995]:

$$d\omega = \frac{\partial \omega}{\partial y} dy + \frac{\partial \omega}{\partial \beta} d\beta = 0$$

$$d\zeta = \frac{\partial \zeta}{\partial y} dy = dz$$

These can be rearranged to give:

$$\begin{bmatrix} \nabla_y \omega & \nabla_\beta \omega \\ \nabla_y \zeta & 0 \end{bmatrix} \begin{bmatrix} dy \\ d\beta \end{bmatrix} = \begin{bmatrix} 0 \\ dz \end{bmatrix} \tag{3.3}$$

Thus for this linear system of equations to have a unique solution with respect to $dy$ and $d\beta$ at $y_o$, the rank of the matrix:

$$\begin{bmatrix} \nabla_y \omega(y_o) & \nabla_\beta \omega(y_o) \\ \nabla_y \zeta(y_o) & 0 \end{bmatrix}$$

must be the number of parameters plus number of states.

As illustrated in Figure 3-1, the objective behind an observability study is to determine if estimates of the system states (or the parameters as in the case of parameter observability) can be obtained from the measurements and the estimator. While the parameter observability criterion in Equation (3.2) contains information about the steady-state process and the measurements, no information about the estimator, $\Phi$, is included. The characteristics of the estimation procedure can have a very significant effect on whether or not the unmeasurable
quantities (parameters and states) can be determined from the measurements. Even when these quantities are observable through the model and measurement equations, a poorly designed estimation procedure may not allow the measurements to be uniquely mapped onto estimates, rendering the unmeasurable quantities unobservable. Therefore, the characteristics of the estimator should be considered.

### 3.2 PARAMETER OBSERVABILITY

The observability criteria presented by Stanley and Mah [1981] and Krishnan [1990] do not consider the effect of the estimation procedure. Their methods for determining observability have been based only on the models that describe the steady-state model equations and process measurements. If the system is unobservable according to the rank criterion in Equation (3.2), then the variables will certainly be unobservable through the whole updating procedure. However, compliance with Equation (3.2) does not guarantee observability through the entire updating process. That is, Equation (3.2) provides a necessary but not sufficient condition for local observability. For a sufficient condition, properties of the estimator would have to be included in formulating a measure of observability. In this section parameter observability for nonlinear steady-state systems will be considered and a new measure of observability will be developed based on statistical principles. The concepts will then be extended to provide measures of degree of observability. First, a definition of parameter observability is provided:

**Definition 4** Parameters are defined to be observable from a given set of process measurements if a unique set of parameter estimates can be determined using a specified updating scheme.

In order to gain insight into how parameters may become unobservable, consider a steady-state system for which the adjustable parameters ($\beta$) have to be estimated using the measurements ($z$) as shown in Figure 3-2.

For the purposes of this work, measurements are assumed to be corrupted with noise and so have a random component. These measurements get mapped to the parameter estimates ($\hat{\beta}$). Thus, the parameter estimates ($\hat{\beta}$) also have a random component. While measurement error may be normally distributed, the same is not necessarily true for the resulting estimates. Figure 3-2 shows the propagation of measurement noise through what may be a nonlinear updating
Fi-we b scheme, which will distort the distribution characteristics. The developments of this chapter assume that the parameter estimates may be locally approximated in some small neighbourhood of the nominal estimates using multivariate normal distribution (i.e., \( \hat{\beta} \sim \mathcal{N}_p(\beta, Q_\beta) \)). The probability density function of \( \hat{\beta} \) for positive definite \( Q_\beta \) can then be expressed as (Chatfield and Collins, 1980):

\[
f(\hat{\beta}) = \frac{1}{(2\pi)^{p/2}|Q_\beta|^{1/2}} \exp \left[ -\frac{1}{2} (\hat{\beta} - \bar{\beta})^T Q_\beta^{-1} (\hat{\beta} - \bar{\beta}) \right]
\]

(3.4)

For a bivariate case, this function represents a bell-shaped surface whose probability contours on the parameter plane are concentric ellipses around \( \bar{\beta} \). In general, the surface contours in the parameter space are p-dimensional ellipsoids. Thus, the function in Equation (3.4) exhibits a single extremum which is a maxima located at \( \bar{\beta} \).

The surface would not possess a unique maxima if the surface were to become flat in which case the updater would not be able to use the measurements to obtain a unique set of parameter estimates. The conditions under which such a situation could arise can be examined by looking at the distribution of \( \hat{\beta} \) more closely. Note that the inverse of the covariance matrix appears in the exponential term in Equation (3.4) and the determinant of \( Q_\beta \) appears in the denominator of the pre-exponential term. One definition of the determinant of \( Q_\beta \) is (Chatfield and Collins, 1980):

\[
|Q_\beta| = \prod_{i=1}^{p} \lambda_i
\]

(3.5)

where \( \lambda_1, ..., \lambda_p \) are the eigenvalues of \( Q_\beta \).

The eigenvalues of \( Q_\beta^{-1} \), \( \eta_i \), are reciprocals of the eigenvalues of \( Q_\beta \) (i.e., \( \eta_i = \frac{1}{\lambda_i}, i = 1, ..., p \)) (Chatfield and Collins, 1980). Now, as an eigenvalue \( \eta_i \) decreases, \( |Q_\beta| \) increases and the probability density function decreases in height. At the same time, the hyper-ellipsoid elongates in
the direction of the corresponding eigenvector of $Q_\beta^{-1}$, $\tau_j$, as will be discussed later. In the limit as $\eta_j \to 0$, the surface becomes flat and exhibits no extremum; at this point a unique set of estimates does not exist and the parameters are unobservable. Then observability can be defined in terms of the properties of $Q_\beta$.

Conditions for observability can also be seen by examining the shape of the joint confidence interval of the parameter estimates. For a prescribed probability $f(\hat{\beta})$ and a given covariance matrix $Q_\beta$, the probability density function can be written as [Chatfield and Collins, 1980]:

$$
\hat{c} = \exp \left[ -\frac{1}{2} (\hat{\beta} - \bar{\beta})^T Q_\beta^{-1} (\hat{\beta} - \bar{\beta}) \right] \tag{3.6}
$$

Taking logarithms of both sides and multiplying by -1 gives the following quadratic equation:

$$
c^2 = \frac{1}{2} (\hat{\beta} - \bar{\beta})^T Q_\beta^{-1} (\hat{\beta} - \bar{\beta}) \tag{3.7}
$$

The random variable $c^2$ follows a chi-squared distribution with $p$ degrees of freedom [Chatfield and Collins, 1980]. For a prescribed value of $c^2$, this equation describes the surface on which the probability density function has a constant value. Since $Q_\beta$ is required to be positive definite for validity of Equation (3.4), the surface in Equation (3.7) is a $p$-dimensional ellipsoid that describes the joint confidence region of the parameter estimates [Sorenson, 1980]. The lengths of the semi-axes of these hyper-ellipsoids indicate the uncertainty in the corresponding eigenvector directions in the space of the parameters [Sorenson, 1980], [Krishnan, 1990]. The semi-axes of the hyper-ellipsoid have magnitudes $\frac{c^2}{\eta_j}$ and have directions defined by the eigenvectors $\tau_j$ [Sorenson, 1980]. For good estimates then, large eigenvalues of $Q_\beta^{-1}$ are desired.

Alternatively, conditioning of the joint confidence region can be studied by examining $Q_\beta^{-1}$ which is the Hessian of $c^2$. As an eigenvalue of $Q_\beta^{-1}$, $\eta_j$, approaches zero, the Hessian becomes very ill-conditioned. As $\eta_j$ approaches zero, the confidence contours in the parameter space stretch out in the direction of $\tau_j$ and in the limit become unbounded as depicted for a bivariate case in Figures 3-3(a) to 3-3(d).

In Figure 3-3(a), the contours are concentric circles which indicate a perfectly conditioned $Q_\beta^{-1}$ (all eigenvalues are equal). As one of the eigenvalues decreases, the contours elongate as shown
in Figures 3-3(b) and (c). Figure 3-3(d) shows the limit case when one of the eigenvalues of $Q^{-1}_\beta$ reaches zero and the contours become unbounded. At this point, a unique $\beta$ does not exist and the parameters become unobservable. Hence an alternate definition of parameter observability can be provided in terms of the eigenvalues of the inverse of the covariance matrix:

**Definition 5** For any updating procedure where parameter estimates ($\hat{\beta}$) (assumed to be locally normally distributed) are to be determined using measurements ($z$), the parameters are observable if all the eigenvalues of $Q^{-1}_\beta$ are strictly positive (positive and nonzero) where $Q_\beta$ is the covariance matrix of $\hat{\beta}$.

In order to demonstrate how parameter observability relates to the covariance matrix of the estimates, a simple linear example is used below. The example will illustrate how parameters
can become unobservable and how unobservability of parameters can be detected.

Example 3.1

Consider a simple problem of estimating parameters \( \beta \) using measurements \( z \) which are related by the model:

\[
z = \chi \beta + \nu
\]

where: \( z \) is a vector of measurements or observations, \( \beta \) is the vector of parameters to be estimated, \( \chi \) is a matrix of operating conditions, and \( \nu \) is a vector of errors in the observations distributed as \( N(\bar{\beta}, Q_v) \), \( Q_v = \sigma^2 I \). Note that the operating conditions in \( \chi \) are variables but not random variables.

The least squares estimate, \( \tilde{\beta} \), is given by the normal equations [Draper and Smith, 1966]:

\[
\tilde{\beta} = (\chi^T \chi)^{-1} \chi^T z
\]

The estimates \( \tilde{\beta} \) are normally distributed with mean \( \bar{\beta} \) and covariance matrix \( Q_{\tilde{\beta}} \); the covariance matrix is given by [Draper and Smith, 1966]:

\[
Q_{\tilde{\beta}} = (\chi^T \chi)^{-1} \sigma^2
\]

Case A:

\[
z = \begin{bmatrix} 22.944 \\ 18.966 \\ 32.041 \end{bmatrix}, \chi = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 0 & 3 \\ 3 & 2 & 4 \end{bmatrix}, \beta = \begin{bmatrix} 2 & 3 & 5 \end{bmatrix}^T, \text{ and } \sigma^2 = 1.
\]

\[
\tilde{\beta} = \begin{bmatrix} 2.08 \\ 3.03 \\ 4.93 \end{bmatrix}^T \text{ and } Q_{\tilde{\beta}} = \begin{bmatrix} 1.186 & 0.3438 & -0.8750 \\ 0.3438 & 0.5469 & -0.4375 \\ -0.8750 & -0.4375 & 0.7500 \end{bmatrix}
\]

The eigenvalues of \( Q_{\tilde{\beta}}^{-1} \) are 0.48, 53.02, and 2.49. Since all the eigenvalues of \( Q_{\tilde{\beta}}^{-1} \) are nonzero, the parameters are observable. Also, the least squares estimates obtained (\( \tilde{\beta} \)) are quite close to the true value of the parameters (\( \beta \)).
Case B: If rank$[\chi] < 3$, the matrix $\left( \chi^T \chi \right)$ would not be invertible and the parameters would not be observable. Consider the case where the third row is dependent on the first two:

$$\chi = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 0 & 3 \\ 3 & 2 & 6 \end{bmatrix}, \quad \beta = \begin{bmatrix} 2 & 3 & 5 \end{bmatrix}^T, \quad \text{and} \quad \sigma^2 = 1.$$ 

Here $Q^{-1}_\beta = \frac{(\chi^T \chi)}{\sigma^2}$ and its eigenvalues are 2.489, 0, and 73.511. The zero eigenvalue of $Q^{-1}_\beta$ indicates that the parameters are unobservable and the least squares estimate cannot be obtained.

Case C: In this case $\chi$ is not singular but is poorly conditioned (the condition number $\kappa_2$, the ratio of the largest eigenvalue of $\chi$ to the smallest, is 285.3):

$$z = \begin{bmatrix} 23.032 \\ 19.152 \\ 41.575 \end{bmatrix}, \quad \chi = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 0 & 3 \\ 3 & 2 & 5.9 \end{bmatrix}, \quad \beta = \begin{bmatrix} 2 & 3 & 5 \end{bmatrix}^T, \quad \text{and} \quad \sigma^2 = 1.$$ 

Here $\tilde{\beta} = \begin{bmatrix} 0.449 & 2.165 & 6.084 \end{bmatrix}^T$, $Q_{\tilde{\beta}} = \begin{bmatrix} 660.250 & 329.875 & -445.000 \\ 329.875 & 165.313 & -222.500 \\ -445.000 & -222.500 & 300.000 \end{bmatrix}$.

The least squares estimate, $\tilde{\beta}$, is a very poor estimate of $\beta$ (in that the estimates are quite far from the true values of the parameters) because the parameters are practically unobservable. This can be seen by examining the eigenvalues of $Q_{\tilde{\beta}}$ which are $8.9 \times 10^{-4}$, 2.43, and 72.3. Although all the eigenvalues are nonzero, one of the eigenvalues is very small, causing the parameters to become practically unobservable. Also, the joint confidence region is very ill-conditioned - the condition number, $\kappa_2 = \frac{\eta_{\text{max}}}{\eta_{\text{min}}}$, is $8.1 \times 10^4$ and so the joint confidence interval is very elongated in the direction corresponding to $\eta_{\text{min}}$. That is, the uncertainty in parameter estimates in the direction corresponding to $\eta_{\text{min}}$ is almost $10^5$ times larger than in the direction corresponding to $\eta_{\text{max}}$.

In this rather simple linear example it is easy to recognize the estimation problem as being poorly posed by examining the condition number of $\chi$. Nonlinear estimation problems can be
checked in a similar manner by linearizing the nonlinear problem about some nominal operating point and then checking the condition number of the resulting matrix. Such an approach will only locally test the estimation problem and will not be able to detect co-linearity of the nonlinear model equations at other operating points. That is, co-linearity of equations at certain points, which can cause the parameters to become practically unobservable, may not be easily detectable. In such situations, testing for local observability by examining the inverse of the covariance matrix of parameter estimates as proposed here, will identify the obtained estimates as being poor. Note that the least squares estimates obtained in Case C are very poor ($\hat{\beta}$ is not close to $\beta$) even though all the eigenvalues of $Q_{\hat{\beta}}^{-1}$ are nonzero and so the updating problem passes the observability test. This highlights the need to consider degree of observability rather than a binary observability test.

3.2.1 DEGREE OF OBSERVABILITY

The observability criterion for parameter observability available in literature by Krishnan [1990] given in Equation (3.2) determines whether or not quantities (states/parameters) are observable. Thus there are only two possible outcomes from the observability test: observable or unobservable. This test provides no information about the quality of estimates. For dynamic systems, Gudi [1995] has used the condition number of the observability matrix $M$ to differentiate between "strong" versus "weak" observability. The approach taken by Gudi [1995] could be applied to parameter observability of steady-state systems by examining the condition number of the augmented Jacobian matrix in Equation (3.2) to get an indication of the degree of observability. However, as has been pointed out earlier, the augmented matrix contains no information about the estimator. In this section, it will be shown how the proposed parameter observability measure naturally leads to a measure of degree of observability that is based on the statistical properties of the parameter estimates.

Degree of observability, in this context, refers to the quality of estimates that can be obtained from a given set of measurements via the updator. In designing experiments for precise parameter estimation, the joint confidence region of the estimates has been used to obtain measures of estimate quality [Sutton and MacGregor, 1977], [Box and Lucas, 1959], [Box and Hunter, 1965]. Quality of parameter estimates is related to the characteristics, both size (volume) and
shape, of the joint confidence region of parameter estimates [Sutton and MacGregor, 1977]. In general, updators yielding confidence regions with small volumes provide better estimates than those resulting in large volumes (of similar shape). Confidence regions that take the shape of a hyper-sphere are more desirable than very elongated regions since the more elongated the hyper-ellipsoid gets, the more correlated the estimates become. Box and Lucas [1959] and Box and Hunter [1965] have used the determinant of $Q_{\beta}$ as measure of the volume of the joint confidence region. The rationale behind using the determinant is that $|Q_{\beta}|$ is the product of the eigenvalues of $Q_{\beta}$ which represent magnitudes of the semi-axes of the hyper-ellipsoid (joint confidence region). Therefore, the larger the determinant, the greater the volume.

However, the volume criterion gives no indication of the shape of the confidence region. An indication of the shape or conditioning of the region can be obtained by looking at the condition number of the Hessian of the function $c^2, Q_{\beta}^{-1}$:

$$\kappa_2 = \frac{\eta_{\text{max}}}{\eta_{\text{min}}}$$

The condition number, $\kappa_2$, takes on its minimum value of unity when the joint confidence region is a hyper-sphere and increases as the region becomes elongated. Another measure of shape provided by Turing [1948] is:

$$R = \frac{1}{p} \left[ \text{trace}(Q_{\beta}) \text{trace}(Q_{\beta}^{-1}) \right]^{\frac{1}{2}}$$

$$= \frac{1}{p} \left[ \sum_{i=1}^{p} \frac{1}{\eta_i} \sum_{i=1}^{p} \eta_i \right]^{\frac{1}{2}}$$

This measure, $R$, also takes on a minimum value of 1 and increases as the region becomes more elongated or ill-conditioned. Note that $R$ is a function of all the eigenvalues of $Q_{\beta}^{-1}$ and so incorporates information about uncertainty in all the $p$ independent directions in the parameter space whereas $\kappa_2$ considers only the best (most certain) and worst (least certain) directions. However, $\kappa_2$ places an upper bound on any measure of conditioning and so will be adopted here.

Thus both the size and shape of the joint confidence region have to be considered in determining the degree of parameter observability. For "strong" observability, small $|Q_{\beta}|$ and $\kappa_2$ are
required. Among regions with similar volumes, the one yielding the smallest value for $\kappa_2$ would be preferred, while among regions with similar conditioning the one encompassing the smallest volume (for a given confidence level) should be chosen.

A simple example is used below to illustrate the use of the shape criterion in selecting among estimators that yield confidence regions of similar volumes.

**EXAMPLE 3.2**

Measurements $z$ are used to update parameters $\beta = \begin{bmatrix} \beta_1 & \beta_2 \end{bmatrix}^T = \begin{bmatrix} 5 & 5 \end{bmatrix}^T$ using two different estimators $A$ and $B$. The inverse of the covariance matrix of the parameter estimates resulting from the two estimators are:

$$
\begin{align*}
(Q^{-1})_A &= \begin{bmatrix} 2 & 3 \\ 1 & 4 \end{bmatrix}, & (Q^{-1})_B &= \begin{bmatrix} 10 & 3 \\ 5 & 2 \end{bmatrix}
\end{align*}
$$

The eigenvalues of $(Q^{-1})_A$ are 1 and 5 and the eigenvalues of $(Q^{-1})_B$ are 11.57 and 0.43. Since $|\begin{bmatrix} (Q^{-1})_A \\ (Q^{-1})_B \end{bmatrix}| = 0.20$, the joint confidence regions from both the estimators enclose the same volume for a given confidence level. However, the condition numbers of $(Q^{-1})_A$ and $(Q^{-1})_B$ are vastly different:

$$
\kappa_{2,A} = 5, \quad \kappa_{2,B} = 26.76
$$

The confidence contours resulting from the two estimators are shown in Figures 3-4 (a) and (b).

The confidence regions resulting from estimator $B$ are much more elongated than those from estimator $A$. Therefore estimator $A$ provides much stronger parameter observability and so should be chosen over $B$.

In this section a criterion for determining whether or not parameters are observable from a given updating scheme and process measurements has been provided. The criterion is based on examining the inverse of the covariance matrix of estimates $(Q^{-1})$. The idea was then extended to obtaining an indication of the degree of observability which again looks at the characteristics of $Q^{-1}$. The rest of the chapter will focus on obtaining estimates of $Q$. 

49
Figure 3-4: Probability Contours for Example 3.2

### 3.3 COVARIANCE MATRIX APPROXIMATION

An approximation to $Q_{\beta}$ can be obtained by representing the updating procedure in Figure 3-2 as a nonlinear map:

$$\hat{\beta} = \Phi(z)$$

which produces parameter estimates from process measurements. When $\Phi$ is at least once continuously differentiable in $z$, changes in the adjustable parameters ($\Delta \hat{\beta}$) in response to small changes in the measurements ($\Delta z$) can be approximated using a first-order Taylor series as:

$$\hat{\beta} - \hat{\beta}_0 \approx \nabla_z \Phi|_{z_0} [z - z_0]$$

which can be expressed as:

$$\Delta \hat{\beta} \approx \frac{d\hat{\beta}}{dz} \Delta z$$

(3.8)

where: $\frac{d\hat{\beta}}{dz}$ is a sensitivity matrix (sensitivity of parameters to measurements).
Thus small changes in $z$, including measurement noise, are approximately mapped to perturbations in $\beta$ through $\frac{d\beta}{dz}$. As such, the propagation of measurement noise through the updator to produce a variance in the parameter estimates, $Q_\beta$, can also be locally approximated using $\frac{d\beta}{dz}$. Forbes [1994] has provided an expression for approximating $Q_\beta$:

$$Q_\beta \approx \frac{d\beta}{dz} Q_z \frac{d\beta}{dz}^T$$

(3.9)

where: $Q_z$ is the covariance matrix of measurement noise.

Thus measurement noise propagates through the updator, the properties of which are captured in $\frac{d\beta}{dz}$, to produce a variance in the parameter estimates. Determination of $\frac{d\beta}{dz}$ will be examined for some estimation techniques in the next section.

It has already been established that any measure of observability should include information about all components of the parameter updating system. $Q_\beta$ depends on $\frac{d\beta}{dz}$ (in addition to $Q_z$) which in turn depends on $\Phi$, the updator. Thus $Q_\beta$ contains information about the whole updating subsystem. How $\frac{d\beta}{dz}$ relates to the components of the updator will also be discussed for some estimation techniques in the next section.

### 3.3.1 ESTIMATION EXAMPLES

Consider a steady-state process described by:

$$\omega(z, \beta) = 0$$

for which the parameters $\beta$ have to be estimated using the measurements $z$. There are many alternative estimation techniques which may be used in updating the adjustable parameters. This section will focus on three common methods (back calculation, optimization-based estimation, and prediction filter based estimation) and illustrate how $\frac{d\beta}{dz}$ can be obtained for each case. The covariance matrix of estimates, $Q_\beta$, can then be approximated using $\frac{d\beta}{dz}$.

Note that since there are no output equations or state variables involved for steady-state systems described by $\omega(z, \beta) = 0$, Krishnan’s [1990] observability criterion in Equation (3.2) will reduce
BACK CALCULATION

The parameters can be back-calculated using given values for measurements (z) by solving the following simultaneous set of (nonlinear) equations for $\hat{\beta}$:

$$\omega (z, \hat{\beta}) = 0$$  \hfill (3.11)

The model equations ($\omega$) are solvable for $\hat{\beta}$ if rank of $\nabla_{\beta} \omega$ is equal to the number of parameters as required by the rank criterion provided by Krishnan [1990] given in Equation (3.10).

The sensitivity matrix can be determined by taking the total differential of Equation (3.11):

$$\frac{\partial \omega}{\partial z} dz - \frac{\partial \omega}{\partial \hat{\beta}} d\hat{\beta} = 0$$

Rearranging yields:

$$\frac{\partial \omega}{\partial \hat{\beta}} d\hat{\beta} = - \frac{\partial \omega}{\partial z} dz$$  \hfill (3.12)

from which $\frac{d\hat{\beta}}{dz}$ can be calculated assuming that rank of $\frac{\partial \omega}{\partial \hat{\beta}}$ (or $\nabla_{\beta} \omega$) is $p$, the number of parameters. $Q_{\hat{\beta}}$ can then be approximated using Equation (3.9). Note that calculation of $\frac{d\hat{\beta}}{dz}$ requires that rank criterion by Krishnan [1990] in Equation (3.10) be satisfied.

Since in back-calculation all the characteristics of the estimator are included in the model equations ($\omega$) themselves, the approach provided by Krishnan [1990] includes information about all components of the estimator. Also, from Equation (3.12) it can be seen that $\frac{d\hat{\beta}}{dz}$ (and therefore $Q_{\hat{\beta}}$) contains all the characteristics of the estimator as well. Thus for back-calculation, both approaches will provide necessary and sufficient conditions for parameter observability.
OPTIMIZATION-BASED ESTIMATION

Parameters are often updated using optimization based methods such as nonlinear regression. A general optimization based estimation can be formulated as:

$$\min_{\hat{\beta}, \epsilon} \phi$$

subject to:

$$f(\hat{\beta}, z, \epsilon) = 0$$

where: $\phi$ is the objective function for parameter-estimation optimization problem, $f$ is a vector containing the appropriate model equations, and $\epsilon$ is a vector of residuals.

The optimization variables in Problem (3.13) are $\hat{\beta}$, and $\epsilon$. Eliminating the residuals from the problem transforms it into its reduced space [Fletcher, 1987] where it becomes an unconstrained optimization problem:

$$\min_{\hat{\beta}} \phi(\hat{\beta}, z)$$

Sufficiency conditions for a minimum require that the reduced gradient ($\nabla_r \phi$) vanish at the optimum and that the reduced Hessian be positive definite for a unique minimum:

$$\nabla_r \phi = 0$$

$$\nabla_r^2 \phi \text{ be positive definite}$$

Forbes [1994] has provided an expression for the reduced gradient (where the appropriate derivatives exist):

$$\nabla_r \phi = \frac{\partial \phi}{\partial \hat{\beta}} - \frac{\partial \phi}{\partial \epsilon} \left( \frac{\partial f}{\partial \epsilon} \right)^{-1} \frac{\partial f}{\partial \hat{\beta}}$$

The sensitivity matrix can be obtained by taking the total differential of the reduced gradient and rearranging:

$$\frac{d\phi}{d\hat{\beta}} = \frac{\partial}{\partial \hat{\beta}} \left( \frac{d\phi}{d\hat{\beta}} \right) d\hat{\beta} + \left( \frac{d\phi}{dz} \right) dz = 0$$

$$\frac{d\hat{\beta}}{dz} = - \left( \nabla_r^2 \phi \right)^{-1} \left( \frac{\partial \nabla_r \phi}{\partial z} \right)$$

(3.15)

Thus $\frac{d\hat{\beta}}{dz}$ depends on the inverse of the reduced Hessian and the effect of perturbations in
the measurements on the reduced gradient. An expression for the reduced Hessian has been provided by Forbes [1994]:

$$\nabla^2 \bar{r}^2 = \sum_{j=1}^p \frac{\partial \bar{r} \partial^2 \bar{r}_j}{\partial \bar{r}^2 \partial \bar{r}_j} - \frac{\partial \bar{r}^T}{\partial \bar{r}} \left( \frac{\partial \bar{r}^T}{\partial \bar{r}} \right)^{-1} \frac{\partial \bar{r}^T}{\partial \bar{r}} - \frac{\partial \bar{r}^T}{\partial \bar{r}} \left( \frac{\partial \bar{r}^T}{\partial \bar{r}} \right)^{-1} \frac{\partial \bar{r}^T}{\partial \bar{r}} \left( \frac{\partial \bar{r}^T}{\partial \bar{r}} \right)^{-1} \frac{\partial \bar{r}^T}{\partial \bar{r}} - \frac{\partial \bar{r}^T}{\partial \bar{r}} \left( \frac{\partial \bar{r}^T}{\partial \bar{r}} \right)^{-1} \frac{\partial \bar{r}^T}{\partial \bar{r}} \left( \frac{\partial \bar{r}^T}{\partial \bar{r}} \right)^{-1} \frac{\partial \bar{r}^T}{\partial \bar{r}}$$

From Equation (3.15) it can be seen that \( \frac{\partial \bar{r}^T}{\partial \bar{r}} \) contains information about all components of the parameter updating procedure including the characteristics of the objective function as well as the steady-state models that describe the process (contained in the vector \( f \)). Similarly, \( \frac{\partial \bar{r}^T}{\partial \bar{r}} \) will also contain information about the objective function as well as the model equations.

Although Equation (3.15) serves well to illustrate the information contained in \( \frac{\partial \bar{r}^T}{\partial \bar{r}} \), this formulation cannot be readily used to compute \( \frac{\partial \bar{r}^T}{\partial \bar{r}} \). An alternate approach to determining \( \frac{\partial \bar{r}^T}{\partial \bar{r}} \) is to use local sensitivity analysis [Seferlis, 1995] which is based on the Implicit Function Theorem [Corwin and Szczesna, 1995] and describes the first-order changes to the optimum subject to small perturbations about a nominal point. The approach to sensitivity analysis taken by Ganesh and Biegler [1987] yields a linear system of equations that allows for easier computation of \( \frac{\partial \bar{r}^T}{\partial \bar{r}} \).

The authors develop sensitivity analysis under the assumption that the following conditions are satisfied at the local minimum, \( \bar{r}^* \):

1. The functions in Problem 3.13 are at least twice continuously differential in \( \bar{r} \) and at least once in \( z \) for a neighbourhood of \((\bar{r}^*, z^*)\).

2. The constraint gradients are linearly independent at \( \bar{r}^* \) and strict complementary slackness [Edgar and Himmelblau, 1988] holds for the functions in Problem 3.13 at \( \bar{r}^* \) with unique Lagrange multipliers, \( \mu \).

3. The second-order sufficiency conditions are met [Ganesh and Biegler, 1987].

From the Karush-Kuhn-Tucker (KKT) conditions [Edgar and Himmelblau, 1988]:

$$\nabla_{\bar{r}} L(\bar{r}^*, z^*, \epsilon^*, \mu^*) = 0$$

$$f(\bar{r}^*, z^*, \epsilon^*) = 0$$
where: $L = o - \mu^T f$ is the Lagrangian of the optimization problem. $\mu$ is a vector of Lagrange multipliers.

Applying the Implicit Function Theorem [Corwin and Szczarba, 1995] and rearranging gives:

$$
\begin{bmatrix}
\nabla_{z\beta} L^* \\
\nabla_{z\epsilon} L^* \\
\nabla_{z\omega} L^*
\end{bmatrix} = -
\begin{bmatrix}
\nabla_{z\beta}^2 L^* & \nabla_{z\beta} \epsilon L^* & \nabla_{z\beta} f^T L^* \\
\nabla_{z\epsilon} \beta L^* & \nabla_{z\epsilon} \epsilon L^* & \nabla_{z\epsilon} f^T L^* \\
\nabla_{z\omega} \beta L^* & \nabla_{z\omega} \epsilon L^* & 0
\end{bmatrix}
\begin{bmatrix}
\nabla_{z\beta} \epsilon^* \\
\nabla_{z\epsilon} \epsilon^* \\
\nabla_{z\omega} \epsilon^*
\end{bmatrix}
$$

(3.16)

from which the sensitivity matrix, $\nabla_z \beta^*$ (or $\frac{d\beta}{dz}$), can be calculated. While analytical solutions can be obtained for small optimization problems, numerical methods would have to be utilized for larger ones. The covariance matrix of parameter estimates ($Q_\beta$) can then be approximated using Equation (3.9).

From this definition of $\frac{d\beta}{dz}$ as well, it can be seen that $\frac{d\beta}{dz}$ contains information about all components of the updating procedure. The Lagrangian $L$ contains the objective function $o$ as well as the model equations (contained in $f$). Thus the characteristics of $o$ are captured in $\nabla_{z\beta} L^*$, $\nabla_{z\epsilon} L^*$: $\nabla_{z\omega} L^*$, $\nabla_{z\beta} \epsilon L^*$, and $\nabla_{z\epsilon} \epsilon L^*$. Information on the model equations are contained in these terms as well as in $\nabla_z f^*$, $\nabla z f^*$, and $\nabla_\epsilon f^*$.

As an example of optimization-based estimation, consider weighted least-squares regression:

$$
\min_{\beta, \epsilon} \epsilon^T \Lambda \epsilon
$$

subject to:

$$
\omega(\beta, z) = \epsilon
$$

(3.17)

where: $\Lambda$ is a weighting matrix.

In this case, $f = \omega(\beta, z) - \epsilon$ and so $\nabla_\beta f = \nabla_\beta \omega$. Therefore, Equation (3.16) becomes:

$$
\begin{bmatrix}
\nabla_{z\beta} L^* \\
\nabla_{z\epsilon} L^* \\
\nabla_{z\omega} L^*
\end{bmatrix} = -
\begin{bmatrix}
\nabla_{z\beta}^2 L^* & \nabla_{z\beta} \epsilon L^* & \nabla_{z\beta} f^T \omega L^* \\
\nabla_{z\epsilon} \beta L^* & \nabla_{z\epsilon} \epsilon L^* & \nabla_{z\epsilon} f^T \omega L^* \\
\nabla_{z\omega} \beta L^* & \nabla_{z\omega} \epsilon L^* & \nabla_{z\omega} f^T \omega L^*
\end{bmatrix}
\begin{bmatrix}
\nabla_{z\beta} \epsilon^* \\
\nabla_{z\epsilon} \epsilon^* \\
\nabla_{z\omega} \epsilon^*
\end{bmatrix}
$$

(3.18)
where the Lagrangian is:

\[ L = \epsilon^T \Lambda \epsilon - \mu^T [\omega(\hat{\beta}, z) - \epsilon] \]

From Equation (3.18) it can be seen that \( \frac{d\hat{\beta}}{dt} \) contains information about all components of the estimator - the model equations in the constraints as well as the objective function. Characteristics of the objective function are contained in the terms \( \nabla_{\beta z} L^*, \nabla_{z, \epsilon} L^*, \nabla_{\hat{\beta}}^2 L^*, \nabla_{\epsilon \beta} L^* \) and \( \nabla_{\epsilon \epsilon} L^* \), while model information is included in these terms as well as in \( \nabla_{z \omega} L^*, \nabla_{\hat{\beta} \omega}^T L^*, \nabla_{\epsilon \omega} L^* \) and \( \nabla_{\epsilon \omega} L^* \). The method presented by Krishnan [1990] examines only the term \( \nabla_{\hat{\beta}} \omega \) and so looks only at the constraints in the estimator in Problem (3.17) and neglects the objective function entirely, providing a necessary but not sufficient condition for parameter observability. Testing for observability using \( Q_{\hat{\beta}} \) on the other hand, provides a sufficient condition since it includes all aspects of the estimator.

**ESTIMATION USING PREDICTION FILTERS**

Filtering is commonly used in control systems and involves using current measurements to update previous estimates of the unmeasured quantities to provide the most up-to-date estimates in a sequential fashion [Ray, 1981]. Filters include Kalman and extended Kalman filters [Chiu, 1987] which incorporate system model information. The Kalman family of filters have been applied very successfully over the past three decades for state estimation. Prediction filters based on Box and Jenkins [1976] methods are also widely used. Other prediction filter design methods include those based on Discounted Least Squares approach [Montgomery and Johnson, 1976] and the Bayesian approach [Montgomery and Johnson, 1976].

In filtering, the updating strategy is to estimate the parameters at the current time-step \( t_k \) \( (\hat{\beta}_{t_k|t_k}) \) using their predictions from the prediction time step \( (\hat{\beta}_{t_k|t_k-1}) \) and a correction term which involves the current measurements \( (z_{t_k}) \) and their predictions from the previous time step \( (\hat{z}_{t_k|t_k-1}) \) [Ray, 1981]. Thus the expression for updating the adjustable parameters is given by:

\[
\hat{\beta}_{t_k|t_k} = \hat{\beta}_{t_k|t_k-1} - K(z_{t_k} - \hat{z}_{t_k|t_k-1})
\]

where: \( \hat{\beta}_{t_k|t_k} \) is the vector of parameter estimates at time \( t_k \) using data up to time \( t_k \), \( \hat{\beta}_{t_k|t_k-1} \) are predicted estimates for time \( t_k \) using data up to time \( t_k-1 \), \( z_{t_k} \) are measurements obtained...
at time $t_k$, $\hat{z}_{tk|t_{k-1}}$ are predicted measurements at time $t_k$ using data up to time $t_{k-1}$, and $K$ is the filter matrix.

Step ahead predictions of parameters $\left(\hat{\beta}_{tk|t_{k-1}}\right)$ and measurements $\left(\hat{z}_{tk|t_{k-1}}\right)$ can be obtained using appropriate prediction models. When such information is not available, one approach is to assume that the measurements and the parameter estimates will remain unchanged over the next time-step:

$$\hat{\beta}_{tk|t_k} = \hat{\beta}_{tk-1|t_{k-1}}$$
$$\hat{z}_{tk|t_k} = z_{tk-1}$$

The updating expression can then be written as:

$$\hat{\beta}_{tk|t_k} = \hat{\beta}_{tk-1|t_{k-1}} + K[z_{tk} - z_{tk-1}]$$

and rearranged to give:

$$\Delta \hat{\beta}_{tk|t_k} = K \Delta z_{tk} \tag{3.19}$$

Comparing Equation (3.19) with Equation (3.8), the sensitivity of the current estimates to the measurements, $\frac{d\hat{\beta}_{tk|t_k}}{dz_{tk}}$, is simply the filter matrix:

$$\frac{d\hat{\beta}_{tk|t_k}}{dz_{tk}} = K$$

Thus the sensitivity matrix will depend on filter design. The covariance matrix of parameter estimates $\left(Q_\beta\right)$ can be obtained using via Equation (3.9) as:

$$Q_\beta \approx KQ_z K^T \tag{3.20}$$

The method for determining parameter observability presented by Krishnan [1990] uses steady-state models ($\omega$) that describe the process as given in Equation (3.10). These models are commonly used in the design of the Kalman family of filters [Chiu, 1987] (in addition to other information such as noise characteristics). However, certain other classes of filters such as
prediction filters based on time-series analysis [Box and Jenkins, 1976] may not directly contain these steady-state models. Moreover, the filter matrix may be user-tuned in which case the filter matrix (K) will not contain any model information. Thus for filter based-estimation, determination of parameter observability using the approach of Krishnan [1990] uses only partial filter information (as in the case of the Kalman family of filters) or no information at all. Therefore, Krishnan's approach has only limited application to some filter designs and no application to other designs. The statistical approach presented in this chapter, however, can be applied to all filters and will provide a sufficient condition for parameter observability since it uses the filter matrix directly in calculating \( Q^{-1} \) as shown in Equation (3.20).

### 3.4 DISCUSSION

Estimation of unmeasured quantities from secondary measurements for steady-state systems is an important problem in the chemical industry. For example, concentrations in distillation columns are often estimated using temperature measurements. However, care should be taken to ensure that unique estimates of these quantities can be obtained from the available measurements and estimator. Moreover, the estimates must have an acceptable level of statistical certainty.

The approach to determining parameter observability for steady-state systems provided by Krishnan [1990] considers only the steady-state models that represent the plant. It does not take into account the characteristics of the estimator. It has been shown in this chapter that this approach cannot provide a sufficient condition for parameter observability. A statistical approach to determining observability of parameters from the measurements and estimator has been presented which takes into account all components of parameter estimation to provide a sufficient condition. The ideas behind parameter observability have been extended to degree of observability which looks at quality of estimates.

The proposed approach to observability and degree of observability involves examining the eigenvalues of the inverse of the covariance matrix of parameter estimates (\( Q^{-1} \)). Since eigenvalues of a matrix are dependent on the scaling applied to the elements of the matrix, degree of observability will also be scale dependent. Gudi [1995] determines degree of state observability
in dynamic systems by looking at the singular values of the observability matrix \((M)\) which are also scale dependent. Therefore, the matrices \(Q^{-1}_\beta\) and \(M\) would have to be pre-scaled (by scaling all elements to the same order of magnitude) before degree of observability can be determined. In the steady-state parameter observability case, \(Q^{-1}_\beta\) should be based on all parameters \((\beta)\) being scaled to the same order of magnitude.

In RTO systems, parameter observability can be used in selecting adjustable parameters. Krishnan [1990] has provided a method for selecting adjustable parameters which involves identifying “key” parameters and then updating these parameters on-line. Key parameters are determined by perturbing each parameter at a time and noting the resulting change in the objective function value and any active set changes. Parameters that cause the most change in objective function value per unit change in parameter, or those that cause the active constraint set to change, are selected as adjustable parameters. However, the objective function in RTO systems is based on process economics which is usually only poorly known. Therefore, the predicted profit could be quite different than the actual profit. Thus selecting adjustable parameters based on objective function changes could lead to poor RTO design. Forbes and Marlin [1996] have provided an alternative approach to adjustable parameter selection which is based on minimizing loss of RTO performance. Loss of RTO performance is determined as the Design Cost which considers performance loss due to: offset from true plant optimum, and variance in predicted optimal setpoints. In the Design Cost approach, those parameters which when updated on-line result in the least Design Cost, are selected as adjustable parameters. However, this strategy (as well as that presented by Krishnan [1990]) does not consider parameter observability. Thus, it could in some cases, lead to the selection of parameters that cannot be estimated from the measurements and estimator and so cannot be updated on-line.

The first step in any parameter selection scheme is to ensure that the selected parameters will be observable from the available measurements and chosen estimation scheme. Parameter observability can be tested in two steps. First, the method presented by Krishnan [1990] can be used which provides a necessary condition for observability. Parameters that fail to satisfy the rank criterion in Equation (3.2) can be discarded from the set of candidate adjustable parameters at this point. Next, the observability approach presented in this chapter should be used on the remaining parameters to test if the parameters would be observable from the
measurements and the estimation scheme. Parameters that are not observable or those that are only weakly observable can also be eliminated. Note that the proposed statistical approach to determining parameter observability will recognize and eliminate parameters that fail to satisfy the rank criterion in Equation (3.2) since it provides a necessary and sufficient condition for parameter observability. However, the second test is specific to a given estimation scheme. Thus if observability through other estimation schemes have to be tested, the parameters eliminated by the first step would not have to be tested again. The above procedure will narrow the set of possible adjustable parameters to those that exhibit an acceptable degree of observability. The Design Cost approach to adjustable parameter selection presented by Forbes and Marlin [1996] can then be applied to the resulting smaller set.

Thus the observability measure developed in this Chapter can be applied to RTO systems as well as to any steady-state system where parameters are to be estimated from secondary measurements.
Chapter 4

BLENDING CONTROL TECHNOLOGY

This chapter builds on the modeling and parameter observability work presented in Chapters 2 and 3 to provide an efficient blend controller. The chapter begins by presenting the perfect or ideal blend controller which is then used as a benchmark for comparing controller performance. In addition to providing a performance benchmark, the ideal/perfect controller provides insight into better controller design. Next, the widely used control strategy and the problems associated with it are examined. Finally, a new control approach that overcomes the shortcomings of the current strategy is presented. Performance of different blend controllers are demonstrated using an automotive gasoline blending case-study throughout the chapter.

4.1 INTRODUCTION

As discussed in Chapter 1, gasoline blending involves combining refinery feedstocks to make products meeting certain quality specifications. The control structure used for blending gasoline is given in Figure 1-4. At the heart of the controller is an RTO layer that is usually based on linear programming with bias updating. The success of this control strategy has been largely due to the practice of blending from well-mixed storage tanks. However, increased competition has forced refiners to reduce on-site tankage inventory by blending out of "running" tanks (or direct in-line blending). "Running" tanks are those intermediate tanks into which feedstocks from upstream processes are being pumped. Also, process streams can be routed directly
to the blender without first being pumped into either an intermediate storage or "running" tank [Agrawal, 1995]. Since blending feedstock qualities are dependent on upstream process operations and upstream process changes (e.g. catalyst deactivation, heat exchanger fouling, crude oil switches, etc.), they may not be constant and may vary significantly during blending.

This chapter focuses on the problem of controlling a gasoline blender which is subject to stochastic disturbances in the feedstock qualities. Such disturbances naturally arise when the blender is using "running" tanks as feeds and upstream process operations change. The objectives of this chapter are to demonstrate the problems that existing blender control systems may encounter when faced with feedstock quality disturbances, to provide a control strategy that can effectively deal with such disturbances, and to illustrate the performance improvements associated with the proposed control approach.

4.2 GASOLINE BLENDING BENCHMARK PROBLEM

An automotive gasoline blending problem is used to compare the performance of blend controllers in this chapter. Different blend controllers will be applied to the benchmark problem.

4.2.1 BLENDING PROBLEM

The blending problem studied here is based on a case-study by Forbes and Marlin [1994] and involves simultaneously blending two grades of automotive gasoline using five feedstocks as shown in Figure 4-1. For the purposes of this illustrative problem, the product specifications for each grade of gasoline will be limited to: minimum limits on $RON$ and $MON$, and a maximum limit on the $RVP$. Constraints are also placed on maximum and minimum product demands and feedstock availabilities. Product specifications and economic data are provided in Table 4.1 and feedstock data are in Tables 4.2 and 4.3.

In this problem, gasoline is to be blended for 24 hours with an RTO interval of 2 hours. As discussed in Chapter 2, the gasoline blending process is simulated using the Ethyl RT-70 [Healy et al., 1959] and the Blending Index [Gary and Handwerk, 1994] models. These models are presented in Equation set (2.16).
<table>
<thead>
<tr>
<th></th>
<th>Regular</th>
<th>Premium</th>
</tr>
</thead>
<tbody>
<tr>
<td>value ($/bbl)</td>
<td>33.00</td>
<td>37.00</td>
</tr>
<tr>
<td>max. demand limit (bbl/day)</td>
<td>8000</td>
<td>10000</td>
</tr>
<tr>
<td>min. demand limit (bbl/day)</td>
<td>7000</td>
<td>10000</td>
</tr>
<tr>
<td>min. RON</td>
<td>88.5</td>
<td>91.5</td>
</tr>
<tr>
<td>min. MON</td>
<td>77.0+</td>
<td>80.0+</td>
</tr>
<tr>
<td>max. RVP (psi)</td>
<td>10.8</td>
<td>10.8</td>
</tr>
</tbody>
</table>

*chosen for this study

Table 4.1: Production Requirements

<table>
<thead>
<tr>
<th></th>
<th>Available (bbl/day)</th>
<th>Cost ($/bbl)</th>
</tr>
</thead>
<tbody>
<tr>
<td>reformate</td>
<td>12000</td>
<td>34.00</td>
</tr>
<tr>
<td>LSR naphtha</td>
<td>6500</td>
<td>26.00</td>
</tr>
<tr>
<td>n-butane</td>
<td>3000</td>
<td>10.30</td>
</tr>
<tr>
<td>catalytic gas.</td>
<td>4500</td>
<td>31.30</td>
</tr>
<tr>
<td>alkylate</td>
<td>7000</td>
<td>37.00</td>
</tr>
</tbody>
</table>

from Forbes and Marlin [1994]

Table 4.2: Feedstock Economic Data

<table>
<thead>
<tr>
<th>Feedstock</th>
<th>reformate (C14a)</th>
<th>LSR naphtha (C10a)</th>
<th>n-butane (C25a)</th>
<th>catalytic gas. (C12a)</th>
<th>alkylate (C7a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RON</td>
<td>94.1</td>
<td>70.7</td>
<td>93.8</td>
<td>92.9</td>
<td>95.0</td>
</tr>
<tr>
<td>MON</td>
<td>80.5</td>
<td>68.7</td>
<td>90.0</td>
<td>80.8</td>
<td>91.7</td>
</tr>
<tr>
<td>Olefin (%)</td>
<td>1.0</td>
<td>1.8</td>
<td>0</td>
<td>48.8</td>
<td>0</td>
</tr>
<tr>
<td>Aromatics (%)</td>
<td>58.0</td>
<td>2.7</td>
<td>0</td>
<td>22.8</td>
<td>0</td>
</tr>
<tr>
<td>RVP (psi)</td>
<td>3.8</td>
<td>12.0</td>
<td>138.0++</td>
<td>5.3</td>
<td>6.6</td>
</tr>
</tbody>
</table>

from Healy et al. [1959]

parentheses under feedstock indicate tables in Healy et al. [1959]

++ chosen for this study

Table 4.3: Feedstock Qualities
4.2.2 STOCHASTIC DISTURBANCES

For the illustrative purposes of this case-study, disturbances are to be added to $RON$, $MON$, and $RVP$ of the feedstocks. In order to simplify the benchmark blending problem, it was assumed that disturbances were present only in the feedstock that affects the optimal operations the most. In order to determine the feedstock whose qualities the optimal blend recipe is most sensitive to, a local sensitivity analysis [Seferlis, 1995] was conducted around the nominal blend. The nominal optimal blend was obtained using NLP with MINOS in GAMS [Brooke et al., 1992] using data given in Tables 4.1, 4.2, and 4.3, and the blending models in Equation set (2.16). The results are summarized in Appendix A. After scaling all the decision variables and parameters to the same order of magnitude, the linear system of equations given in Ganesh and Biegler [1987] was solved analytically using MAPLE [Char et al., 1991] for the parametric sensitivity matrix ($\nabla_\beta x^*$) of the optimal process variables ($x^*$) to the parameters ($\beta$). Five submatrices of $\nabla_\beta x^*$, each corresponding to a feedstock, were obtained and their norms (largest singular values) computed. The results are summarized in Table 4.4.
Table 4.4: Feedstock Sensitivity

<table>
<thead>
<tr>
<th>Feedstock</th>
<th>Submatrix Norm</th>
</tr>
</thead>
<tbody>
<tr>
<td>reformate</td>
<td>3.66</td>
</tr>
<tr>
<td>LSR naphtha</td>
<td>1.20</td>
</tr>
<tr>
<td>n-butane</td>
<td>0.005</td>
</tr>
<tr>
<td>catalytic gas.</td>
<td>1.63</td>
</tr>
<tr>
<td>alkylate</td>
<td>0</td>
</tr>
</tbody>
</table>

The submatrix corresponding to the reformate qualities yielded the largest singular value. Thus, stochastic disturbances were added to the reformate stream, for the purposes of this example, as:

\[
q_{ref,t} = \bar{q}_{ref} + \begin{bmatrix} 1 \\ 0.85 \\ -0.1 \end{bmatrix} d_t \tag{4.1}
\]

where: \( q_{ref,t} = \begin{bmatrix} RON \\ MON \\ RVP \end{bmatrix} \) is a vector of reformate qualities at time \( t \), \( \bar{q}_{ref} \) is a vector of nominal reformate qualities, and \( d_t \) is a scalar disturbance.

The scalar disturbance, \( d_t \), was modeled as steps of random height entering a well mixed tank. The tank was assumed to hold one third the availability of reformate (as given in Table 4.3) per eight-hour shift, resulting in the following transfer function:

\[
d_t = \frac{(1 - 0.56)z^{-1}}{(1 - 0.56z^{-1})} s_t \tag{4.2}
\]

where: \( z^{-1} \) is the backward shift operator and \( s_t \) are steps of random height.

A noise vector was generated for each 2 hour time interval over the blend horizon and noise was assumed to remain unchanged during each RTO interval. Noise was then added to the reformate qualities over the whole blend horizon. The resulting \( RON \), \( MON \), and \( RVP \) of the reformate stream over the 24 hour period is shown in Figure (4-2).

### 4.2.3 CONTROLLER PERFORMANCE

Controller performance is measured by the profit earned from applying the controller on the benchmark problem posed in this section. When a controller produces blends that meet all
quality specifications, the profit level can easily be computed using the economic data provided in Table 4.2. However, if the products at the end of the 24 hour blend horizon are found to be off-specification, they may not be suitable for sale as produced, and would likely be routed to ‘slop’ tanks and reblended. In such situations, profit calculation is not as simple.

One option is to include the cost of reblending in determining profit level. Alternatively, the off-specification portions of blends (products made during RTO intervals that are causing the whole 24 hour blend to be off-specification) can be “removed” from the blend. The profit can then be calculated based on the modified smaller blend that does meet quality specifications. Although blend portions cannot be “removed” or unblended from a blended product in practice, it can easily be done for simulation studies for the purposes of accessing controller performance. Since the economic data required for determining loss of profit due to reblending is not available for this study, the second alternative of “removing” off-specification products is adopted.

Small violations of quality specifications can often be tolerated since product quality measurements are limited by analyzer sensitivity. For the purposes of this study, it is assumed that
violations of up to -0.03 octane number for RON and MON, and +0.005 psi for RVP can be tolerated. That is, blended qualities that fall outside these tolerance limits are deemed off-specification.

4.3 IDEAL BLEND CONTROLLER

An ideal blend controller is one that gives the maximum possible profit from the blending process, while meeting all blended quality specifications, and satisfying demand and availability limits. In order to achieve perfect control, the controller must have perfect knowledge of the blending process. That is, it should employ blending models that capture the true blending behaviour. In addition, the controller must have perfect knowledge of all feedstock qualities at all times throughout the entire blending time horizon. For batch blending of gasoline (blending to a storage tank for a given length of time as in the benchmark problem), the ideal blending control problem can be formulated as an optimization problem where the objective is to maximize profit over the entire blending time horizon, subject to meeting quality constraints and demand/availability limits at the end of the blend. This problem has the form:

$$\max_x \int_{t_o}^{t_f} c^T x dt$$
subject to:

$$\int_{t_o}^{t_f} g(R(t), x(t)) dt \leq \left\{ \int_{t_o}^{t_f} [w^T(t)x(t)] dt \right\} s$$
$$\int_{t_o}^{t_f} h(x) dt \leq 0$$

where: c is a constant vector containing process economics, x are the feedstock or component flows, R is a matrix containing known feedstock qualities, g is a vector of blending equations that represent the true blending behaviour, w is a weighting vector (usually containing only ones and zeros to indicate the presence of a specific stream in a blend), s are the blended quality specifications, h contains product demand and feedstock availability constraints, and t_o and t_f are the initial and final blend times, respectively.

The controller works to maximize profit over the whole blend by integrating blending economics from the start of the blend (t_o) to the end of the blend (t_f), rather than at any point in time.
The first set of constraints:

\[
\int_{t_o}^{t_f} \mathbf{g}(\mathbf{R}(t), \mathbf{x}(t)) \, dt \leq \left\{ \int_{t_o}^{t_f} \left[ \mathbf{w}^T(t) \mathbf{x}(t) \right] \, dt \right\} \mathbf{s}
\]

ensure that quality specifications are met at the end of the blend. These constraints use perfect knowledge of the feedstock qualities (\( \mathbf{R} \)) over the entire blend horizon (from \( t_o \) to \( t_f \)) as well as perfect blending models in vector \( \mathbf{g} \). The second set of constraints:

\[
\int_{t_o}^{t_f} \mathbf{h}(\mathbf{x}) \, dt \leq 0
\]

integrate mass balance information over the blend horizon in order to satisfy all product demand and feedstock availability limits.

Problem (4.3) contains integrals in the objective function as well as in the constraints and so would have to be solved using dynamic programming techniques [Bellman and Lee, 1984]. Alternatively, the problem can be discretized and solved using standard NLP methods [Avriel, 1976]. The solution to Problem (4.3) will provide optimal feedstock flows (\( \mathbf{x}(t) \)) over the whole blending horizon which is the optimal blend trajectory. The value of the objective function at the optimum represents the theoretical maximum profit that can be earned from the blending process.

The ideal controller in Problem (4.3) requires future knowledge of feedstock qualities and so cannot be realized in practice. However, it can serve as a benchmark against which performance of other controllers can be evaluated, and so it can provide insight into better controller design.

### 4.3.1 Optimal Blend Trajectory for Benchmark Problem

The perfect controller as formulated in Problem (4.3) was applied to the benchmark blending problem. Vector \( \mathbf{g} \) contained blending models for \( RON \), \( MON \), and \( RVP \) for both gasoline grades. The blending models and constraints used here were the same as those used for simulating the blending process given in Equation (2.16). The demand/availability constraints in vector \( \mathbf{h} \) use mass balances and assume no density changes upon blending. Feedstock flows \( \mathbf{x} \)
at time $t$, and the weighting vector $w$ are given as:

$$
\begin{align*}
\mathbf{x}_t^T &= \begin{bmatrix} x_{t,1} & x_{t,2} & x_{t,3} & x_{t,4} & x_{t,5} & x_{t,6} & x_{t,7} & x_{t,8} & x_{t,9} & x_{t,10} \end{bmatrix} \\
\mathbf{w}^T &= \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}
\end{align*}
$$

where: $x_{t,1}, \ldots, x_{t,5}$ are flows at time $t$ to regular gasoline of reformate, LSR naphtha, n-butane, catalytic gasoline, and alkylate, respectively; $x_{t,6}, \ldots, x_{t,10}$ are flows at time $t$ to premium gasoline of reformate, LSR naphtha, n-butane, catalytic gasoline, and alkylate, respectively.

The demand/availability limits are of the form:

\[
\begin{align*}
\int_{t_0}^{t_f} \sum_{i=1}^{5} x_{t,i} \, dt &\leq (\text{demand})_{\text{regular}}^\text{max} \\
\int_{t_0}^{t_f} \sum_{i=6}^{10} x_{t,i} \, dt &\leq (\text{demand})_{\text{premium}}^\text{max} \\
\int_{t_0}^{t_f} (x_{t,1} - x_{t,6}) \, dt &\leq (\text{availability})_{\text{reformate}}^\text{max} \\
\int_{t_0}^{t_f} (x_{t,2} - x_{t,7}) \, dt &\leq (\text{availability})_{\text{LSR}}^\text{max} \\
\int_{t_0}^{t_f} (x_{t,3} - x_{t,8}) \, dt &\leq (\text{availability})_{\text{n-butane}}^\text{max} \\
\int_{t_0}^{t_f} (x_{t,4} - x_{t,9}) \, dt &\leq (\text{availability})_{\text{cat gas}}^\text{max} \\
\int_{t_0}^{t_f} (x_{t,5} - x_{t,10}) \, dt &\leq (\text{availability})_{\text{alkylate}}^\text{max}
\end{align*}
\]

The perfect controller was applied to the blending problem by approximating the integrals in Problem (4.3) with summations, and solving using MINOS/GAMS. The optimal blend trajectory and the active constraints during each RTO interval are provided in Appendix B. The theoretical maximum profit was found to be $\$66.276.55$ for the 24 hour blend.

4.4 CONVENTIONAL CONTROLLER

As has been discussed in Chapter 1, at the heart of the blender control system is an RTO layer that is usually based on linear programming with bias updating. The objective of the on-line optimizer is usually optimization of steady-state economic performance (i.e., maximization of profit flow). Thus the blending control problem is most often formulated as:
\[
\max_x \quad c^T x
\]
subject to:
\[
\tilde{R} x \leq (w^T x) s + b
\]
\[
h(x) \leq 0
\]

where: \( c \) is a constant vector containing process economics. \( \tilde{R} \) is a constant matrix containing the feedstock quality blending indices. \( s \) are the blended quality specifications. \( x \) are the feedstock or component flows. \( w \) is a weighting vector (usually containing only ones and zeros to indicate the presence of a specific stream in a blend), \( b \) are the biases used to update the blending model to maintain its accuracy. and \( h \) is a vector of linear equations for the maximum and minimum product demands and feedstock availabilities.

The matrix \( \tilde{R} \) contains blending indices such as Blending Octane Numbers (BO.N's) that blend linearly as volumetric averages. However, as discussed in Chapter 2, most important gasoline qualities (such as octane number, Reid Vapour Pressure, and the ASTM Distillation points) blend nonlinearly. Since linear blending models are unable to capture the true blending behaviour, structural mismatch is introduced into the optimizer. Bias updating is used to compensate for such plant/model mismatch as well as other modeling inaccuracies.

The RTO layer works by:

1. taking measurements of blended qualities.
2. calculating biases as the difference between measured blended qualities and those predicted by the linear model \( \tilde{R} x_{k-1} \), where \( x_{k-1} \) are the current feedstock flows,
3. solving Problem (4.4) using the newly calculated biases to obtain new blender feedstock flows \( (x_k) \).
4. implementing blend recipe and waiting for steady-state.

The process iterates over the whole blend horizon. That is, the above four steps are carried out at each RTO interval until end of blend is reached.

In the bias update formulation of Problem (4.4), the only adjustable parameters are the bias terms while all the feedstock qualities are treated as fixed parameters. Forbes and Marlin [1994]
have shown that a bias update approach can lead to a substantial loss in blender profitability given even a small variation in the feedstock qualities. Thus the current blender control structure cannot adequately address the blending problem where the component qualities are varying.

The conventional LP with bias updating controller suffers from two limitations: inability to incorporate the inherent blending nonlinearities, and ineffectiveness in dealing with fluctuating feedstock qualities. The effect of these limitations on controller performance is demonstrated by applying the controller to the gasoline blending problem described in Section 4.2.

4.4.1 CONVENTIONAL CONTROLLER PERFORMANCE STUDY

The traditional LP with bias updating blending controller given in Problem (4.4) was used on the blending problem posed in Section 4.2. Blending Octane Numbers (BON's) [Gary and Handwerk, 1994] were used for RON and MON and blending indices (RVPBI's) were used for RVP blending [Gary and Handwerk, 1994]. Hence, matrix $\tilde{R}$ contained the BON’s and RVPBI’s for all the feedstocks. The linear models used in the RTO layer result in structural mismatch in octane blending.

The demand/availability constraints use mass balances and assume no density changes upon blending. Feedstock flows at time $t$, $x_t$, and the weighting vector, $w$, are given as:

$$
\begin{align*}
  x_t^T &= \begin{bmatrix}
    x_{t,1} & x_{t,2} & x_{t,3} & x_{t,4} & x_{t,5} & x_{t,6} & x_{t,7} & x_{t,8} & x_{t,9} & x_{t,10}
  \end{bmatrix} \\
  w^T &= \begin{bmatrix}
    1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1
  \end{bmatrix}
\end{align*}
$$

where: $x_{t,1}, \ldots, x_{t,5}$ are flows at time $t$ to regular gasoline of reformate, LSR naphtha, n-butane, catalytic gasoline, and alkylate, respectively; $x_{6}, \ldots, x_{10}$ are flows at time $t$ to premium gasoline of reformate, LSR naphtha, n-butane, catalytic gasoline, and alkylate, respectively.

The demand/availability limits at time $t$ are formulated as:
The following steps were carried out at the $k^{th}$ RTO interval:

1. simulate blending process using $x_{k-1}$ and the blending models in Equation (2.16) to get "measured" blended qualities,

2. calculate biases for next step,

3. solve Problem (4.4) to calculate $x_k$.

Blended Octane

Figure 4-3: Blended Octane using LP + Bias Controller

The above steps were repeated at each RTO interval, and Problem (4.4) was solved using linear programming in GAMS [Brooke et al., 1992]. The optimization results (feedstock flowrates and
active constraints) for each RTO interval are given in Appendix C. The product qualities at
the end of the 24 hour blending period are shown in Figures 4-3 and 4-4 as deviations from
specification.

While there is significant quality giveaway in $RON$ and $MON$ of regular and $RON$ of pre-
mium gasoline, $RVP$'s of both grades of gasoline are above the maximum specified and the
$MON$ of premium grade is below the minimum allowed. In addition, $RVP$ of both grades is
off-specification throughout the blend. As a result, both grades of gasoline produced are off-
specification and may not be suitable for sale. Since both grades are off-specification throughout
the blend horizon, portions of blends cannot be removed to obtain blends that do meet speci-
fications. Hence, a profit level for the conventional controller could not be computed.

In this case-study, the conventional controller fails to make products meeting quality specifi-
cations. Poor controller performance can be attributed to a combination of structural plant/model
mismatch resulting from the use of linear blending models, and parametric mismatch arising
from fluctuations in reformate qualities.

![Blended RVP](image)

Figure 4-4: Blended RVP using LP + Bias Controller

73
4.5 PARAMETRIC MISMATCH CASE

As discussed in Chapter 2, linear gasoline blending models are not able to capture the true blending behaviour because most important gasoline qualities blend nonlinearly. Since blending nonlinearity is one of the major sources of blending inaccuracy, accurate modeling of properties such as octane number and boiling points is crucial to the success of the blend controller [Ramsey Jr. and Truesdale, 1990]. Recognizing the problems associated with blending nonlinearity, some refiners have tried incorporating nonlinear blending models in their controllers. An approach to incorporating nonlinear blending models has been to linearize the models and then use sequential linear programming (SLP) which retains the controller formulation given in Problem (4.4) (e.g. Diaz and Barsamian, [1994]). Another approach is to incorporate the nonlinear models directly in the blender control problem by formulating the on-line optimizer as a nonlinear programming (NLP) problem with bias updating (e.g. Ramsey Jr. and Truesdale, 1990):

\[
\max_x \quad c^T x
\]

subject to:

\[
\begin{align*}
g(x) &\leq (w^T x)s + b \\
h(x) &\leq 0
\end{align*}
\]

where: \( g(x) \) is a vector of nonlinear blending models.

Note that Problem (4.5) differs from the LP + bias update controller in Problem (4.4) only in the blending models used and can be solved using standard NLP techniques [Avriel, 1976].

4.5.1 PARAMETRIC MISMATCH PERFORMANCE STUDY

The NLP + bias update controller given in Problem (4.5) was used on the benchmark automotive gasoline blending problem posed in Section 4.2. The controller was designed to eliminate all sources of plant/model mismatch by using the same blending models as used in simulating the blending process (see Section 2.4). Since the feedstock qualities used in the RTO were fixed at their nominal values for all feedstocks except reformate, bias updating was used to compensate for fluctuations in reformate qualities. Product demand and feedstock availability limits were
the same as used in the LP + bias update case and the quality constraints were of the form:

\[
g_1(RON, MON, O, A, x) \geq (RON)_{\text{regular}}^{\text{min}}
g_2(RON, MON, O, A, x) \geq (RON)_{\text{premium}}^{\text{min}}
g_3(RON, MON, O, A, x) \geq (MON)_{\text{regular}}^{\text{min}}
g_4(RON, MON, O, A, x) \geq (MON)_{\text{premium}}^{\text{min}}
g_5(RVP, x) \leq (RVP)_{\text{regular}}^{\text{max}}
g_6(RVP, x) \leq (RVP)_{\text{premium}}^{\text{max}}
\]

where: \(g_1\) and \(g_2\) are the \(RON\) blending model applied to regular and premium grades, respectively, \(g_3\) and \(g_4\) are the \(MON\) blending model for regular and premium grades, and \(g_5\) and \(g_6\) are the \(RVP\) blending model for regular and premium gasoline. The blending models are given in Equations (2.16).

Simulation of blending control was conducted as described for the LP + bias update case except that the blend recipe at each RTO interval was obtained using NLP with MINOS in GAMS [Brooke et al., 1992]. The complete blend recipe can be found in Appendix D. Upon completion of the blend, four of the blended qualities in the product tanks were found to be off-specification as summarized in Table 4.5.

For the purposes of this study, deviations of up to -0.03 octane number for \(RON\) and \(MON\) and +0.005 psi for \(RVP\) were deemed acceptable. These tolerance levels were satisfied for both grades when gasoline produced during the 1\textsuperscript{st}, 9\textsuperscript{th}, 10\textsuperscript{th}, and 12\textsuperscript{th} intervals were excluded from the final products. The excluded gasoline was routed for reblending.

Eliminating products from 4 of the 12 RTO intervals resulted in much smaller batches and the profit earned from the blends is $44,105.96, much less than the theoretical maximum of

<table>
<thead>
<tr>
<th>Quality</th>
<th>( RON ) (regular)</th>
<th>( RVP ) (regular)</th>
<th>( MON ) (premium)</th>
<th>( RVP ) (premium)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Deviation</td>
<td>-0.1</td>
<td>0.015 psi</td>
<td>-0.05</td>
<td>0.01 psi</td>
</tr>
</tbody>
</table>

Table 4.5: Deviation from Specification at End of Blend
$66,276.55. However, performance of the NLP+bias update controller is far better than that of the conventional LP+bias controller used in Section 4.4.1. Thus eliminating structural mismatch from the conventional LP+bias controller improves controller performance dramatically. However, the bias updating strategy is not able to adequately handle parametric mismatch arising from stochastic feedstock disturbances, resulting in the production of off-specification products.

4.6 TIME-HORIZON CONTROLLER

Comparing the performance of the LP+bias controller of Section 4.4.1 and the NLP+bias controller of section 4.5.1 clearly shows that the use of appropriate nonlinear blending models is crucial to the success of the blend controller. By eliminating structural plant/model mismatch, a very significant improvement in controller performance was obtained for the benchmark problem. However, as shown in the case-study, the resulting NLP+bias updating controller can still lead to the production of off-specification blends when disturbances are present in feedstock qualities. This is because in the bias updating structure, the feedstock qualities are treated as fixed parameters in the controller while they vary in the actual plant. The resulting parametric mismatch cannot be compensated for by bias update [Forbes and Marlin, 1994]. Thus, such a blender control strategy is not well suited for control application where feedstock qualities are fluctuating.

Several control practitioners have recognized the problems associated with fluctuating component qualities and have offered some partial solutions by incorporating multi-period optimization capabilities into their blender control systems (e.g. McDonald et al. [1992], Rigby et al. [1995]). These methods approach the problem of feedstock quality changes by infrequent feedback of feedstock properties from laboratory analyses, and predicting future control actions using these laboratory based measurements. The update interval for such systems is typically a day and component qualities are assumed to remain unchanged in the future. Thus, they cannot effectively deal with the higher frequency disturbances associated with upstream process operation changes. Another approach involves using model predictive control technology where on-line blended quality measurements are used to predict disturbances in these qualities [Vermeer et al., 1996]. However, in their work Vermeer et al. assumed disturbances in the blended qualities
as step disturbances that persist over the blend horizon. Although a move in the right direction, this method does not utilize noise models that exploit feedstock quality disturbance dynamics to predict feedstock qualities in the future. As a result, existing methods cannot adequately address the issue of handling stochastic feedstock disturbances.

In this section, a new blender control approach will be presented that can effectively deal with changes in feedstock qualities. Model predictive control (MPC) schemes (e.g. Cutler and Ramaker [1979]) have enjoyed considerable success both in academia and in industry in the last 15 years since their development. MPC systems have been widely applied to systems subject to stochastic disturbances [Garcia et al., 1989], [Ogunnaike and Ray, 1994]. The success of MPC systems can be attributed in large part to their ability to exploit knowledge of process dynamics to predict future plant behaviour using appropriate models. However, to date, such strategies have not been applied to RTO systems. In this work, the disturbance handling capabilities of MPC systems are adopted in developing a new blend controller which is based on insights provided by the ideal controller.

The ideal controller in Problem (4.3) cannot be implemented because it requires future knowledge of feedstock qualities. Although perfect knowledge of feedstock qualities at all times during the blend is not realizable, past feedstock qualities can be used to predict these qualities into the future. Thus at each RTO interval, predicting feedstock qualities during the remaining blending time horizon will allow future control actions to be based on knowledge of feedstock behaviour over the whole blend horizon (past and future). This requires the blending problem to be posed as an optimization problem over the whole blend horizon as in the case of the ideal controller. This approach generates blend recipes for the remaining blend horizon. The recipe for the current time-step can be implemented and the process of prediction/optimization repeated at each time-step in a receding horizon fashion until end of blend is reached.

Such a blender control strategy is very similar to MPC in that they both involve predicting disturbances over a time horizon and basing control action by optimizing over a time horizon. In both cases, only the current control action is implemented and the whole process is repeated in receding horizon fashion. However, while the length of the prediction as well as the control (optimization) horizons are tuning parameters in MPC, only the prediction horizon is user tuned in the blend controller. This is because the optimization horizon in the blend controller
is fixed at each RTO interval as the remaining blend horizon.

The blender control strategy discussed above and the ideal controller work towards meeting quality specifications only at the end of the blend. If blending has to be terminated prior to reaching end of blend, the products made thus far could be far from being on specification. In order to guard against such situations, an additional constraint may be added to the optimization problem that would ensure that product specifications are met at all times in the future. This control strategy can be mathematically formulated as:

$$\max_x \int_{t_p}^{t_f} c^T x dt$$

subject to:

$$\int_{t_o}^{t_p} g(R(t), x(t)) dt + \int_{t_p}^{t_f} g(\hat{R}(t), x(t)) dt$$

$$\leq \left\{ \int_{t_o}^{t_f} [w^T(t)x(t)] dt \right\}_s$$

$$g(\hat{R}(t), x(t)) \leq [w^T(t)x(t)]_s$$

$$\int_{t_o}^{t_f} h(x) dt \leq 0$$

where: $R$ is a matrix containing past and present measured feedstock qualities. $\hat{R}$ is a matrix containing the predicted feedstock qualities, $g$ is a vector of blending equations which may be linear or nonlinear, and $t_o, t_p, t_f$ are the initial, present, and final blend times, respectively, and $h$ contains product demand and feedstock availability constraints.

Note that the Problem (4.6) is very similar to the perfect controller in Problem (4.3). The proposed blend controller differs from the ideal controller in that the blend horizon is divided into two parts: past (and present) and future. Also, Problem (4.6) contains an additional constraint to ensure that product specifications are met during blending. The objective functions in Problems (4.6) and (4.3) are equivalent even though Problem (4.6) integrates blending economics only from $t_p$ to $t_f$ rather than over the whole blend horizon. This is because the economics due to the past blended products is a constant and will not affect decisions on future control action. In other words, future control action cannot change economics due to past blended products.
The first set of constraints:

\[ \int_{t_o}^{t_p} g(R(t), x(t)) \, dt + \int_{t_p}^{t_f} g(\hat{R}(t), x(t)) \, dt \leq \left\{ \int_{t_o}^{t_f} [w^T(t)x(t)] \, dt \right\} s \]

look at predicted end of blend qualities which are composed of past blended qualities \((t_o \text{ to } t_p)\) and future predicted blended qualities. The future predicted blended qualities are obtained by integrating the blending models from \(t_p \text{ to } t_f\) using predicted feedstock qualities, \(\hat{R}(t)\). Feedstock qualities can be predicted using conventional prediction filter techniques \((e.g. \ Box \text{ and } Jenkins. \ [1976], \ Chiu, \ [1987])\). These constraints ensure that products meet quality specification at end of the blend.

The second set of constraints:

\[ g(\hat{R}(t), x(t)) \leq [w^T(t)x(t)] s \]

look at future blended qualities based on blending models and predicted feedstock qualities. These constraints attempt to blend products such that each partial batch made during individual RTO intervals meet specifications. Finally, the third set of constraints:

\[ \int_{t_o}^{t_f} h(x) \, dt \leq 0 \]

integrate mass balances from the start of the blend to the end of the blend in order to satisfy all demand and availability limits over the whole blend.

Like the ideal controller, the time-horizon based controller in Problem (4.6) can be solved using dynamic programming \([Bellman \text{ and } Lee. \ 1984]\) or the problem can be discretized and then solved with NLP \([Avriel, \ 1976]\).

The blender control problem in Problem (4.6) is unique compared to other blend controllers in that, at each RTO interval, the controller looks back in time to what has been blended so far while anticipating future trends in feedstock qualities. It then adaptively alters the blend recipe in order to maximize profit while satisfying all constraints. The advantages of the time horizon formulation are that during each RTO interval the controller has an opportunity to:

1. compensate for past measured off-specification products,
2. pre-compensate for anticipated trends in feedstock qualities,

3. re-capture any past quality "giveaway".

Therefore, the controller should be able to effectively deal with stochastic disturbances in feedstock qualities and provide better performance than the bias update approach. The effectiveness of the time-horizon controller will be demonstrated using the benchmark automotive gasoline blending case-study of Section 4.2.

The time-horizon based controller requires that some of the feedstock qualities be forecasted into the future. First, though, the feedstock qualities that are to be updated on-line and forecasted have to be identified. It is desirable to keep the number of adjustable parameters low since the more parameters that need to be updated on-line, the more measurements that would be required. However, the selected adjustable feedstock qualities should be able to capture the effects of major disturbances. Selection of adjustable parameters for RTO systems is discussed in Section 3.4 where a selection strategy based on the Design Cost criterion [Forbes and Marlin, 1996] is recommended. The suggested adjustable parameter selection strategy incorporates parameter observability information. Parameter observability is discussed in Chapter 3 where a new measure of observability is developed based on fundamental statistical principles. Even when a rigorous selection strategy is not applied, those parameters that exhibit strong observability (have well conditioned joint confidence regions) from the available measurements and given estimation scheme should be selected over those that only have a low degree of observability.

4.6.1 TIME-HORIZON CONTROLLER PERFORMANCE STUDY

The proposed time-horizon based controller in Problem (4.6) was discretized (by approximating integrals with summations) and used on the blending problem posed in Section 4.2. The blending models used in the vector \( \mathbf{g} \) contained no structural mismatch with the simulated blending process and are as given in Equations (2.16). Product and feedstock availability constraints were as described for the ideal controller in Section 4.2.

In this simulation case-study, disturbances are known to be present only in reformate \( RON \), \( MON \), and \( RVP \). Therefore, feedstock qualities to be forecasted (adjustable parameters) did
not have to be selected. Also, it was assumed for this case-study that the reformate qualities (RON, MON, and RVP) are measured on-line. As a result, an observability test on these parameters was not conducted. Generally, however, feedstock qualities are not measured and have to be estimated from other measurements. In such situations, observability (from the available measurements and estimator) of the qualities to be forecasted will have to be ensured using the methods developed in Chapter 3.

The three reformate qualities were forecasted in the time-horizon based controller using a prediction filter. In this simulation study, the actual noise model was used in designing the prediction filter. In general, the noise model would not be known and can be developed using identification techniques [e.g. Ljung, 1987]. The prediction filter made minimum mean squared error forecasts [Box and Jenkins, 1976] of the reformate qualities using the noise model given in Equation (4.2). The prediction filter equations are provided in Appendix H.

Three time-horizon based controllers were designed which differed in their size of the prediction horizon. 1-step, 2-steps, and 3-steps ahead predictions were used. The prediction filter used the noise model given in Equation (4.2) and two samples of historical reformate quality data to make 1-step, 2-steps, and 3-steps ahead minimum mean squared error forecasts [Box and Jenkins, 1976] of the reformate qualities for each RTO interval. The qualities were forecasted at each RTO interval from \( t_0 \) to \( t_{f-1} \) and the predictions were held constant for all intervals beyond the prediction horizon.

The three controllers (with 1, 2, and 3 step ahead prediction horizons) were used on the blending problem with NLP using MINOS in GAMS [Brooke et al., 1992]. The results from the controllers at each RTO instant are provided in Appendices E, F, and G. While controllers with prediction horizons of 2 and 3 steps yielded products meeting quality tolerance levels, RON and RVP in regular gasoline produced using 1-step ahead prediction filter failed to meet quality specifications within the specified tolerances. Excluding regular gasoline produced during the last interval brought the RON up and the RVP down to within tolerance at the cost of reducing the size of the blend, thus decreasing the profit level.

Profit earned from the controllers for the 24 hour blend are given in Table 4.6.
Table 4.6: Comparison of Time-Horizon Controllers

<table>
<thead>
<tr>
<th>Controller</th>
<th>Profit</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-step</td>
<td>$64,621.99</td>
</tr>
<tr>
<td>2-steps</td>
<td>$65,491.29</td>
</tr>
<tr>
<td>3-steps</td>
<td>$65,914.78</td>
</tr>
<tr>
<td>ideal</td>
<td>$66,276.55</td>
</tr>
</tbody>
</table>

All three controllers provide profit levels that are quite close to the theoretical maximum of $66,276.55 but performance of time-horizon controllers increase slightly as the size of the prediction horizon increases since longer prediction horizons are able to exploit more of the noise dynamics.

4.7 DISCUSSION

A gasoline blending case-study has been used in this chapter to compare the performance of blend controllers. The conventional LP – bias update controller was found to perform quite poorly on the benchmark problem and it has been shown that the conventional controller can lead to a large performance loss when stochastic disturbances are present in feedstock qualities.

Next, all structural plant/model mismatch was eliminated in formulating the NLP – bias controller. In this controller, the feedstock qualities were assumed to be fixed and bias updating was used to compensate for parametric mismatch resulting from fluctuations in reformate qualities. The NLP – bias controller was found to provide significant performance improvements over the conventional LP – bias controller on the benchmark blending problem. However, the controller can still lead to the production of off-specification blends as illustrated in the case-study.

Further performance improvements can be obtained for such systems where stochastic disturbances are present in the feedstock qualities. by using the proposed time-horizon based controller. The proposed controller differs from the NLP – bias update controller in that it optimizes the blending problem over the whole blend horizon rather than at a point in time. In addition, it updates the feedstock qualities directly, thus addressing the issue of parametric mismatch directly. The performance of three time-horizon based controllers and the NLP – bias controller are compared in Figure 4-5. Controller performance is based on the amount
of theoretical maximum profit uncaptured by each controller. The profit levels for the NLP + bias update and the 1-step ahead prediction time-horizon based controller were calculated using modified blends that meet quality specifications.

![Controller Performance](image)

**Figure 4-5: Uncaptured Profit for 24 hour Blend**

As is evident from Figure 4-5, the proposed time-horizon based controllers are far more efficient at handling stochastic disturbances than the controller based on the conventional bias updating approach. This is because the time-horizon controllers update feedstock qualities directly and work to maximize profit over the whole blend horizon rather than at a point in time.
Chapter 5

SUMMARY, CONCLUSIONS, & RECOMMENDATIONS

5.1 SUMMARY

This thesis has focused on the design of the gasoline blend controller. The widely used blend controller (LP + bias update) has to deal with structural plant/model mismatch and also is not capable of effectively handling feedstock quality disturbances as shown in Chapter 4. In this thesis, a blend controller that incorporates suitable gasoline blending models and one that can effectively handle predictable changes in feedstock qualities has been presented and shown to out-perform the conventional controllers.

Chapter 2 examines gasoline blending models for use in the blend controller. Models for octane number, Reid vapour pressure, and ASTM distillation points are discussed with respect to predictive accuracy and ease with which the model can be updated on-line in order to maintain its predictive accuracy. The Ethyl RT-70 [Healy et al., 1959] model for octane number blending, and the Blending Index method [Gary and Handwerk, 1994] for RVP blending were found to be the most suitable for control purposes among published models.

Since some of the model parameters would have to be updated on-line in the blend controller, it is important to ensure that estimates of these parameters be can obtained using the available measurements and chosen estimator. Chapter 3 develops a method of determining parameter observability for such steady-state systems.
The design of the new blend controller that incorporates appropriate nonlinear blending models is then presented in Chapter 4. The proposed controller adopts concepts from MPC systems which allows it to deal with stochastic disturbances in feedstock qualities.

5.2 CONCLUSIONS

The use of LP with bias updating for the control of gasoline blending can lead to a large performance loss when stochastic disturbances are present in feedstock properties as shown in the case-study in Chapter 4. As a first step towards capturing more profit, plant/model mismatch should be minimized. The use of NLP with bias updating increases controller performance, but can still lead to the production of off-specification blends as illustrated in the case-study. This is because in, the bias update approach, the feedstock qualities are treated as fixed parameters even though they are changing in the real process.

The time-horizon based blend controller proposed in this thesis directly addresses the issue of feedstock quality fluctuations by treating these qualities as adjustable parameters that are updated on-line. Moreover, the control strategy predicts feedstock qualities over the blend horizon to plan blending operations over the entire blend horizon. At each RTO interval, the controller predicts feedstock qualities over a time horizon, and optimizes the blending problem over the remaining blend horizon. It then implements control action for the current time-step and repeats the process at the next time step in a receding horizon fashion until end of blend. Thus the proposed time-horizon controller can be thought of as an economic optimizing model-predictive control system that is analogous to the process control technology that petroleum refiners have widely deployed throughout their plants [e.g. Cutler and Ramaker, 1979]. Although computationally more intensive, the time-horizon based controller offers a new approach to handling feedstock quality disturbances, and can provide efficient control of the gasoline blender as illustrated in Chapter 4.

The time-horizon RTO approach developed for the blend controller can be applied to on-line optimization of any process that experiences stochastic disturbances that cause the optimal operations to drift with time. The proposed RTO approach would predict trends in major disturbances entering the plant and optimize the steady-state process over a time horizon so as
to include predicted future plant behaviour in determining optimal operations. In addition, the time-horizon optimization approach can be applied to off-line optimization applications such as refinery planning and scheduling where predictable trends exist. Here again, predictable disturbances can be exploited in order to optimize operations over a period of time rather than at a point in time.

The parameter observability test developed in Chapter 3 is based on fundamental statistical principles and has been shown to provide a necessary and sufficient condition for observability of parameters from available measurements and estimator for steady-state systems. The approach naturally leads to a measure of degree of observability that looks at the joint confidence region of the parameter estimates. The observability and degree of observability concepts developed in this thesis can be used in the design of all RTO systems. The tests can be used for selecting adjustable parameters such that they have an acceptable degree of observability. Moreover, the observability concepts and tests developed in Chapter 3 are not limited to RTO systems. Rather, they are applicable to any steady-state system where secondary measurements are used to obtain estimates of unmeasured quantities.

5.3 RECOMMENDATIONS

Future work stemming from this thesis include applications of the parameter observability work of this thesis for RTO design, as well as further work on the design of the gasoline blend controller.

The approach to determining parameter observability developed in this thesis can be used for developing RTO design practices. That is, it can be used as a basis for selecting adjustable model parameters as well as for selecting process measurements for updating these parameters. In developing a method for selecting adjustable parameters and/or measurements, the test developed in this thesis can be used to ensure that the adjustable parameters exhibit an acceptable degree of observability.

The time-horizon blend controller is based on forecasting some of the feedstock qualities into the future using a prediction filter. The prediction filter only looks at the behaviour of the feedstock qualities in the past in order to make future predictions. It does not directly include
any information on upstream process operations changes and how these changes affect blender feedstock qualities. The proposed blend controller can be improved by developing models between some upstream process variables (measured disturbances) and the feedstock qualities of interest. The models can then be used in a feed forward configuration in order to allow the controller to handle feedstock disturbances (arising from measured changes in upstream process operations) more effectively.

Also, the developments of this thesis have only been applied to the design of the RTO layer in the blend controller. The ideas should be extended to the off-line optimization layer as well. That is, blending models selected in Chapter 2 and the time-horizon optimization approach developed in Chapter 4 should be adopted in the off-line scheduler and planner for increased blender efficiency.
Nomenclature

A \quad \text{system matrix in Problem (3.1)}
A \quad \text{aromatics content (\% volume)}
ai \quad \text{correlation coefficients in Ethyl RT-70 model, } i=1,\ldots,6
\bar{a} \quad \text{constant in the Stewart model for octane blending}
\bar{a} \quad \text{constant in Soave-Redlich-Kwong equation of state}
\bar{a}_{ij} \quad \text{constant in Soave-Redlich-Kwong equation of state}
B \quad \text{matrix in Problem (3.1) that relates rate of change of state variables to controlled variables}
b \quad \text{bias vector}
\bar{b} \quad \text{constant in Soave-Redlich-Kwong equation of state}
C \quad \text{matrix in Problem (3.1) that relates observations to states}
c \quad \text{cost vector}
c \quad \text{random variable defined in Problem (3.7)}
\dot{c} \quad \text{random variable defined in Problem (3.6)}
\bar{c} \quad \text{constant in the Stewart method for octane blending}
c_i \quad \text{parameters in Transformation method}
Di \quad \text{variable for feedstock } i \text{ defined in the Stewart method for octane blending}
d \quad \text{number of gasoline grades}
d_t \quad \text{scalar disturbance at time } t
F \quad \text{mass of feed to } RVP \text{ test chamber}
f \quad \text{probability density function of parameter estimates}
g \quad \text{vector of blending models}
H \quad \text{adjustment factor for hydrocarbon type in Transformation method}
h \quad \text{vector of demand and availability limits}
\( I_{i,k} \) interaction coefficient between feedstocks \( i \) and \( k \) in octane blending
\( \bar{I}_{i,k} \) interaction coefficient between feedstocks \( i \) and \( k \) in RVP blending
\( \mathbf{K} \) filter matrix
\( K_0, K_1 \) constant in Soave-Redlich-Kwong equation of state
\( k \) number of components over all feedstocks
\( k_1, k_2 \) parameters in Transformation method
\( k_3, k_4 \) parameters in Zahed method
\( L \) Lagrangian of optimization problem
\( \bar{L} \) mass of liquid phase
\( \mathbf{M} \) observability matrix for dynamic systems
\( M_0 \) model parameter in Zahed method
\( M_i \) model parameters in Zahed method, \( i = 1, \ldots, n \)
\( m \) motor octane number
\( (MW)_i \) molecular weight of \( i \)
\( \mathbf{N} \) union of a finite number of convex sets that defines plant operation region
\( N \) normal distribution
\( N_i \) convex regions that define the plant operating region, \( N_i \subset \mathbb{R}^q \)
\( n \) number of feedstocks in blend
\( O \) olefin content (\% volume)
\( P \) paraffin content (\% volume)
\( \bar{P} \) pressure
\( p \) number of adjustable parameters
\( \mathbf{Q}_\beta \) covariance matrix of parameter estimates
\( \mathbf{Q}_z \) covariance matrix of process measurements
\( Q_0 \) model parameter in Zahed method
\( Q_i \) model parameters in Zahed method, \( i = 1, \ldots, n \)
\( \mathbf{q}_{\text{ref}} \) vector of reformate qualities
\( q \) number of state variables in dynamic system
\( \mathbf{R} \) \hspace{1em} matrix containing feedstock qualities
\( \hat{\mathbf{R}} \) \hspace{1em} matrix containing feedstock blending indices
\( R \) \hspace{1em} measure of shape of joint confidence region
\( \hat{R} \) \hspace{1em} gas constant
\( r \) \hspace{1em} research octane number
\( S \) \hspace{1em} feasible set of states in steady-state system
\( S' \) \hspace{1em} closure of set \( S \) consisting of \( S \) and all its limit points
\( s \) \hspace{1em} vector of quality specifications
\( s \) \hspace{1em} octane sensitivity (research octane number - motor octane number)
\( s_t \) \hspace{1em} steps of random height at time \( t \)
\( s'_t \) \hspace{1em} random impulses at time \( t \)
\( T \) \hspace{1em} temperature
\( u \) \hspace{1em} vector of controlled variables
\( u_i \) \hspace{1em} volume fraction of feedstock \( i \) in blend
\( V \) \hspace{1em} set from which measurement noise realizations are obtained
\( \hat{V} \) \hspace{1em} mass of vapour phase in \( RVP \) test chamber
\( V_i \) \hspace{1em} volume of feedstock \( i \) in blend
\( v \) \hspace{1em} measurement noise vector
\( v \) \hspace{1em} gas volume
\( \hat{v} \) \hspace{1em} percent volume evaporated
\( v_o \) \hspace{1em} expanded liquid volume
\( w \) \hspace{1em} weighting vector
\( x \) \hspace{1em} decision variables in gasoline blending problems (feedstock flowrates)
\( y \) \hspace{1em} state variables \( \in \mathbb{R}^q \)
\( \dot{y} \) \hspace{1em} rate of change of \( y \)
\( y_0 \) \hspace{1em} initial states of process
\( z \) \hspace{1em} process measurement vector
\( z^{-1} \) \hspace{1em} backward shift operator
\begin{itemize}
\item $\alpha_1, \alpha_2$ constants in blending model in Equation (2.14)
\item $\alpha_3, \alpha_4$ constants in blending model in Equation (2.15)
\item $\beta$ adjustable parameters $\in \mathbb{R}^p$
\item $\hat{\beta}$ adjustable parameter estimates $\in \mathbb{R}^p$
\item $\tilde{\beta}$ mean of adjustable parameter estimates, $\hat{\beta}$
\item $\gamma_i$ activity coefficient of component $i$
\item $\zeta$ vector of steady-state equations that relate measurement to states
\item $\eta_i$ $i^{th}$ eigenvalue of $Q_{\bar{\beta}}^{-1}$
\item $\kappa_2$ condition number of a matrix based on $L_2$ norm
\item $\Lambda$ weighting matrix
\item $\lambda_i$ $i^{th}$ eigenvalue of $Q_{\bar{\beta}}$
\item $\mu$ Lagrange multipliers
\item $\theta_i$ mole fraction of component $i$ in the liquid phase
\item $\epsilon$ vector of residuals in Problem (3.13)
\item $\xi$ noise vector in Problem (3.1)
\item $\xi_0$ initial noise vector in Problem (3.1)
\item $\rho_i$ density of $i$ at 100 $^\circ$F (pound-moles per barrel)
\item $\rho_{M_i}$ molar density of component $i$ (pound-moles per barrel as liquid at 1 atm and 60 $^\circ$F)
\item $\rho_{\text{blend}}$ density of blend as saturated liquid at 60 $^\circ$F (pound-moles per barrel)
\item $\sigma^2$ variance of measurement noise in Example 3.1
\item $\tau_i$ $i^{th}$ eigenvector of $Q_{\bar{\beta}}^{-1}$
\item $\phi$ objective function of optimization-based estimation problem in Problem (3.13)
\item $\Phi$ map (possibly nonlinear) representing parameter estimation problem
\item $\chi$ matrix of operating conditions in Example 3.1
\item $\omega$ vector of steady-state plant model equations
\end{itemize}
OPERATORS

∇ gradient
∇² Hessian
|A| determinant of matrix A
Aᵀ transpose of matrix A

SUPERSCRIPTS

* optimal value
^ predicted value
## Glossary of Terms

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>ASTM</td>
<td>American Society for Testing and Materials</td>
</tr>
<tr>
<td>bias updating</td>
<td>model updating by applying an error term</td>
</tr>
<tr>
<td>BON</td>
<td>Blending Octane Number</td>
</tr>
<tr>
<td>LP</td>
<td>Linear Programming</td>
</tr>
<tr>
<td>LSR</td>
<td>Light Straight Run</td>
</tr>
<tr>
<td>MIP</td>
<td>Mixed Integer Programming</td>
</tr>
<tr>
<td>MON</td>
<td>Motor Octane Number</td>
</tr>
<tr>
<td>MPC</td>
<td>Model Predictive Control</td>
</tr>
<tr>
<td>NLP</td>
<td>Nonlinear Programming</td>
</tr>
<tr>
<td>ON</td>
<td>Octane Number</td>
</tr>
<tr>
<td>PID</td>
<td>Proportional-Integral-Derivative</td>
</tr>
<tr>
<td>RON</td>
<td>Research Octane Number</td>
</tr>
<tr>
<td>RTO</td>
<td>Real-Time Optimization</td>
</tr>
<tr>
<td>RVP</td>
<td>Reid Vapour Pressure</td>
</tr>
<tr>
<td>RVPBI</td>
<td>Reid Vapour Pressure Blending Index</td>
</tr>
<tr>
<td>SLP</td>
<td>Sequential Linear Programming</td>
</tr>
</tbody>
</table>
Bibliography


Appendix A: Nominal Blend

Results for the optimization problem for the nominal blend of Section 4.2 are provided in this appendix.

<table>
<thead>
<tr>
<th>Feedstock</th>
<th>Regular</th>
<th>Premium</th>
</tr>
</thead>
<tbody>
<tr>
<td>reformate</td>
<td>5430</td>
<td>3870</td>
</tr>
<tr>
<td>LSR naphtha</td>
<td>2570</td>
<td>1500</td>
</tr>
<tr>
<td>n-butane</td>
<td>1.99</td>
<td>13.0</td>
</tr>
<tr>
<td>catalytic gas.</td>
<td>0</td>
<td>4500</td>
</tr>
<tr>
<td>alkylate</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Regular</th>
<th>Premium</th>
</tr>
</thead>
<tbody>
<tr>
<td>$RON$</td>
<td>88.5</td>
<td>91.6</td>
</tr>
<tr>
<td>$MON$</td>
<td>77.8</td>
<td>80.0</td>
</tr>
<tr>
<td>$RVP$ (psi)</td>
<td>10.8</td>
<td>10.8</td>
</tr>
</tbody>
</table>

Optimal Blend Recipe
feedstocks in bbl/day

<table>
<thead>
<tr>
<th>Constraint</th>
<th>Lagrange multiplier</th>
</tr>
</thead>
<tbody>
<tr>
<td>maximum $RVP$ in regular gasoline</td>
<td>$1737 \frac{\text{day}}{\text{psi}}$</td>
</tr>
<tr>
<td>maximum $RVP$ in premium gasoline</td>
<td>$2023 \frac{\text{day}}{\text{psi}}$</td>
</tr>
<tr>
<td>minimum $RON$ in regular gasoline</td>
<td>$3110.5 \frac{\text{day}}{\text{ON}}$</td>
</tr>
<tr>
<td>minimum $MON$ in premium gasoline</td>
<td>$5679.3 \frac{\text{day}}{\text{ON}}$</td>
</tr>
<tr>
<td>maximum demand of regular gasoline</td>
<td>$1.57 \frac{\text{bbl}}{\text{day}}$</td>
</tr>
<tr>
<td>maximum demand of premium gasoline</td>
<td>$4.58 \frac{\text{bbl}}{\text{day}}$</td>
</tr>
<tr>
<td>maximum availability of catalytic gas.</td>
<td>$2.38 \frac{\text{bbl}}{\text{day}}$</td>
</tr>
<tr>
<td>all available catalytic gas. to premium gas.</td>
<td>$0.15 \frac{\text{bbl}}{\text{day}}$</td>
</tr>
<tr>
<td>no alkylate to regular gasoline</td>
<td>$4.36 \frac{\text{bbl}}{\text{day}}$</td>
</tr>
<tr>
<td>no alkylate to premium gasoline</td>
<td>$0.43 \frac{\text{bbl}}{\text{day}}$</td>
</tr>
</tbody>
</table>

Active Constraints
Appendix B: Ideal controller on benchmark problem

The optimization results for the ideal controller on the benchmark problem of Section 4.2 are provided in this appendix.

<table>
<thead>
<tr>
<th>RTO Interval</th>
<th>Reformate</th>
<th>LSR Naphtha</th>
<th>n-Butane</th>
<th>Catalytic Gas</th>
<th>Alkylate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.136</td>
<td>0.473</td>
<td>0.005</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>1.051</td>
<td>0.432</td>
<td>0.005</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
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<td>0.004</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
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<td>0</td>
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</tr>
<tr>
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<td>0.544</td>
<td>0.218</td>
<td>0.003</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>0.534</td>
<td>0.214</td>
<td>0.003</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>0.721</td>
<td>0.290</td>
<td>0.004</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>9</td>
<td>0.077</td>
<td>0.030</td>
<td>5.02*10^{-4}</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>10</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>11</td>
<td>0.205</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>12</td>
<td>0.168</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Ideal Blend Recipe for Regular Gasoline
feedstock flows in 10^4 bbl/day
Reformate LSR Naphtha n-Butane Catalytic Gas. Alkylate

<table>
<thead>
<tr>
<th>RTO Interval</th>
<th>Reformate</th>
<th>LSR Naphtha</th>
<th>n-Butane</th>
<th>Catalytic Gas.</th>
<th>Alkylate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.583</td>
<td>0.184</td>
<td>0.18</td>
<td>0.450</td>
<td>0.064</td>
</tr>
<tr>
<td>2</td>
<td>0.505</td>
<td>0.166</td>
<td>0.016</td>
<td>0.450</td>
<td>0.052</td>
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<tr>
<td>3</td>
<td>0.412</td>
<td>0.145</td>
<td>0.014</td>
<td>0.450</td>
<td>0.037</td>
</tr>
<tr>
<td>4</td>
<td>0.480</td>
<td>0.161</td>
<td>0.016</td>
<td>0.450</td>
<td>0.048</td>
</tr>
<tr>
<td>5</td>
<td>0.453</td>
<td>0.155</td>
<td>0.015</td>
<td>0.450</td>
<td>0.044</td>
</tr>
<tr>
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<td>0.371</td>
<td>0.136</td>
<td>0.013</td>
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<td>9</td>
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<td>0.012</td>
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<td>0.207</td>
<td>0.096</td>
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<td>0.450</td>
<td>0.007</td>
</tr>
<tr>
<td>11</td>
<td>0.205</td>
<td>0.095</td>
<td>0.010</td>
<td>0.450</td>
<td>0.007</td>
</tr>
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<td>0.168</td>
<td>0.086</td>
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<td>0.002</td>
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</table>

Ideal Blend Recipe for Premium Gasoline

feedstock flows in $10^4$ bbl/day

<table>
<thead>
<tr>
<th></th>
<th>Regular</th>
<th>Premium</th>
</tr>
</thead>
<tbody>
<tr>
<td>RON</td>
<td>88.5</td>
<td>91.5</td>
</tr>
<tr>
<td>MON</td>
<td>77.5</td>
<td>80.0</td>
</tr>
<tr>
<td>RVP (psi)</td>
<td>10.8</td>
<td>10.8</td>
</tr>
</tbody>
</table>

Final Blended Qualities

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Constraint

maximum availability of catalytic gas.
maximum demand of regular gasoline
maximum demand of premium gasoline

Active constraints over whole blend

103
<table>
<thead>
<tr>
<th>CONSTRAINT</th>
<th>INTERVAL</th>
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<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>maximum ( RVP ) in regular gasoline</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>maximum ( RVP ) in premium gasoline</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td></td>
<td></td>
</tr>
<tr>
<td>minimum ( RON ) in regular gasoline</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td></td>
<td></td>
</tr>
<tr>
<td>minimum ( RON ) in premium gasoline</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>minimum ( MON ) in premium gasoline</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>maximum catalytic gas. to premium</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>minimum catalytic gas. to regular</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>minimum alkylate to regular gasoline</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>maximum alkylate to premium gasoline</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Active constraints during each RTO interval

\( x \) indicates the constraint is active
Appendix C: LP plus bias controller on benchmark problem

This appendix summarizes results for the optimization problem for the conventional LP+bias controller on the benchmark problem in Section 4.2.

The blend recipe implemented by the controller at each RTO interval is given below:

<table>
<thead>
<tr>
<th>RTO Interval</th>
<th>Reformate</th>
<th>LSR Naphtha</th>
<th>n-Butane</th>
<th>Catalytic Gas.</th>
<th>Alkylate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.592</td>
<td>0.157</td>
<td>0.012</td>
<td>0.0396</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>0.463</td>
<td>0.175</td>
<td>0.075</td>
<td>0.153</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>0.353</td>
<td>0.204</td>
<td>0.004</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>0.270</td>
<td>0.206</td>
<td>0</td>
<td>0.324</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>0.190</td>
<td>0.191</td>
<td>0</td>
<td>0.419</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>0.164</td>
<td>0.186</td>
<td>0</td>
<td>0.450</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>0.164</td>
<td>0.186</td>
<td>0</td>
<td>0.450</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>0.164</td>
<td>0.186</td>
<td>0</td>
<td>0.450</td>
<td>0</td>
</tr>
<tr>
<td>9</td>
<td>0.164</td>
<td>0.186</td>
<td>0</td>
<td>0.450</td>
<td>0</td>
</tr>
<tr>
<td>10</td>
<td>0.164</td>
<td>0.186</td>
<td>0</td>
<td>0.450</td>
<td>0</td>
</tr>
<tr>
<td>11</td>
<td>0.164</td>
<td>0.186</td>
<td>0</td>
<td>0.450</td>
<td>0</td>
</tr>
<tr>
<td>12</td>
<td>0.164</td>
<td>0.186</td>
<td>0</td>
<td>0.450</td>
<td>0</td>
</tr>
</tbody>
</table>

Blend Recipe for Regular Gasoline

feedstock flows in $10^4 \frac{bbl}{day}$
RTO Interval | Reformate | LSR Naphtha | n-Butane | Catalytic Gas. | Alkylate |
---|---|---|---|---|---|
1 | 0.500 | 0.644 | 0.025 | 0.410 | 0 |
2 | 0.567 | 0.178 | 0.020 | 0.295 | 0 |
3 | 0.635 | 0.136 | 0.020 | 0.210 | 0 |
4 | 0.714 | 0.138 | 0.021 | 0.126 | 0 |
5 | 0.807 | 0.139 | 0.023 | 0.031 | 0 |
6 | 0.863 | 0.109 | 0.027 | 0 | 0 |
7 | 0.893 | 0.075 | 0.032 | 0 | 0 |
8 | 0.913 | 0.052 | 0.035 | 0 | 0 |
9 | 0.926 | 0.037 | 0.037 | 0 | 0 |
10 | 0.940 | 0.021 | 0.039 | 0 | 0 |
11 | 0.957 | 0.002 | 0.041 | 0 | 0 |
12 | 0.932 | 0 | 0.040 | 0 | 0.027 |

Blend Recipe for Premium Gasoline

feedstock flows in $10^4 \text{ bbl}_{\text{day}}$

<table>
<thead>
<tr>
<th></th>
<th>Regular</th>
<th>Premium</th>
</tr>
</thead>
<tbody>
<tr>
<td>$RON$</td>
<td>89.6</td>
<td>92.8</td>
</tr>
<tr>
<td>$MON$</td>
<td>79.0</td>
<td>79.7</td>
</tr>
<tr>
<td>$RVP$ (psi)</td>
<td>10.9</td>
<td>11.0</td>
</tr>
</tbody>
</table>

Final Blended Qualities
<table>
<thead>
<tr>
<th>CONSTRAINT</th>
<th>INTERVAL</th>
</tr>
</thead>
<tbody>
<tr>
<td>maximum RVP in regular gasoline</td>
<td>x x x x x x x x x x</td>
</tr>
<tr>
<td>maximum RVP in premium gasoline</td>
<td>x x x x x x x x x x</td>
</tr>
<tr>
<td>minimum RON in regular gasoline</td>
<td>x x x x x x x x x x</td>
</tr>
<tr>
<td>minimum RON in premium gasoline</td>
<td>x x x x x x x x x x</td>
</tr>
<tr>
<td>minimum MON in regular gasoline</td>
<td>x x x x x x x x x x</td>
</tr>
<tr>
<td>minimum MON in premium gasoline</td>
<td>x x x x x x x x x x</td>
</tr>
<tr>
<td>maximum demand regular gasoline</td>
<td>x x x x x x x x x x</td>
</tr>
<tr>
<td>maximum demand premium gasoline</td>
<td>x x x x x x x x x x</td>
</tr>
<tr>
<td>maximum catalytic gas. to premium</td>
<td>x x x x x x x x x x</td>
</tr>
<tr>
<td>minimum alkylate to regular gasoline</td>
<td>x x x x x x x x x x</td>
</tr>
<tr>
<td>maximum alkylate to premium gasoline</td>
<td>x x x x x x x x x x</td>
</tr>
<tr>
<td>minimum butane to regular gasoline</td>
<td>x x x x x x x x x x</td>
</tr>
<tr>
<td>minimum catalytic gas. to premium</td>
<td>x x x x x x x x x x</td>
</tr>
</tbody>
</table>

Active constraints during each RTO interval

x indicates the constraint is active
Appendix D: NLP plus bias controller on benchmark problem

Results for the optimization problem for the NLP+bias controller (Section 4.5.1) on the benchmark problem of Section 4.2 are provided in this appendix.

The blend recipe implemented by the controller at each RTO interval is given below:

<table>
<thead>
<tr>
<th>RTO Interval</th>
<th>Reformate</th>
<th>LSR Naphtha</th>
<th>n-Butane</th>
<th>Catalytic Gas</th>
<th>Alkylate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.543</td>
<td>0.257</td>
<td>0.0002</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>0.562</td>
<td>0.253</td>
<td>0.002</td>
<td>0</td>
<td>0</td>
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<tr>
<td>3</td>
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<td>0.232</td>
<td>0.003</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>0.568</td>
<td>0.239</td>
<td>0.003</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>0.566</td>
<td>0.231</td>
<td>0.003</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>0.567</td>
<td>0.230</td>
<td>0.003</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
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<td>0.569</td>
<td>0.228</td>
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<td>0</td>
<td>0</td>
</tr>
<tr>
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<td>0.0030</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>9</td>
<td>0.568</td>
<td>0.229</td>
<td>0.003</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>10</td>
<td>0.573</td>
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<td>0.004</td>
<td>0</td>
<td>0</td>
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<tr>
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<td>0.580</td>
<td>0.215</td>
<td>0.005</td>
<td>0</td>
<td>0</td>
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<td>0.583</td>
<td>0.213</td>
<td>0.005</td>
<td>0</td>
<td>0</td>
</tr>
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</table>

Blend Recipe for Regular Gasoline

feedstock flows in $10^4 \frac{bbl}{day}$

108
<table>
<thead>
<tr>
<th>RTO Interval</th>
<th>Reformate</th>
<th>LSR Naphtha</th>
<th>n-Butane</th>
<th>Catalytic Gas.</th>
<th>Alkylate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.387</td>
<td>0.150</td>
<td>0.013</td>
<td>0.450</td>
<td>0</td>
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<tr>
<td>2</td>
<td>0.414</td>
<td>0.120</td>
<td>0.016</td>
<td>0.450</td>
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</tr>
<tr>
<td>3</td>
<td>0.418</td>
<td>0.115</td>
<td>0.017</td>
<td>0.450</td>
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</tr>
<tr>
<td>4</td>
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<td>0.017</td>
<td>0.450</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>0.419</td>
<td>0.114</td>
<td>0.017</td>
<td>0.450</td>
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</tr>
<tr>
<td>6</td>
<td>0.420</td>
<td>0.113</td>
<td>0.017</td>
<td>0.450</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>0.423</td>
<td>0.109</td>
<td>0.017</td>
<td>0.450</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>0.423</td>
<td>0.109</td>
<td>0.018</td>
<td>0.450</td>
<td>0</td>
</tr>
<tr>
<td>9</td>
<td>0.422</td>
<td>0.110</td>
<td>0.018</td>
<td>0.450</td>
<td>0</td>
</tr>
<tr>
<td>10</td>
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<td>0.018</td>
<td>0.450</td>
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</tr>
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</tr>
</tbody>
</table>

**Blend Recipe for Premium Gasoline**

feedstock flows in $10^4 \text{ bbl/ day}$

The following constraints were found to be active during all RTO intervals over the blend:

1. maximum $RVP$ in regular gasoline
2. maximum $RVP$ in premium gasoline
3. minimum $RON$ in regular gasoline
4. minimum $MON$ in premium gasoline
5. maximum demand of regular gasoline
6. maximum demand of premium gasoline
7. maximum supply of catalytic gas.
8. minimum alkylate to regular gasoline
9. maximum alkylate to premium gasoline.
Appendix E: 1-Step ahead controller on benchmark problem

The optimization results for the time-horizon based 1-step ahead prediction controller on the benchmark problem of Section 4.2 are summarized in this appendix.

<table>
<thead>
<tr>
<th>RTO Interval</th>
<th>Reformate</th>
<th>LSR Naphtha</th>
<th>n-Butane</th>
<th>Catalytic Gas.</th>
<th>Alkylate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.072</td>
<td>0.030</td>
<td>0.0003</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>0.655</td>
<td>0.271</td>
<td>0.003</td>
<td>0</td>
<td>0</td>
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<tr>
<td>3</td>
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<tr>
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<td>0.147</td>
<td>0.002</td>
<td>0</td>
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<tr>
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<td>0.071</td>
<td>0.001</td>
<td>0</td>
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</tr>
<tr>
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<td>0.927</td>
<td>0.373</td>
<td>0.005</td>
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<tr>
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Blend Recipe for Regular Gasoline

feedstock flows in $10^4 \text{ bbl/day}$
### Blend Recipe for Premium Gasoline

<table>
<thead>
<tr>
<th>RTO Interval</th>
<th>Reformate</th>
<th>LSR Naphtha</th>
<th>n-Butane</th>
<th>Catalytic Gas.</th>
<th>Alkylate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.371</td>
<td>0.141</td>
<td>0.013</td>
<td>0.450</td>
<td>0.025</td>
</tr>
<tr>
<td>2</td>
<td>0.370</td>
<td>0.140</td>
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<td>0.450</td>
<td>0.027</td>
</tr>
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<td>3</td>
<td>0.371</td>
<td>0.137</td>
<td>0.013</td>
<td>0.450</td>
<td>0.029</td>
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</tr>
<tr>
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<td>0.137</td>
<td>0.013</td>
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</tr>
<tr>
<td>9</td>
<td>0.371</td>
<td>0.137</td>
<td>0.013</td>
<td>0.450</td>
<td>0.029</td>
</tr>
<tr>
<td>10</td>
<td>0.370</td>
<td>0.129</td>
<td>0.014</td>
<td>0.450</td>
<td>0.038</td>
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<tr>
<td>11</td>
<td>0.369</td>
<td>0.124</td>
<td>0.014</td>
<td>0.450</td>
<td>0.043</td>
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<tr>
<td>12</td>
<td>0.370</td>
<td>0.127</td>
<td>0.014</td>
<td>0.450</td>
<td>0.040</td>
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</tbody>
</table>

**Blend Recipe for Premium Gasoline**

feedstock flows in $10^4 \text{ MLL/day}$

<table>
<thead>
<tr>
<th></th>
<th>Regular</th>
<th>Premium</th>
</tr>
</thead>
<tbody>
<tr>
<td>$RON$</td>
<td>88.5</td>
<td>91.5</td>
</tr>
<tr>
<td>$MON$</td>
<td>77.5</td>
<td>80.0</td>
</tr>
<tr>
<td>$RVP$ (psi)</td>
<td>10.8</td>
<td>10.8</td>
</tr>
</tbody>
</table>

**Final Blended Qualities**

<table>
<thead>
<tr>
<th>Constraint</th>
</tr>
</thead>
<tbody>
<tr>
<td>maximum availability of catalytic gas.</td>
</tr>
<tr>
<td>maximum demand of regular gasoline</td>
</tr>
<tr>
<td>maximum demand of premium gasoline</td>
</tr>
</tbody>
</table>

**Active constraints over whole blend**

The following constraints were found to be active during each RTO interval for the “current” time-step:

1. maximum $RVP$ in regular gasoline
2. maximum $RVP$ in premium gasoline
3. minimum $RON$ in regular gasoline
4. minimum $RON$ in premium gasoline
5. minimum $MON$ in premium gasoline
6. minimum catalytic gas. to regular gasoline.
Appendix F: 2-step ahead controller on benchmark problem

The optimization results for the time-horizon based 2-step ahead prediction controller on the benchmark problem of Section 4.2 are provided in this appendix.

<table>
<thead>
<tr>
<th>RTO Interval</th>
<th>Reformate</th>
<th>LSR Naphtha</th>
<th>n-Butane</th>
<th>Catalytic Gas</th>
<th>Alkylate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.072</td>
<td>0.030</td>
<td>0.0003</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>1.200</td>
<td>0.497</td>
<td>0.006</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>1.200</td>
<td>0.487</td>
<td>0.006</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>1.200</td>
<td>0.478</td>
<td>0.007</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>0.0005</td>
<td>0.0002</td>
<td>2.3*10^{-6}</td>
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<td>0</td>
</tr>
<tr>
<td>6</td>
<td>1.200</td>
<td>0.481</td>
<td>0.007</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>7</td>
<td>0</td>
<td>0.00001</td>
<td>0</td>
<td>0</td>
<td>0.0006</td>
</tr>
<tr>
<td>8</td>
<td>0.0004</td>
<td>0.0002</td>
<td>2.4*10^{-6}</td>
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<td>0.0002</td>
<td>2.8*10^{-6}</td>
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</tr>
<tr>
<td>10</td>
<td>1.200</td>
<td>0.450</td>
<td>0.009</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>11</td>
<td>0.780</td>
<td>0.279</td>
<td>0.007</td>
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<td>0</td>
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<tr>
<td>12</td>
<td>0.0005</td>
<td>0.0005</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
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</table>

Blend Recipe for Regular Gasoline

feedstock flows in $10^4 \text{ M day}^{-1}$
<table>
<thead>
<tr>
<th>RTO Interval</th>
<th>Reformate</th>
<th>LSR Naphtha</th>
<th>n-Butane</th>
<th>Catalytic Gas.</th>
<th>Alkylate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.371</td>
<td>0.141</td>
<td>0.013</td>
<td>0.450</td>
<td>0.025</td>
</tr>
<tr>
<td>2</td>
<td>0.379</td>
<td>0.142</td>
<td>0.013</td>
<td>0.450</td>
<td>0.028</td>
</tr>
<tr>
<td>3</td>
<td>0.385</td>
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<td>0.450</td>
<td>0.032</td>
</tr>
<tr>
<td>4</td>
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<td>0.014</td>
<td>0.450</td>
<td>0.034</td>
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<tr>
<td>5</td>
<td>0.334</td>
<td>0.132</td>
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<td>0.450</td>
<td>0.020</td>
</tr>
<tr>
<td>6</td>
<td>0.391</td>
<td>0.140</td>
<td>0.014</td>
<td>0.450</td>
<td>0.034</td>
</tr>
<tr>
<td>7</td>
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<td>0</td>
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<tr>
<td>8</td>
<td>0.355</td>
<td>0.132</td>
<td>0.013</td>
<td>0.450</td>
<td>0.027</td>
</tr>
<tr>
<td>9</td>
<td>0.363</td>
<td>0.135</td>
<td>0.013</td>
<td>0.450</td>
<td>0.028</td>
</tr>
<tr>
<td>10</td>
<td>0.410</td>
<td>0.136</td>
<td>0.015</td>
<td>0.450</td>
<td>0.046</td>
</tr>
<tr>
<td>11</td>
<td>0.780</td>
<td>0.123</td>
<td>0.014</td>
<td>0.450</td>
<td>0.041</td>
</tr>
<tr>
<td>12</td>
<td>0.0005</td>
<td>0.117</td>
<td>0.012</td>
<td>0.450</td>
<td>0.028</td>
</tr>
</tbody>
</table>

**Blend Recipe for Premium Gasoline**

feedstock flows in $10^4 \frac{bbd}{day}$

The following constraints were found to be active for the whole blending problem:

1. maximum availability of catalytic gas.,

2. maximum demand of regular gasoline,

3. maximum demand of premium gasoline.

The following constraints were found to be active during each RTO interval for the “current” time-step:

1. maximum $RVP$ in regular gasoline,

2. maximum $RVP$ in premium gasoline,

3. minimum $RON$ in regular gasoline,

4. minimum $RON$ in premium gasoline,
5. minimum MON in premium gasoline,

6. minimum catalytic gas. to regular gasoline.
Appendix G: 3-step ahead controller on benchmark problem

The optimization results for the time-horizon based 3-step ahead prediction controller on the benchmark problem of Section 4.2 are provided in this appendix.

<table>
<thead>
<tr>
<th>RTO Interval</th>
<th>Reformate</th>
<th>LSR Naphtha</th>
<th>n-Butane</th>
<th>Catalytic Gas</th>
<th>Alkylate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.072</td>
<td>0.030</td>
<td>3.1*10^-4</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>1.200</td>
<td>0.497</td>
<td>0.006</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>1.200</td>
<td>0.487</td>
<td>0.006</td>
<td>0</td>
<td>0</td>
</tr>
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<td>1.1*10^-6</td>
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<td>0</td>
<td>0</td>
</tr>
<tr>
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<td>1.200</td>
<td>0.477</td>
<td>0.007</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
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<td>2.4*10^-6</td>
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<td>2.1*10^-4</td>
<td>2.9*10^-6</td>
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</tr>
<tr>
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<td>1.200</td>
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<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Blend Recipe for Regular Gasoline
feedstock flows in 10^4 bbl/day
The following constraints were found to be active over the blending problem:

1. maximum availability of catalytic gas.,

2. maximum demand of regular gasoline,

3. maximum demand of premium gasoline.

The following constraints were found to be active during each RTO interval for the “current” time-step:

1. maximum \( RVP \) in regular gasoline,

2. maximum \( RVP \) in premium gasoline,
3. minimum $RON$ in regular gasoline,

4. minimum $RON$ in premium gasoline,

5. minimum $MON$ in premium gasoline,

6. minimum catalytic gas. to regular gasoline.
Appendix H: Prediction Filter

This appendix describes the prediction filter used in forecasting the feedstock qualities in Section 4.6.1.

The reformate qualities are given in Equation (4.1) as:

\[ q_{\text{ref},t} = \bar{q}_{\text{ref}} + \begin{bmatrix} 1 \\ 0.85 \\ -0.1 \end{bmatrix} d_t \]

In order to predict the reformate qualities, \( q_{\text{ref},t} \), the scalar disturbances are first calculated using the above equation (with known \( \bar{q}_{\text{ref}} \)). The scalar disturbances are then forecasted and used to calculate predictions of \( q_{\text{ref}} \) using Equation (4.1).

The scalar disturbance given in Equation (4.2) can be written as:

\[ d_t = \frac{(1 - 0.56)z^{-1}(1 - z^{-1})}{(1 - 0.56z^{-1})} s_t' \]

where: \( s_t' \) are random impulses that are integrated to give steps of random height, \( s_t \).

One, two, and three step ahead forecasts of \( d_t \) are made using minimum mean squared error forecasts [Box and Jenkins, 1976]. The filter equations are given below:

\[
\begin{align*}
\hat{d}_t(1) &= 0.56d_t + 0.44s_t' + 0.44s_{t-1}' \\
\hat{d}_t(2) &= 0.56\hat{d}_t(1) + 0.44s_t' \\
\hat{d}_t(3) &= 0.56\hat{d}_t(2)
\end{align*}
\]
where: \( \hat{d}_t(1), \hat{d}_t(2), \) and \( \hat{d}_t(3) \) are 1, 2, and 3 step ahead forecasts of \( d_t \), respectively.

Forecasting was started using two samples of historical data and by initially setting \( s'_{t-1} \) and \( s'_t \) to zero. The impulses were then calculated using:

\[
\begin{align*}
    s'_t &= d_t - \hat{d}_{t-1}(1) \\
    s'_{t-1} &= d_{t-1} - \hat{d}_{t-2}(1)
\end{align*}
\]
IMAGE EVALUATION
TEST TARGET (QA-3)