MODEL STRUCTURE AND ADJUSTABLE PARAMETER SELECTION FOR OPERATIONS OPTIMIZATION

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A Thesis Submitted to the School of Graduate Studies in Partial Fulfilment of the Requirements for the Degree of Doctor of Philosophy

McMaster University

Doctor of Philosophy (1994) McMaster University
(Chemical Engineering) Hamilton, Ontario

TITLE: **Model Structure and Adjustable Parameter Selection For Operations Optimization**

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NUMBER OF PAGES: xii, 241

MODELLING FOR OPERATIONS OPTIMIZATION

ABSTRACT

The value of model-based process optimization systems for competitive advantage in many industries, has been widely recognized. Such model-based optimization systems include Real-Time Optimization, On-Line Optimizing Control, off-line process scheduling, and any other economic process optimization scheme which uses a process model to predict optimal plant operation. The thesis investigates the design of these model-based optimization systems, particulary with respect to model structure and adjustable parameter selection..

The main contributions of this work include design phase methods, based on fundamental principles of optimization and statistics theory, for determining whether a model-based optimization system can attain the plant optimum, as well as methods for discriminating between design alternatives. Three necessary conditions for zero-offset from the optimal plant operation are presented. These include Point-Wise Model Adequacy, Augmented Model Adequacy and Point-Wise Stability. Recognizing that achieving zero-offset from the plant optimum may not always be possible, or may not be the only design objective, a Design Cost method is presented for selecting among design alternatives. This Design Cost method provides a natural "trade-off" between offset elimination and variance of the predicted optimal manipulated variable values.

Finally, the thesis is completed with a larger-scale case study involving the Williams-Otto Plant [1960]. In the case study selection of a process model and adjustable parameter set for implementation in a closed-loop Real-Time Optimization system is investigated.

ACKNOWLEDGEMENTS

I would like to thank my supervisor, Professor T.E. Marlin, for his confidence, encouragement and support throughout my thesis work. My supervisory committee, including Professors J.F. MacGregor, C.M. Crowe and D.W. Butterfield, provided many useful suggestions which enhanced the quality of this work. I would like to add a special note of thanks to Professor C.M. Crowe for the many stimulating discussions and timely advice. Funding supplied by the Natural Science and Engineering Research Council helped make the research possible.

Finally, I would like to express my deepest gratitude to my wife, Barbara, for her understanding and patience during the span of this work.

Model Structure and Adjustable Parameter Selection
For Operations Optimization

Table Of Contents

List of Figures

List of Tables

1. Introduction

Optimization of steady-state process operations has enjoyed considerable industrial interest during the past several decades and has assumed increasing importance as the operation of existing plants has become a dominant factor in achieving competitive advantage [Cutler and Perry (1983), Darby and White (1988)]. Although there are many different process optimization techniques, they can be classified into two general categories: direct search and model-based optimization [Garcia and Morari (1981)]. This thesis considers model-based process optimization systems. Such systems encompass Real-Time Optimization (RTO), On-Line Optimizing Control, off-line process scheduling, or any other control methodology which utilizes a process model to determine an optimum operations policy. The results presented in this work are applicable to all forms of model-based process optimization; however, they are particularly vital in the design of closed-loop RTO systems and, as a result, investigations will focus on closed-loop, real-time, model-based process optimization.

Any control system built for optimizing process economics, and not some form of deviation from setpoints, is commonly called an Online Optimizing Controller or a Real-Time Optimizer (RTO). Real-Time Optimization provides the link between process scheduling and the process control system. Its purpose is to maintain an optimal operations policy with respect to process economics, for processes whose behaviour varies with time. Process variation can be due to disturbances, such as catalyst deactivation and so forth, or operations changes, such as feed grade switches. Although the potential rewards for Real-Time

Optimization are considerable, attempts at implementation have met with mixed success [Darby and White (1988)]. One of the major barriers to the successful implementation of operations optimization systems is the current lack of design procedures. RTO design decisions include selection of such system components as: the process model, parameter estimation technique, optimization method, process measurements and sensors, data filtering techniques, data validation procedures, and so forth. This thesis develops design methods for Real-Time Optimization systems derived from fundamental principles of optimization and statistics theory. The concepts presented in this work provide insight into what is required of the integrated optimization system to yield a successful implementation, as well as providing some useful tools for evaluating competing design alternatives.

The major portion of this chapter is devoted to a review of the current state of process operations optimization technology, and the motivation for the subject matter of the thesis. The final two sections of the chapter provide an overview of the thesis contents, as well as a summary of the terms and conventions used throughout the work.

1.1 Process Operations Optimization Overview

Currently there are two basic philosophies in optimizing the economic performance of a plant. These are Direct Search and Model-Based techniques [Garcia and Morari (1981)]. Direct Search methods explore the response surface of the plant profit directly for the optimum operating conditions. Model-Based algorithms use process models to predict process behaviour, and thus the process model's response surface is searched for the optimal operations policy.

Regardless of philosophy, all Real-Time Optimization systems have three essential features:

i) Data Validation, where the consistency of the current data set is decided,

ii) an optimization step, where the optimum operating policy is determined,

iii) Results Analysis, where the optimization results are validated.

With the exception of Results Analysis, there has been considerable research in each of these fields, although not always with the goal of integrated RTO system design. The purpose of this section is to survey the main ideas in each area. The survey will begin by exploring both classes of process operations optimization philosophies. It will continue by examining the current state of Data Validation technology. Finally, the current status of Results Analysis will be reviewed.

1.1.1 Direct Search Methods

The early ideas for on-line optimization concentrated on the various forms of pattern searching the process response surface. During the 1950s and 1960s, Box [(1951), (1954), and (1957)] laid the basis for on-line process optimization in a series of application papers, the culmination of which was the formulation of the Evolutionary Operations (EVOP) technique [Box and Draper (1969)]. The idea central to EVOP is the performance of a set of plant experiments around the current operating point. Using statistical tests, each experimental point is tested for a significant improvement in process performance with respect to current operations. The process is then moved to the point which shows the largest plant performance improvement and the procedure is repeated.

EVOP has several properties which make its use attractive. The method is easily understood, implemented and maintained. It is particularly useful when little is known regarding plant operation. As the method proceeds to the optimal operations policy, a large quantity of information can be garnered from the plant experiments. Finally, with the exception of the required plant experimentation, every process change which EVOP makes produces improved performance.

The current state of Direct Search optimization consists of splitting the problem into several phases [Bamberger and Iserman (1978), Garcia and Morari (1981), and McFarlane and Bacon (1989)]:

i) plant experimentation,

ii) dynamic plant model identification,

iii) performance function gradient calculation,

iv) optimizer step determination.

Generally, these techniques differ only in the type of dynamic model being used to estimate the local dynamic behaviour of the plant. Steady-state information can then be extracted from the dynamic model and the direction of performance improvement determined.

The structure of the dynamic model is pre-specified for each of the methods and is not updated online. In many cases a linear structure is assumed [Garcia and Morari (1981), and McFarlane and Bacon (1989)] and in some cases a general nonlinear form is assumed [Bamberger and Iserman (1978)]. The performance gain in these methods is mainly due to the algorithm's ability to mimic local plant behaviour. This knowledge can then be exploited to give an improved estimate of the direction of the optimum. If some knowledge of the plant physical phenomena were available and could be incorporated into the dynamic model structure of the optimization method, then the method could be generalized to:

i) estimate the parameters of a dynamic process model based on plant experimentation,

ii) use the model to estimate the steady-state behaviour of the plant and, as a result, the direction of the true process optimum.

As Golden and Ydstie [1989] argue, embedding knowledge of the plant phenomena in the process model would give further performance gains by allowing not only the direction but the location of the plant extremum to be estimated; however, it must be noted that such an algorithm would closely approximate the methods of current model-based process operations optimization systems.

All of the Direct Search methods suffer from the same failing, in that they do not use any *a priori* knowledge of the process behaviour. Consequently, Direct Search optimization methods require an extensive amount of plant experimentation to find the process optimum, which increases geometrically with problem dimensionality. Since for many of these techniques, steady-state must be attained between each experiment, processes with large time constants can require an unacceptable amount of time to reach an optimum. Thus, the Direct Search methods can be significantly slower in approaching the process optimum, when started at a distance from it, than ideal model-based systems.

Plant experimentation is, typically, expensive to perform. Most of the Direct Search methods discard all but the most recent plant information and, as a result, are inefficient users of experimental data. Theoretically, model-based process optimization systems could minimize plant experimentation to the determination of a few parameters, which would allow the prediction of plant behaviour over a wide range of operation. Then, convergence speed and minimization of plant experimentation are the main driving forces for model-based optimization systems.

1.1.2 Model-Based Methods

The underlying idea in model-based process optimization is that optimum operations policy is computed using some form of a process model. If the model is very accurate, the true optimum can be found in a very few steps. Generally as model fidelity decreases, there is little performance difference between these methods and the direct search techniques. Typically, a model-based optimization system has two core components [Roberts (1979)]: one for updating the process model using measurements, and another for performing the optimization using the updated model.

Model-based optimization methods can use either steady-state or dynamic models. Optimization using steady-state models is attractive for finding the optimal steady-state operating conditions, as it is directly solving the problem as posed. Optimization using dynamic models [Bamberger and Iserman (1978), Chen and Joseph (1987), and Golden and Ydstie (1989)] has the advantage of direct measurement of the process gradients. These are particularly useful in any gradient-based optimization algorithm; however, dynamic models require some form of integration to yield an estimate of the steady-state behaviour of the process. Integration of sets of non-linear differential equations, in real-time, can drastically increase the required computing resources for optimization system implementation. Thus, investigations in this thesis will be limited to model-based optimization using steady-state models.

The model-based optimization strategy may find the true process optimum by:

1) using an accurate model of the process to predict the optimum process operation,
2) moving in the direction of this optimum and waiting for steady-state,

3) updating the process model to reflect process behaviour at the new steady-state,

4) repeating the process.

It is important to note the crucial role that process model updating plays in this optimization procedure. Arkun and Stephanopoulos [1981] give a good discussion of the main problems associated with using steady-state models for on-line optimization. They point out that:

> *"Any model-based optimizing control should address directly the problem of inaccuracies in the model and its parameters"*

For operations optimization purposes it is desirable to use simplified process models which reflect the major physical phenomena of the process, yet are not so complex as to be prohibitive from a computing point of view. Accuracy of the simplified models is often ensured by updating them using current process measurements. Roberts [1979] has shown that optimization systems using approximate steady-state models, will not necessarily converge to the actual process optimum, even with model updating.

Rather than addressing the issue of model adequacy directly, researchers have concentrated on modification of the optimization problem. Both Roberts [1979], and Golden and Ydstie [1989] provide methods which may overcome model deficiencies; however, their techniques require that process dynamics be determined by "persistent excitation" of the process inputs. Thus, these methods suffer from the same difficulties as the direct search methods and as a result have not been widely accepted by industry.

Then, one of the primary issues in model-based optimization design is model fidelity. Ensuring model fidelity requires selection of a process model with an adequate structure and a model updating scheme which will maintain model accuracy.

1.1.3 Data Validation

In any set of process measurements there are, potentially, two types of errors present. The first are those due to normal randomness inherent to the process, sometimes called process noise. The second type are biases caused by such things as instrumentation failure, leaks, and so forth. Both of these types of error pose their own unique problems for any operations optimization system. Biases in the process measurements can cause a failure to close process material or energy balances, and subsequently a poor estimate of the direction of the process optimum. Random errors create difficulty in uniquely identifying the location of the process optimum.

To deal with these two separate demands, Data Validation is split into two phases: Gross Error Detection and Data Reconciliation. Gross Error Detection techniques attempt to identify and correct any biases in the process measurement data [Crowe et al. (1983), Crowe (1988)]. Good surveys of Gross Error Detection techniques can be found in Tamhane and Mah [1985], and Rosenberg et al. [1987].

Data Reconciliation adjusts given sets of data so that process balances are closed in some statistical sense with respect to the expected properties of normal process measurement variation. Unfortunately adjusting the process measurements can affect the results of parameter estimation. Recognizing this problem, MacDonald and Howatt [1988] have proposed a method for combining Data Reconciliation and parameter estimation into a single problem using the Error-In-Variables Model [Britt and Luecke (1973), and Reilly and Patino-Leal (1981)]. Kim et al. [1990] presents an approach to solving the combined Data Reconciliation / parameter estimation problem which they claim is more robust.

Recognizing the interaction between Gross Error Detection and Data Reconciliation, Tjoa and Biegler [1990] have combined the two problems. There has been no research to date which addresses the interaction among all three problems (Gross Error Detection, Data Reconciliation and parameter estimation).

1.1.4 Results Analysis

At the end of each cycle the optimization system produces estimates of the setpoints corresponding to the optimal plant operation. Such setpoints may contain considerable uncertainty. This uncertainty arises due to modelling errors, measurement errors, uncertainty in parameter estimates, and so forth. Results Analysis attempts to determine the level of certainty associated with the predicted optimum setpoints and whether calculated changes should be made.

Sensitivity Analysis [Fiacco (1983)] provides the cornerstone for analyzing the optimization results. The key idea behind this technique is to determine how the prediction of the process optimum is affected by changes in the model parameters. This method allows the variance of estimates for the magnitude of the process optimum and its location to be estimated in terms of parametric sensitivity and parameter covariance. Konickx [1988] gives a good treatment of the various uses to which this variance information can be put. These include on-line accuracy checks of the expected optimal performance and setpoints, expected gain from on-line optimization, and optimizer self-checking. Using the methods proposed by Konickx [1988], a predicted process optimum can be tested for significant changes in the expected performance and setpoints. Setpoint change decisions can then be made on the basis of statistical evidence.

Process operations optimization research has focussed in each of the individual system component areas. Although the importance of considering the interaction of system components has been recognized by some researchers [Roberts (1979), Krishnan (1990)], there is currently little research on the effects of such interactions within an integrated optimization system. Design methods and tools, which consider the optimization system in its entirety, are required to ensure successful optimization system implementation.

1.2 Thesis Scope

As discussed in the previous section, this thesis concentrates on the design of model-based optimization systems for steady-state process operations. In particular this work emphasizes the RTO design issues involving process model and adjustable parameter selection in optimization system design. Thus, to facilitate the development of the work the following assumptions are made:

i) it is possible to determine when the process has reached steady-state,

ii) there are no gross errors in the process data reaching the optimization layer,

iii) the "best" control technology available has been implemented beneath the optimization layer.

The last assumption is particularly important so as to ensure feasible operation regardless of optimization system output and to provide a fail-safe mechanism.

Figure 1.1 presents the general anatomy of a model-based optimization system. Typically, a successful design has five basic features:

1) a sensing system to provide the necessary information to keep the process model accurate,

2) a process model which is suitable for use within the optimization application,

3) a model updating method which is consistent with the process model and optimization strategy,

4) an optimization algorithm,

5) a flexible control system to enforce the optimal operations policy.

All of these features have received some attention in the literature. Krishnan [1990] showed that selection of process sensors and model parameter updating methods for on-line optimization must be considered with respect to the process model. Roberts [1979] illustrated the necessity of tailoring the parameter estimation and optimization strategies to the characteristics of the process model. It follows that for model-based process optimization systems, model selection is a critical design decision, upon which success of the system depends. Determination of the suitability of a process model for use in an optimization system is one of the main contributions of this work and has been published in Forbes et al. [(1992a), (1993a), and (1994)]. The Point-Wise Model Adequacy methods of Chapter 2 have been used to examine the bias update method used in many model predictive controllers. These extensions form the basis of Chapter 3 and have been published in Forbes et al. [(1992b) and (1993b)].

Figure 1.1 serves to illustrate the inter-dependence of the optimization system components. Roberts [1979], Durbeck [1965], and Krishnan [1990] have highlighted the importance of considering some of the subsystem interactions; however, to date no comprehensive design method is available which considers the entire closed-loop optimization system.

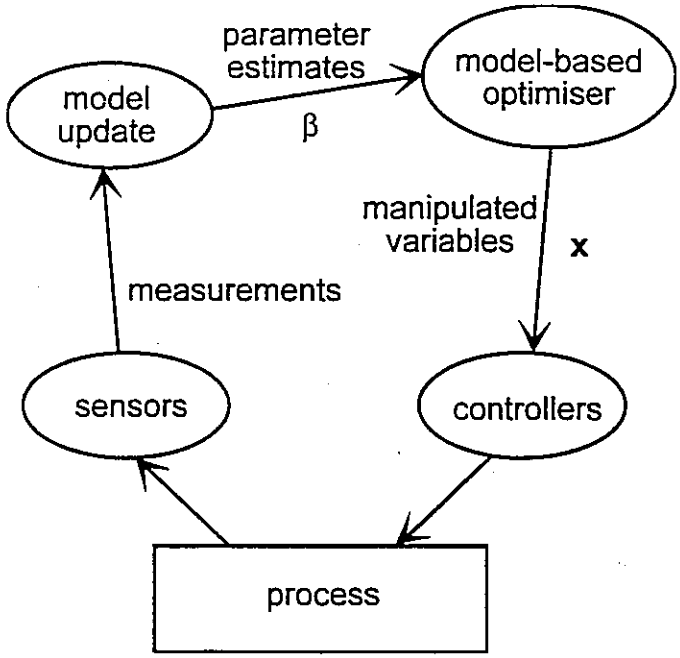

Figure 1.1: Process Optimization System Anatomy

Chapter 5 develops the Design Cost approach to optimization systems synthesis based on some fundamentals of statistics and optimization theory, as well as process economics. Although, the Design Cost method is applied to model structure and adjustable parameter selection in this thesis, it can provide a basis for development of a comprehensive design procedure for the entire closed-loop model-based optimization system. This structured Design Cost approach to model-based optimization system design is another major contribution of this work. The Design Cost method has been presented in Forbes and Marlin [(1993b) and (1994)]. Design Cost is shown to be a function of both offset from optimal operation and variation in the predicted optimal operation. Chapter 4 gives a set of necessary conditions for offset elimination in steady-state, model-based operations optimization. These offset elimination conditions have been presented in Forbes and Marlin [1993d]. The procedure presented in Chapter 5 for selection of which model parameters will be adjusted in real-time, based on Design Cost, has been published in Forbes and Marlin [(1993b) and (1994)].

Although the methods of this thesis have been limited to model structure and adjustable parameter selection, they are more broadly applicable and can be extended to the other operations optimization design issues.

1.3 Thesis Conventions

This section serves to document the conventions and terms that have been adopted to simplify discussions, throughout the thesis.

The **process model**, or more simply the **model**, is generally used to refer not only to the system of equations which describe the material and energy balances, thermodynamic relationships, and so forth, but also process operating constraints. This recognizes the possibility of model parameters occurring in both the equality and inequality constraints of the model-based optimization problem. Further, it may be necessary to include the actions of the control system / process operator in the model when these are considered to have a significant effect on steady-state process operation.

The process variables are usually split into two sets throughout this thesis. **Manipulated variables (x)**, or the independent process variables, are considered to be the set of process variables which can be independently adjusted for optimizing plant performance. **Dependent variables (u)** are those process variables whose values are uniquely determined once values for the manipulated variables are set. As a results of this division of process variables, extensive use is made of reduced space concepts [Fletcher (1987)] throughout the thesis. The term **Reduced Space** is taken to mean the space of possible manipulated variable values, once the dependent variables have been eliminated from the model-based optimization problem.

Much of the subject matter of this thesis deals with a comparison of plant and model behaviour with respect to optimization. In order to avoid confusion when referring to an optimum: the term **true plant optimum**, or more simply **plant optimum**, is taken to mean the optimal operations of the process, and **model optimum** is used to indicate the optimum of the model-based optimization problem. This work concentrates on determining whether a model-based optimization system is capable of predicting the **location** of the plant optimum. The location of an optimum refers to the values of the manipulated variables which correspond to the optimal value of the plant performance. The term **plant profit** is used to indicate the actual profit that would be realized by operating the process at a given set of manipulated variable values.

Throughout the thesis, **Real-Time Optimization (RTO)**, **On-Line Optimization**, **Process Operations Optimization**, and so forth, are used interchangeably. Also, **Model updating** is limited to parameter estimation, without restricting the possible methods of parameter estimation.

In the Design Cost discussions of Chapter 5, the term **Design Cost Metric** is used to describe the objective function in the Design Cost problems presented in the chapter. In this context, the term "metric" can used interchangeably with the term "measure".

Throughout this thesis, and particularly in the apendices, conventions are adopted for differentiation of functions with respect to vectors. In this thesis the derivative of a scalar-valued function with respect to a vector variable, whose elements are organized in a column, is a row vector containing as elements the partial derivatives of the scalar function with respect to the individual elements of the vector variable. The derivative of a vector-valued function, which is organized in a column, with respect vector variable, which is also organized in a column, is a matrix whose rows are the derivatives of the individual elements of the vector-valued function with respect to the vector variable. Conversely, for the derivative of a vector-valued function, whose elements are organized in a row, with respect to a vector variable, whose elements are organized in a clomun, the results is a matrix whose columns are the derivatives of the individual elements of the vector-valued function with respect to the vector variable.

Finally, whenever a term or convention is introduced for the first time in this thesis, it is explained.

2. Point-Wise Model Adequacy

During the development of a model-based Real-Time Optimization (RTO) system, key design decisions include selection of the process model and adjustable parameter set. Typically there are many modelling alternatives, and an important RTO system design task involves elimination of candidate process models which are not adequate for the task of process optimization. This chapter deals with the development of necessary conditions which a model must meet for a successful RTO implementation. The necessary conditions presented here are the least restrictive conditions which test the ability of the model-based optimization system to have an optimum coincident with the process optimum.

Perhaps the most common currently used method for differentiating among modelling alternatives is comparison of their accuracy in predicting key process variables, given a set of operating conditions. This method would select process optimization models based on their ability to accurately predict process outputs given a set of process inputs; however, as Durbeck [1965] showed, and is reinforced in this work, this method will not guarantee an adequate model for use in a process optimization system. A more appropriate requirement of a candidate process model is that it allows the optimization system to predict the manipulated variable values which coincide with the values of the plant optimum operations. Under this premise, the only match between the process and the model that is necessary, for a successful RTO system, is the optimal values of the manipulated variables. Further, from this perspective, an accurate estimate of profit level of the process operation is of little value for determining optimal operations, although it may be useful for monitoring plant performance.

From the preceding discussion, it is evident that an estimate of the optimum values of the manipulated variables for the true plant is required to evaluate process models using the model adequacy criteria. One possibility for such knowledge is when the plant optimum, for some nominal conditions, has been found by direct process search [Box and Draper (1969), Garcia and Morari (1980), MacFarlane and Bacon (1989)]. More typically, in the design stages of the process optimization system some nominal model will be used to represent the process. The nominal model will not be perfect, but will represent important effects to the extent that it is topologically similar to the real process. This nominal model will then provide a base-line against which the modelling alternatives can be compared. In this case, RTO modelling alternatives may consist of anything from fixing some of the parameters in the nominal model to various levels of model reduction, (e.g. tray-to-tray, collocation, sectional and lumped distillation models). Regardless of how the optimum manipulated variable values were determined, they are assumed to be available for the developments of this thesis and will be referred to as the plant optimum throughout this work.

Then, with the plant optimum available, model adequacy for the system of Figure 1.1 can be briefly stated as:

> *for at least one set of values of the adjustable model parameters, optimizing an adequate process model will yield the values of the manipulated variables which are the same as the optimum values for the plant.*

Since generally, processes and their models are nonlinear, model adequacy at a single point is valid for that point only and will not guarantee adequacy anywhere else. As some plants may have several sets of "normal" operating conditions, corresponding to different feed or product specifications and so forth, the model adequacy checks would typically be performed for each condition. Although checking several sets of conditions increases the effort, this entire procedure is performed only during the design phase of an optimization system and is intended to exclude process model alternatives that cannot yield a successful system.

In this chapter, discussions will be broken into two parts. Developments will start by considering the partially-constrained case, where there are fewer active constraints than manipulated variables at the plant optimum. Such optimization problems frequently arise in nonlinear plants when all safety, product quality, equipment performance and product rate requirements can be satisfied by adjusting some plant operating conditions, and additional degrees of freedom exist, which can be used to increase profit. The chapter continues with a discussion of the fully-constrained case, in which there are as many active constraints as manipulated variables at the true plant optimum. The chapter concludes with a discussion of the limitations of the methods.

2.1 Model Adequacy for Partially Constrained Systems

Consider a nonlinear plant with "n" independent manipulated variables, where the optimum operation occurs at the intersection of "m" constraints, with linearly independent tangent hyperplanes. Then, the dimension of the operating space for the plant can be reduced from "n" to "n-m". That is only "n-m" of the manipulated variables have to be specified to uniquely determine the process operation. For any physical plant two possibilities exist:

i) if $m = n$, the reduced operating space has zero dimension (a point) and the optimum is uniquely determined by the active constraints. This is termed the fully constrained case for the purposes of model adequacy testing.

ii) if $m < n$, the reduced operating space has some dimension greater than zero and the optimum is not uniquely determined by the active constraints. This is termed the partially constrained case for the purposes of model adequacy testing.

In either of these cases there may be more than "m" active constraints at the process optimum, that do not have more than "m" linearly independent tangent hyperplanes. The choice of which subset of the constraints to use for adequacy testing is arbitrary and may be based on considerations other than those which are the considered in this chapter.

In this section, discussions will concentrate on the determination of model adequacy when the process optimum occurs strictly within a sub-space, having dimension higher than zero, of the plant operating region. The fully constrained case is dealt with in Section 2.2.

2.1.1 Theoretical Development

As indicated in the introduction to this chapter, model adequacy testing is based on matching the optimal manipulated variable values for the plant. This will require the model-based optimization system to meet certain optimality conditions at such manipulated variable values. For the general inequality constrained optimization problem, optimality is defined by the Karush-Kuhn-Tucker (KKT) conditions [Edgar and Himmelblau, 1988]. A natural approach to determining the adequacy of a process model would be to determine whether it is possible for the model-based optimization to satisfy the KKT conditions at the values of the manipulated variables which represent the plant optimum.

Biegler et al. [1985] successfully used this concept in a related problem. They employed the KKT conditions directly to show that the "inside-out" method of Boston and Britt [1978], when applied to flowsheet optimization, does not guarantee convergence to the optimum of the more rigorous model. The "inside-out" method employs a rigorous process model in the outside optimization loop and an approximate model in the inner loop. The rigorous model is used to update a set of adjustable model parameters in the inner loop. Flowsheet optimization is performed mainly in the inner loop, using the approximate model. The "inside-out" methodology is similar to the process optimization system presented in Figure 1.1, where the outer loop includes the process, which provides process measurements for model updating, and the inner loop is the model-based optimization.

In their work, Biegler et al. required that the optimum of the rigorous model be a KKT point for the approximate model in the inner loop. Implicit in the formulation of their adequacy criteria were the following assumptions:

i) all process variables in the rigorous model are included in the approximate model,

ii) the process operating constraints (equality and inequality) consist of the same equations for both the approximate and rigorous problems,

iii) the approximate and rigorous problems should have the same KKT multipliers.

These assumptions lead to the conclusion that an inner model is adequate for use in the "inside-out" method, if the gradients of the process model, with respect to the process variables and fixed plant parameters, can be forced to match those of the outer model, by an appropriate selection of adjustable parameter values.

This method was very successful in illustrating the shortcomings of the "inside-out" method, but it assumes more correspondence between the approximate and rigorous models than necessary for plant operations optimization. Typically, a process model is a simplification of reality and as such may not contain all of the process variables. In the extreme, the model could include only those variables which can be manipulated. Thus, the only necessary correspondence between the plant and the process model is that they both must contain the same set of the manipulated variables. Similarly, the operating constraint set for a process may be much more complex than that implemented in an approximation. Since there may be little direct correspondence between the structure of the plant and that of the model used in the optimizer, beyond the manipulated variables, the actual values of the dual and non-manipulated variables should not be used in determining the adequacy of a process model.

A more appropriate approach to determining model adequacy for operations optimization would be the use of reduced space concepts [Avriel (1976), Fletcher (1987)]. The central idea in reducing the optimization space of a problem is the use of equality and active inequality constraints to eliminate some of the variables in the optimization problem, thereby transforming a constrained optimization problem into an unconstrained one.

Consider the general model-based optimization problem (which will be used throughout this work):

$$\begin{aligned} &\underset{\mathbf{x},\mathbf{u}}{\text{minimize}} \quad P(\mathbf{x},\mathbf{u},\boldsymbol{\alpha},\boldsymbol{\beta}) \\ &\text{subject to:} \\ &\qquad \mathbf{f}(\mathbf{x},\mathbf{u},\boldsymbol{\alpha},\boldsymbol{\beta}) = 0 \\ &\qquad \mathbf{g}(\mathbf{x},\mathbf{u},\boldsymbol{\alpha},\boldsymbol{\beta}) \geq 0 \end{aligned} \qquad 2.1$$

where **f** is the set of model equations, **g** is the set of operating constraints, P is the objective function, **u** is the set of dependent process variables, **x** is the set of manipulated variables, α and β are the fixed and adjustable model parameters, respectively. In order to express criteria for Point-Wise Model Adequacy in the reduced space of the model-based problem, expressions for the reduced properties of an optimization problem are required (see Appendix A). The main results of Appendix A give the following expressions for the reduced gradient of the objective function (P) :

$$\nabla_r P = \left[\nabla_x P \;\; \nabla_u P\right] \mathbf{Z} \qquad 2.2$$

and the reduced Hessian of the objective function:

$$\nabla_r^2 P = \mathbf{Z}^T \begin{bmatrix} \nabla_{\mathbf{x}}^2 L & \nabla_{\mathbf{x},\mathbf{u}}^2 L \\ \nabla_{\mathbf{u},\mathbf{x}}^2 L & \nabla_{\mathbf{u}}^2 L \end{bmatrix} \mathbf{Z} \qquad 2.3$$

in terms of partial derivatives of the objective function or Lagrangian (L) with respect to the independent manipulated variables (**x**) and the dependent process variables (**u**), and a set of basis vectors (**Z**) for the null space of the Jacobian of the active constraint set. In the reduced space, the KKT conditions require stationarity of the reduced gradient and the appropriate definiteness of the reduced Hessian (positive for a minimum and negative for a maximum), at the optimum of the resulting unconstrained optimization problem.

From Problem 2.1 it is clear that the relationship between the dependent and independent process variables depends on both the process model structure and parameters. It follows from Equations 2.2 and 2.3 that the reduced properties of the objective function also depend on both of these. Then, a process model can only be considered adequate if there is a set of adjustable parameters (β) which allows the model-based problem to have an extremum which coincides with that of the plant, in the reduced operating space. Thus, criteria for determining adequacy at a given point develop naturally from the necessary and sufficient conditions for optimality in the reduced space of the optimization problem.

The main advantage of a reduced space formulation of model adequacy is that only those variables which determine the location of the process optimum (the manipulated variables) must be considered. Exact matching of the process gradients is required only for the reduced gradient of the objective function at the optimum and the reduced Hessian need only be matched qualitatively. The dual variables can be disregarded and there need be no correspondence between the dependent process variables of the plant and process model. Model adequacy can then be defined as:

Definition 2.1: **Point-wise Model Adequacy**

For the manipulated variable values $\mathbf{x}^*_p$ *representing an unique (local) plant optimum, there must exist at least one set of values for the adjustable parameters* ($\boldsymbol{\beta}$) *such that the model-based optimization possesses an optimum at* $\mathbf{x}^*_p$, *in order for the candidate process model to be considered Point-Wise Adequate. Further, if this (local) optimum of model-based problem is unique with respect to* $\mathbf{x}$, *then the candidate process model is strongly Point-Wise Adequate.*

A mathematical expression of Point-Wise Model Adequacy is:

Criteria 2.1: **Point-Wise Model Adequacy (Partially-Constrained Case)**

If $\mathbf{x}^*_p$ *is an unique plant minimum and* $\exists$ *at least one set of values for the adjustable parameters* ($\boldsymbol{\beta}$) *such that:*

$$\nabla_r P_m \Big|_{x_p^*} \equiv 0$$

and:

$$x^T \nabla_r^2 P_m \Big|_{x_p^*} x \geq 0 \qquad \forall\, x \in S$$

when:

$$x^T \nabla_r^2 P_p \Big|_{x_p^*} x > 0 \qquad \forall\, x \in S$$

then the process model is Point-Wise Adequate. Furthermore, if the inequality constraints on the reduced Hessian of the model-based problem are strictly satisfied, the model is strongly Point-Wise Adequate.

Direct use of the Point-Wise Adequacy criteria is illustrated with a simple example.

Example 2.1.1: Minimal Approximation

In this example, for illustrative purposes, the model adequacy criteria are applied to a very simple system. A minimal representation, involving only the manipulated variables (**x**), for the Williams-Otto [1960] reactor is examined. For the reactor, the independent manipulated variables are the reactor temperature (T_R) and flow-rate of reactant B (F_B). All of the process details are given with the case studies in Section 2.1.3; however, these process details are not required for this simple illustration of analytical model adequacy testing, since the use of a empirical, quadratic model is examined. Consider the case where the model-based optimizer is a response surface method using the quadratic form:

$$\min_{\mathbf{x}} \; -P(\mathbf{x}) = -P^{*} - \boldsymbol{\beta}^{T}\mathbf{x} - \frac{1}{2}\mathbf{x}^{T}\mathbf{Q}\mathbf{x}$$

where:

$$\mathbf{x} \equiv \begin{bmatrix} F_B \\ T_R \end{bmatrix}$$

In this example P^{*} and $\mathbf{Q}$ are fixed, and $\boldsymbol{\beta}$ is adjusted in real-time. Consider the specific case where:

$$\mathbf{Q} = -\begin{bmatrix} 0.3714 & 1.714\times10^{-3} \\ 1.714\times10^{-3} & 2.138\times10^{-4} \end{bmatrix}$$

By definition, using the plant optimum given in the case studies section ($\mathbf{x}^{*}_{p}$=[4.7836 kg/s 89.647 °C]^{T}), this approximation is Point-Wise Adequate if:

$$\nabla_{r}P\Big|_{\mathbf{x}^{*}_{p}} = -\boldsymbol{\beta}^{T} - (\mathbf{x}^{*}_{p})^{T}\mathbf{Q} = 0$$

can be satisfied by at least one set of values for the adjustable parameters. Clearly, this criterion can be satisfied by $\boldsymbol{\beta}$ = [1.930 0.02737]^{T}. No adjustable parameters appear in the second-order criterion, since:

$$\nabla_{r}^{2}P = -\mathbf{Q}$$

and the model is strongly adequate since $\mathbf{Q}$ is negative definite.

Notice that the adequacy results are independent of the actual profit level, as P^{*} does not affect adequacy; in fact, the above expressions could be multiplied by any positive scalar without affecting the Point-Wise Adequacy of the approximation. Also, the Hessian of the approximation was chosen as an arbitrary negative definite matrix, illustrating that the reduced Hessians of the plant performance and the model-based optimization problem need match only qualitatively with respect to definiteness. Although this is a trivial example, it is useful for illustrating what is necessary in an adequate model. The adjustable parameters (β) must be capable of taking on the values necessary for the reduced gradient to vanish. Notice that we have not selected a method for determining β based on plant data; thus, the determination of model adequacy is independent of the model updating scheme used in the RTO system.

If this example is reformulated by fixing an element of β, it is possible to make the model inadequate by not allowing the reduced gradient to vanish at $\mathbf{x}^*_p$. The problem can be made weakly adequate by choosing a negative semi-definite $\mathbf{Q}$. An indefinite $\mathbf{Q}$ will render the model Point-Wise inadequate. In general, since some adjustable parameters may appear in the expressions for the reduced gradient and Hessian, both the first- and second-order model adequacy criteria must be checked when assigning values to the adjustable parameters.

The purpose of the Point-Wise Adequacy criteria is to provide the system designer with a tool which can be used to determine and eliminate those modelling alternatives which cannot suitably approximate the plant behaviour at the process optimum. The proposed model adequacy testing procedure requires simultaneous solution of the active constraint and reduced gradient equations, subject to restrictions on the reduced Hessian, given the plant optimum manipulated variables ($\mathbf{x}^*_p$) and the values of the fixed parameters (α). For the general non-linear case, this will not easily be accomplished analytically; thus analytical methods will be used for solving only the simplest problems. Most industrial-scale problems will require a numerical method due to their complexity.

2.1.2 Numerical Methods

Checking the Point-Wise Adequacy of a process model involves determining whether or not some adjustable parameter values (β) exist such that the given fixed point (x^*_p) is an optimum of the model-based optimization problem. If values for such a parameter set exists, the process model may be deemed Point-Wise Adequate at the given point. This criterion requires that an appropriate set of simultaneous, nonlinear equations must be solved to determine the adequacy of a process model. Thus, given x^*_p and α, a value for β must be found such that:

$$\begin{aligned} f(x^*_p, u_m, \alpha, \beta) &= 0 \\ g_L(x^*_p, u_m, \alpha, \beta) &= 0 \\ g_I(x^*_p, u_m, \alpha, \beta) &> 0 \\ \nabla_r P \Big|_{x^*_p} &= 0 \\ \lambda_i &\geq 0 \quad \forall\, i=1,2,\ldots,n \end{aligned} \qquad 2.4$$

where:

λ ≡ eigenvalues of $\nabla_r^2 P$

The non-negativity condition on the eigenvalues of the reduced Hessian is equivalent to requiring positive semi-definiteness [Ortega (1988)].

When there is at least one set of values for β which satisfies Equations 2.4, then the process model is Point-Wise Adequate. If this problem has no feasible solution, then the candidate model is not adequate for operations optimization.

Since x^*_p is determined based on the plant and no correspondence between the dependent variables of the model-based problem and plant is required, there are *(m+p)* adjustable quantities (u_m and β) available to meet the model adequacy criteria. From Equations 2.4, the Point-Wise Adequacy criteria require of the process model:

i) m independent quantities for feasibility (f and g_L),

ii) n independent quantities for stationarity,

iii) n independent quantities to manipulate the problem geometry in the reduced space.

Then, it follows that for the general Point-Wise adequate model with at least one independent adjustable parameter in each equation, $(m+p) \geq (m+2n)$. Model structure may ensure that certain principal sub-matrices of the Hessian have the required definiteness properties; thus it may be possible to have an adequate process model where $(m+2n) > (m+p) \geq (m+n)$. The minimal approximation in Example 2.1 is such a case. The dependent variables were eliminated from the minimal approximation, thus $m = 0$. The Hessian of the approximation was fixed, negative definite. Thus, only two adjustable parameters were required to ensure stationarity and Point-Wise Model Adequacy.

It is not unusual for a process model to contain at least one parameter for each model equation. Hence, there are many plant parameters which could be updated or adjusted on-line to satisfy Equation 2.4. Typically, not all model parameters are observable from available process measurements [Krishnan (1990)]; however, the set of observable model parameters can be large. Further, in the case of real plants, the manipulated variables can constitute a small subset of the plant variables. For such situations, it is possible that there may be more adjustable parameters than manipulated variables, since the number of model equations and parameters are of the same order. More simply, in many industrial-scale problems, there are an excess of degrees of freedom for meeting the adequacy criteria. When there are excess degrees of freedom in the adequacy problem, it follows that there exist multiple solutions for β in an adequate process model.

An adequacy testing method can exploit these excess degrees of freedom to enhance the predictive characteristics of the process model. When some of the process model's dependent variables have physical meaning, a natural choice is to match those dependent plant variables, for which values are available at the plant optimum, as closely as possible. Since a process model is a simplification of actual process behaviour, not all of the dependent plant variables will be represented in the model (i.e. $\mathbf{u}_m$ has lower dimension the $\mathbf{u}_p$). Also, some of the dependent variables within the process model could be composites of plant variables. Thus, the numerical problem of Equations 2.4 could be re-formulated in such a fashion as to allow the adequacy criteria to be met with minimal adjustment to those dependent variables which can be compared to available plant data. Such a formulation would be:

$$\min_{\beta} \; (\mathbf{u}_m^* - \mathbf{T}\mathbf{u}_p^*)^T \mathbf{W} (\mathbf{u}_m^* - \mathbf{T}\mathbf{u}_p^*)$$

subject to:

$$\begin{aligned} \mathbf{f}(\mathbf{x}_p^*, \mathbf{u}_m^*, \boldsymbol{\alpha}, \boldsymbol{\beta}) &= 0 \\ \mathbf{g}_L(\mathbf{x}_p^*, \mathbf{u}_m^*, \boldsymbol{\alpha}, \boldsymbol{\beta}) &= 0 \\ \mathbf{g}_I(\mathbf{x}_p^*, \mathbf{u}_m^*, \boldsymbol{\alpha}, \boldsymbol{\beta}) &> 0 \\ \nabla_r P \big|_{\mathbf{x}_p^*} &= 0 \\ \lambda_i \big|_{\mathbf{x}_p^*} &\geq 0 \qquad \forall\, i = 1,2,\ldots,n \end{aligned} \qquad 2.5$$

The advantage of solving the adequacy problem in this manner lies in the interpretation of results. When $\mathbf{u}_m$ and β have physical meaning, the solution of Problem 2.5 can be examined for validity (e.g. parameters within plausible ranges, deviation between plant and model dependent variables reasonable with respect to measurement uncertainty, and so forth).

Although the optimization Problem 2.5 will solve the adequacy problem, it involves the explicit calculation of eigenvalues. These eigenvalue computations are more complex than are required for use in an adequacy calculation. Since the reduced Hessian of the model-based problem's objective function is real and symmetric, the restrictions on its eigenvalues can be replaced by [Horn and Johnson, 1985]:

1) for strong Point-Wise Adequacy,

$$|Y_i|_{x_p^*} > 0 \qquad \forall\, i=1,\ldots,n \tag{2.6}$$

2) for weak Point-Wise Adequacy,

$$\begin{aligned} |Y_i|_{x_p^*} &\geq 0 \qquad \forall\, i=1,\ldots,n \\ \max(|Y_i|_{x_p^*}) &> 0 \end{aligned} \tag{2.7}$$

where:

$$Y_i \equiv \text{principle submatrices of } \nabla_r^2 P.$$

The formulation of the model adequacy Problem 2.5 may be further modified by adding inequality constraints to bound possible parameter and dependent variable values. Such bounds would be used when elements of $\mathbf{u}_m$ and $\boldsymbol{\beta}$ have physical meaning, with known limiting values.

Implementation of the numerical method for determining Point-Wise Model Adequacy, in either Equations 2.4 or Problem 2.5, requires a considerable effort to produce the necessary derivatives ($\nabla_r P$ and $\nabla_r^2 P$) in high-order non-linear models. These difficulties could be greatly alleviated through the use of symbolic processing software such as MAPLE [Char et al., 1991] or MATHEMATICA

[Wolfram, 1991]. If such software is not available and the problem under consideration prohibits manually determining the various derivatives, it is possible to generate approximations by finite differences [Gill, Murray and Wright, 1981]. This will require converging the plant at points about the optimum, in the reduced space.

The model adequacy problem as posed in Problem 2.5, Equations 2.6 and 2.7 can prove difficult for NLP solvers to handle, even with symbolic computation or difference approximation of the reduced gradient and Hessian. Further, care must be exercised when the reduced Hessian is semi-definite at the plant optimum. In such cases higher-order derivatives of the objective function must be checked to determine the geometry of the model-based optimization problem [Ray and Szekely, 1973], increasing the difficulty in solving the adequacy problem. An alternative formulation, which can avoid the computational complexities of determining derivatives of the objective function, based on the definition of an optimum [Avriel, 1976]:

if $\mathbf{x}^*$ is a minimum of the function $P(x)$ then,

$$P(\mathbf{x}^*) \leq P(\mathbf{x}^* + \boldsymbol{\delta}\mathbf{x}) \qquad \forall\ \boldsymbol{\delta}\mathbf{x} \in \mathbf{B}$$

where $\mathbf{B}$ is some finite neighbourhood of $\mathbf{x}^*$,

replaces the conditions on the reduced gradient and Hessian with a set of inequality constraints. If a mesh of points were to be set up around the plant optimum ($\mathbf{x}^*_p$), the constraints on the reduced properties in Problem 2.5 could be replaced with the provision that the value of the objective function at each of these grid points must be greater than that of the optimum point. Then, any method based on this idea eliminates the need for calculation of the reduced properties, at the expense of converging the plant at points in the neighbourhood of the plant optimum. Thus, the model adequacy problem can be posed as:

$$\min_{\beta} \; (u_m^* - Tu_p^*)^T W (u_m^* - Tu_p^*)$$

subject to:

$$\begin{aligned} f_m(x_p^*, u_m^*, \alpha, \beta) &= 0 \\ g_L(x_p^*, u_m^*, \alpha, \beta) &= 0 \\ g_I(x_p^*, u_m^*, \alpha, \beta) &> 0 \\ P(x_p^*, u_m^*, \alpha, \beta) &\leq P(x_p^* \pm \delta x_i, u_m^*(x_p^* + \delta x_i), \alpha, \beta) \end{aligned} \qquad 2.8$$

$$i = 1, \ldots, n$$

In order to ensure that x^*_p is the optimum of the model-based problem, according to the definition of a local optimum, it is necessary to check every feasible point in some small neighbourhood about x^*_p. Since it is not practical to test all neighbouring points, a grid geometry for some small number of points must be chosen. For the purposes of testing for model adequacy, a grid was chosen which contains two points for each element of x and one at the plant optimum. The distance between grid points (δx_i) was selected to be small with respect to the curvature of plant performance, yet sufficiently large that flowsheet convergence tolerances are not significant relative to the grid spacing.

The choice of the number and positions of the grid points can be crucial to the success of this method. Figure 2.1 demonstrates some of the possible difficulties which can arise when using the numerical adequacy method of Problem 2.8. Figure 2.1(a) shows the ideal placing of the grid. The optimum of the approximate problem is contained within it. However, even in this case the plant optimum and the optimum of the model-based problem do not exactly coincide. This will be of little concern when the grid spacing is sufficiently small. Figure 2.1(b) illustrates a possible solution to the problem of Problem 2.8, which does not have an optimum that coincides with the plant optimum. Such a situation can occur no matter how fine the grid is, whenever the condition number of the reduced Hessian is large. Although it is possible to eliminate the problem by the addition of grid points, a simpler approach would be to rotate the original grid to align with the eigenvectors of the reduced Hessian of the profit function, as in Figure 2.1(c), and re-solve Problem 2.8. Finally it is also possible that an inadequate model is a solution to the optimization Problem 2.8, as is shown in Figure 2.1(d). In this case rotating the grid along the eigenvectors of the reduced Hessian will help, as will adding extra points to the grid or calculating the reduced Hessian for the approximate problem and checking its eigenvalues.

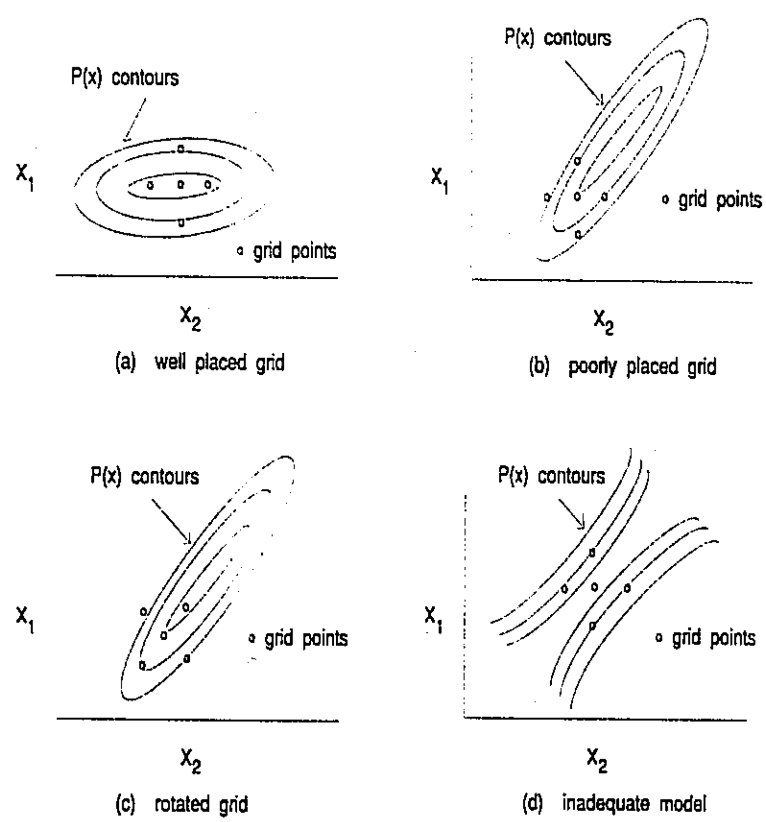

Figure 2.1: Grid Placement for Adequacy Testing

Thus, checking model adequacy using the formulation of Problem 2.8 is an iterative procedure. An initial grid is set up, and the adequacy problem solved. For this solution to the adequacy problem, the eigensystem of the reduced Hessian of the objective function is then examined. If necessary, the grid is modified, either by rotation or adding grid points, and the entire procedure repeated.

Upper bounds, based on a quadratic approximation to the response surface of the model-based optimization problem, for the distance (ε) between the plant optimum (x_p^*) and that of a process model (x_m^*) which satisfies the adequacy Problem 2.8 are presented in Appendix B. The main results are:

i) for the rectangular grid structure proposed here,

$$\|\epsilon\| < \frac{\max\{\|\boldsymbol{\delta x}_i\|\}}{\sqrt{2}}\kappa_2 \qquad 2.9$$

ii) for the rectangular grid structure aligned with the eigenvectors of the reduced Hessian,

$$\|\epsilon\| < \frac{\max\{\|\boldsymbol{\delta x}_i\|\}}{\sqrt{2}} \qquad 2.10$$

Of the two proposed numerical methods, that outlined in Problem 2.5 is preferable, because of its ability to ensure model adequacy when a solution is found, along with providing information on the ability of the model to match process outputs and geometry. The method of Problem 2.8 is easier to implement, so it may be preferable for larger problems in which analytical determination of reduced properties of the objective function is prohibitive. Use of this method is illustrated with a simple example.

Example 2.2: Minimal Approximation

Example 2.1 used a minimal approximation of the form:

$$P(\mathbf{x}) = P^{*} + \boldsymbol{\beta}^{T}\mathbf{x} + \frac{1}{2}\mathbf{x}^{T}\mathbf{Q}\mathbf{x}$$

to illustrate model adequacy for the Williams-Otto reactor. It was shown to be adequate for the specific value of **Q** given in Example 2.1. Consider the case where **Q** is fixed at another value:

$$\mathbf{Q} = -\begin{bmatrix} 2.518\times10^{4} & 856.9 \\ 856.9 & 12.96 \end{bmatrix}$$

If the numerical adequacy testing procedure of Problem 2.8 is used with a grid of five points at $\mathbf{x}^{*}_{p}$, $\mathbf{x}^{*}_{p}\pm\delta\mathbf{x}_{1}$ and $\mathbf{x}^{*}_{p}\pm\delta\mathbf{x}_{2}$, for $\delta\mathbf{x}_{1}$ = [0.0126 kg/s 0°C]^{T} and $\delta\mathbf{x}_{2}$ = [0 kg/s 0.556°C]^{T}, the Point-Wise Adequacy problem was successfully solved with:

$$\boldsymbol{\beta} = \begin{bmatrix} 1.973\times10^{5} \\ 5.261\times10^{3} \end{bmatrix}$$

with a profit of approximately $2/s more at $\mathbf{x}^{*}_{p}$ than at the other grid points.

Before accepting the model as Point-Wise adequate, the definiteness of the reduced Hessian of the model-based problem should be checked. The reduced Hessian (**Q**) in this example is indefinite, and therefore $\mathbf{x}^{*}_{p}$ corresponds to a saddle point in the reduced space. This situation is illustrated in Figure 2.1(d). The model is clearly not Point-Wise Adequate according to Criteria 2.1, regardless of its passing the preliminary numerical testing procedure and serves to illustrate the care with which numerical adequacy results must be treated. Rather than checking the reduced Hessian, the same result could be found by rotating the grid to align with the eigenvectors of the reduced Hessian, and then re-running the adequacy check. When the grid was aligned with the eigenvectors of the reduced Hessian, the NLP solver did not find a solution to Problem 2.8, also indicating an inadequate model.

2.1.3 Williams-Otto Reactor Examples

Use of the Point-Wise Model Adequacy criteria can be illustrated using the reactor from the Williams-Otto plant [1960] as modified by Roberts [1979]. Figure 2.2 provides a flow diagram for the reactor. (The entire Williams-Otto plant is treated in detail in Chapter 6).

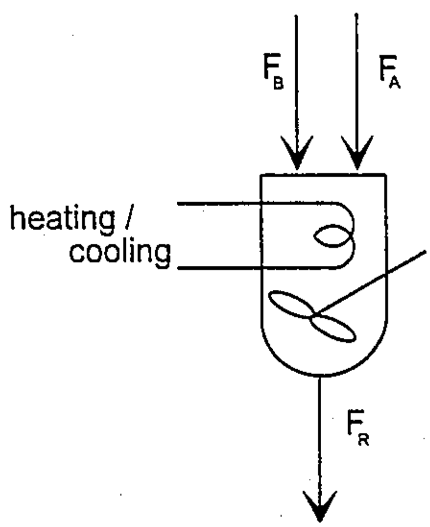

Figure 2.2: Williams-Otto Reactor

This is an ideal CSTR with the reaction sequence:

$$
\begin{aligned}
A + B &\rightarrow C & \ldots\ k_1 &= 1.6599\times10^{6}\, e^{-6666.7/T_R} \\
B + C &\rightarrow P + E & \ldots\ k_2 &= 7.2117\times10^{8}\, e^{-8333.3/T_R} \\
C + P &\rightarrow G & \ldots\ k_3 &= 2.6745\times10^{12}\, e^{-11111/T_R}
\end{aligned}
$$

In this example instantaneous profit is to be maximized. Profit is expressed as a function of feed and product flowrates:

$$P(\mathbf{x},\mathbf{u}) = 1143.38\ X_P F_R + 25.92\ X_E F_R - 76.23\ F_A - 114.34\ F_B$$

As in Roberts [1979], the case study was simplified as follows:

i) the flowrate of Reactant A to the reactor (F_A) is fixed at 1.8275 kg/s,
ii) the recycle stream flowrate in the original problem definition is set to zero,
iii) the flowrate of Reactant B to the reactor (F_B) and reactor temperature (T_R) are the manipulated variables, thus in this case $x = [F_B\ T_R]^T$.
iv) all other variables are dependent,
v) upper and lower limits on the manipulated variables are the only inequality constraints,
vi) excess heat generated by the chemical reactions can be removed from the reactor without significant cost (i.e. equipment cooling / heating duties within the reactor are not limiting),
vii) only steady-state operation is considered.

As a result, the reactor model consisted solely of material balances and simple bounds. Figure 2.3 displays a plot of the profit function of the plant versus the manipulated variables, for a typical operating range.

In the reduced space of the optimization problem, for the given operating range, the plant profit surface is strictly convex. It has a unique local optimum at :

$$T_R = 89.647\ ^{\circ}\mathrm{C}$$
$$F_B = 4.7836\ \mathrm{kg/s}.$$

This was found using MINOS 5.1, in GAMS [Brooke et al. (1988)], based on cost information supplied in Williams and Otto [1960]. This optimum was different from that found by Roberts [1979]; however, since his costing information was unavailable, this is expected.

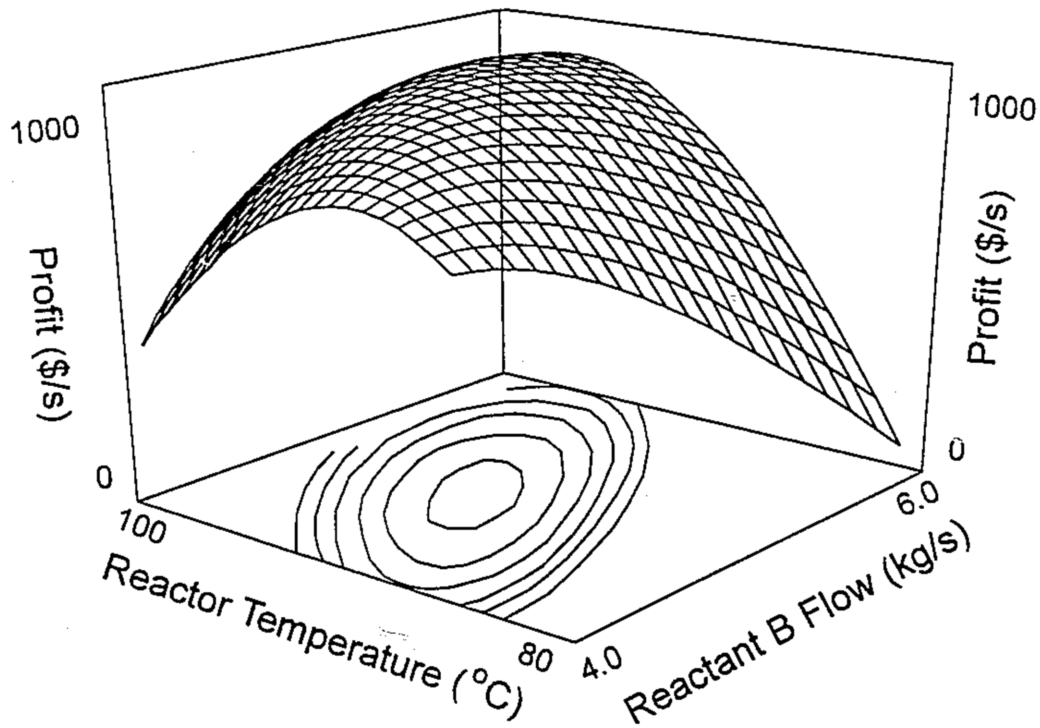

Figure 2.3: Williams-Otto Reactor Profit Surface

In most cases, the process model used by the optimization system would not have the same structure as the true plant. Thus, for the purposes of these examples, two possible approximations to the reaction system are considered for use in an operations optimization system. These elementary reaction systems are:

1) the single reaction approximation,

$$A + 2B \rightarrow P + E$$

2) the two reaction approximation,

$$A + 2B \rightarrow P + E$$
$$A + B + P \rightarrow G$$

Although there are other elements of the reactor which could be approximated, discussions are limited to the reaction kinetics to simplify the examples.

Single Reaction Approximation

Roberts [1979] approximated the Williams-Otto reaction sequence with a single reaction. In this approximation, components which are present in small amounts, and the reactions which produce them, are disregarded. Further, components which do not explicitly appear in the profit function are neglected. These considerations produced the single reaction system:

$$A + 2B \rightarrow P + E \quad \ldots \; k = \beta_1 e^{-\beta_2/T_R}$$

In a case study, Roberts [1979] demonstrated that operations optimization of the form shown in Figure 1.1, using the single reaction model, does not converge to the plant optimum. He termed this approach a conventional two-step method because the model updating and optimization were performed sequentially and independently during each iteration. In his study, model parameters are estimated using the common prediction error formulation and the updated model parameters are used in the model-based optimization to predict the optimal manipulated variable values at each iteration. The reason this two-step method failed for the single reaction approximation to the reactor kinetics is apparent from Figure 2.4, which gives the geometry of the optimization problem. The response surface for this approximation is negative semi-definite, whereas the actual process response surface is negative definite. As such, the single reaction approximation is only weakly Point-Wise Adequate and not appropriate for use in the operations optimization system of Figure 1.1, as the model-based optimization problem lacks strict convexity. This result can be shown analytically.

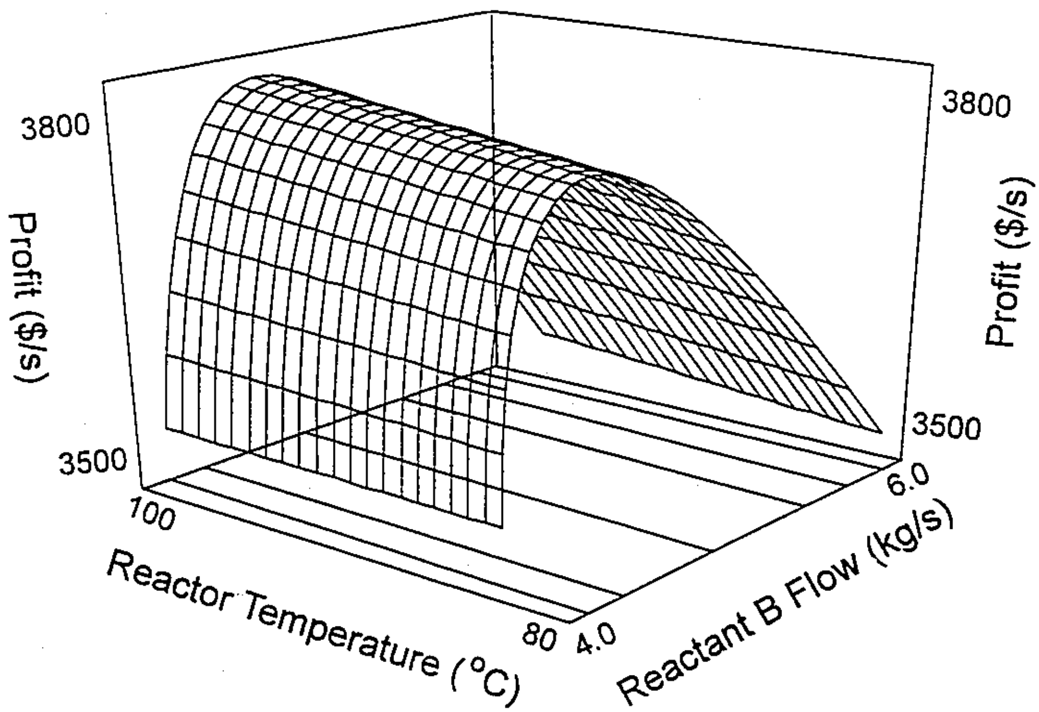

Figure 2.4: Profit Surface for Single Reaction Model (using parameters in Table 2.1)

The model for the single reaction approximation to the Williams-Otto reactor consists of the following equations:

material balances,

$$1.8275 - F_R X_A - r X_A X_B^2 = 0$$
$$F_B - F_R X_B - 2 r X_A X_B^2 = 0$$
$$2 r X_A X_B^2 - F_R X_E = 0$$
$$r X_A X_B^2 - F_R X_P = 0$$
$$F_R - 1.8275 - F_B = 0$$

reaction rate expression,

$$r - v \beta_1 \; e^{-\beta_2/T_R} = 0.$$

The objective function is:

$$P(\mathbf{x},\mathbf{u}) = 1143.38\ F_R\ X_P + 25.92\ F_R\ X_E - 114.34\ F_B - 139.31$$

The manipulated and dependent variables are:

$$\mathbf{x} = [F_B\ \ T_R]^T \text{ and } \mathbf{u} = [F_R\ \ X_A\ \ X_B\ \ X_E\ \ X_P\ \ r]^T,$$

respectively.

Then, from Equation 2.2, an expression for the reduced gradient is:

$$\nabla_r P = [-114.34\ \ \ 0] - \mathbf{c}^T \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ -1 & 0 \\ 0 & -\dfrac{v\,\beta_1\beta_2 e^{-\beta_2/T_R}}{T_R^2} \end{bmatrix}$$

where:

$$\mathbf{c} = \begin{bmatrix} -X_A & -X_B & -X_E & -X_P & 1 & 0 \\ -F_R - rX_B^2 & -2rX_B^2 & 2rX_B^2 & rX_B^2 & 0 & 0 \\ -2rX_AX_B & -F_R - 4rX_AX_B & 4rX_AX_B & 2rX_AX_B & 0 & 0 \\ 0 & 0 & -F_R & 0 & 0 & 0 \\ 0 & 0 & 0 & -F_R & 0 & 0 \\ -X_AX_B^2 & -2X_AX_B^2 & 0 & 0 & 0 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 1143.83X_P + 25.92X_E \\ 0 \\ 0 \\ 25.92F_R \\ 1143.83F_R \\ 0 \end{bmatrix}$$

simplifying:

$$\nabla_r P = [-114.34\ \ \ 0] + \begin{bmatrix} c_5 - c_2 & \dfrac{c_6 v\,\beta_1\beta_2 e^{-\beta_2/T_R}}{T_R^2} \end{bmatrix}$$

The derivation of this result made use of the observation that the Jacobian of the constraint equations and the partial derivative of the profit function, with respect to the dependent variables, are explicit functions of the dependent variables only.

No model parameters are present in these structures. Thus, their product is a constant matrix, dictated by the values of the dependent variables necessary to ensure feasibility. Finally, the Jacobian of the constraint equations with respect to the dependent variables is full rank and therefore invertible.

Stationarity requires that the reduced gradient of the objective function vanishes at the optimum. Thus, it follows that at the optimum x^*_p:

$$c_2 - c_5 = -114.34$$

$$\frac{c_6 V \beta_1 \beta_2 e^{-\beta_2/T_R}}{T_R^2} = 0$$

Since reactor temperature must be finite and the reactor volume is non-zero,

$$\frac{1}{T_R^2} \neq 0 \quad \text{and} \quad e^{-\beta_2/T_R} \neq 0 \qquad \forall \, |\beta_2| < \infty$$

hence:

$$\beta_1 \beta_2 = 0.$$

However, since there is product present in the reactor effluent, some reaction must be taking place. Therefore the parameter β_1 must be non-zero. Stationarity then requires that $\beta_2 = 0$ and the model must have a reaction rate which is independent of reactor temperature. The value of the remaining parameter (β_1) can be adjusted so as to make the first element of the reduced gradient vanish.

Since stationarity can only be met when the single reaction approximation is independent of temperature and reactor temperature appears nowhere else in the model, the reduced Hessian of the objective function is at best negative semi-definite for any set of adjustable model parameters. Thus, the single reaction approximation is only weakly adequate. This example is much simpler than a typical industrial-scale problem. However, it provides a clear example of the importance of structure on model adequacy for operations optimization.

The single reaction approximation was tested using the numerical methods presented in Section 2.1.2. The results are shown in Table 2.1:

Table 2.1: Single reaction approximation numerical Point-Wise Adequacy results.

Method	β_1	β_2
algebraic (Problem 2.5)	179.8	0.000
grid (Problem 2.8)	179.8	0.000

The results of the two numerical methods agreed with the analytical values, as shown in Table 2.1. The grid spacing was chosen at the assumed accuracy of the instrumentation, 0.6 °C for reactor temperature and 0.0126 kg/s for Reactant B flow-rate. Model convergence tolerances were set to within one-tenth of these values. The results in Table 2.1 were checked by fixing the reactor temperature at the optimum value and calculating the optimum flow-rate of reactant B. This produced the same flow as the plant optimum.

Figure 2.4 verifies the results of the model adequacy testing procedures by showing that the response surface for the single reaction approximation can have a maximum at the plant optimum, but it is not a unique extremum. Setting the operating conditions at a flowrate of 4.7836 kg/s and any reactor temperature would yield the same profit measure. This is a very poorly posed problem for any conventional optimization algorithm. Thus, this approximation is not adequate for use in the operations optimization system of Figure 1.1.

Two Reaction Approximation

The simplifications which led to the single reaction approximation of the Williams-Otto reactor, eliminated the curvature of the plant profit surface in the temperature direction. This can be recovered by observing that one of the plant reactions consumes the primary product P. This reaction is much more temperature sensitive than the others, thus producing strict convexity with respect to reactor temperature. Perhaps, a more natural plant approximation would involve the reaction sequence:

$$A + 2B \rightarrow P + E \qquad \ldots\ k_1 = \beta_1 e^{-\beta_2/T_R}$$
$$A + B + P \rightarrow G \qquad \ldots\ k_2 = \beta_3 e^{-\beta_4/T_R}$$

with all the β_i's adjustable. The response surface for this approximation is given in Figure 2.5, using the adjustable parameter values in Table 2.2. Figure 2.5 shows that the two reaction approximation exhibits curvature in both directions and appears to be capable of adequately representing the true process at the optimum.

The model for the two reaction approximation to the Williams-Otto reactor consists of the following equations:

material balances,

$$1.8275 - F_R X_A - r_1 X_A X_B^2 - r_2 X_A X_B X_P = 0$$
$$F_B - F_R X_B - 2 r_1 X_A X_B^2 - r_2 X_A X_B X_P = 0$$
$$2 r_1 X_A X_B^2 - F_R X_E = 0$$
$$3 r_2 X_A X_B X_P - F_R X_G = 0$$
$$r_1 X_A X_B^2 - F_R X_P = 0$$
$$F_R - F_B - 1.8275 = 0$$

reaction rate expressions,

$$r_1 - v\,\beta_1 \quad e^{-\beta_2/T_R} \qquad = 0$$

$$r_2 - v\,\beta_3 \quad e^{-\beta_4/T_R} \qquad = 0.$$

The objective function is:

$$P(\mathbf{x},\mathbf{u}) \;=\; 1143.38\ F_R\ X_P + 25.92\ F_R\ X_E - 114.34\ F_B - 139.31$$

The manipulated and dependent variables are:

$$\mathbf{x} = [F_B \;\; T_R]^T \text{ and } \mathbf{u} = [F_R \;\; X_A \;\; X_B \;\; X_E \;\; X_G \;\; X_P \;\; r_1 \;\; r_2]^T,$$

respectively.

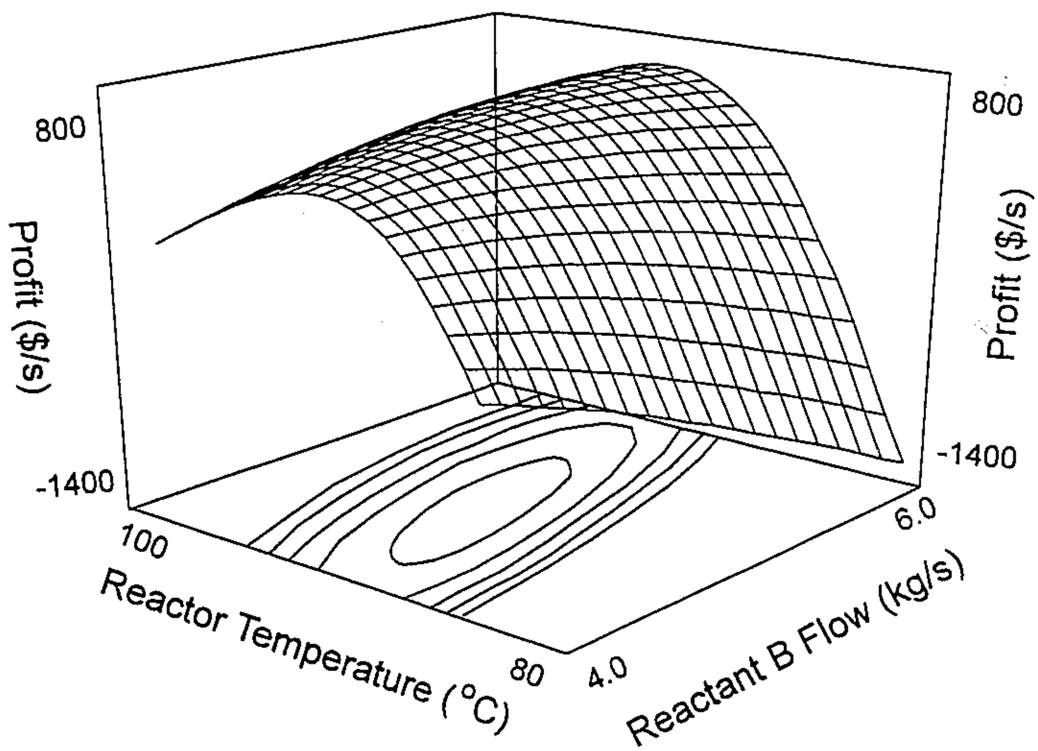

Figure 2.5: Profit Surface for Two Reaction Model (using parameters in Table 2.2)

Following the procedure described in the single reaction approximation case, the reduced gradient of the performance function is:

$$\frac{dP}{dx} = \begin{bmatrix} -114.34 \\ 0 \end{bmatrix} - \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\dfrac{\beta_1\beta_2 e^{-\beta_2/T_R}}{T_R^2} & -\dfrac{\beta_3\beta_4 e^{-\beta_4/T_R}}{T_R^2} \end{bmatrix} \begin{bmatrix} C_1 \\ 0 \\ C_3 \\ C_4 \\ C_5 \\ C_6 \\ 0 \\ C_8 \\ C_9 \\ C_{10} \\ C_{11} \end{bmatrix}$$

simplifying:

$$\frac{dP}{dx} = \begin{bmatrix} -114.34 \\ 0 \end{bmatrix} + \begin{bmatrix} C_9 - C_5 \\ \dfrac{C_{10}\,\beta_1\beta_2 e^{-\beta_2/T_R}}{T_R^2} + \dfrac{C_{11}\,\beta_3\beta_4 e^{-\beta_4/T_R}}{T_R^2} \end{bmatrix}$$

The second expression can be simplified to:

$$\beta_1\beta_2 e^{-\beta_2/T_R} + \gamma\,\beta_3\beta_4 e^{-\beta_4/T_R} = 0$$

where:

$$\gamma = \frac{C_{11}}{C_{10}}$$

This has an infinite number of solutions for finite T_R and non-zero β_i. Since the stationarity condition can easily be met with this approximation, the definiteness of the performance function's reduced Hessian must also be checked. This is not easily accomplished, analytically, and serves to highlight the need for a numerical method. However, Figure 2.5 clearly shows that the reduced Hessian is negative definite. Thus, for an appropriate set of model parameters the two reaction approximation to the Williams-Otto reactor is strongly Point-Wise Adequate.

Table 2.2 presents the results of numerical adequacy testing.

Table 2.2: Two reaction approximation numerical Point-Wise Adequacy results.

Method	β_1	β_2	β_3	β_4
algebraic (Problem 2.5)	4.611×10^{10}	13,153	2.582×10^{14}	18,808
grid (Problem 2.8)	4.040×10^{10}	13,066	2.357×10^{14}	18,749

The same grid was used as in testing the single reaction approximation, 0.6 °C for reactor temperature and 0.0126 kg/s for Reactant B flow-rate. Several starting points were chosen for the algebraic and grid methods, in each case they converged to the values given in Table 2.2. Both methods yielded very similar results, in comparable convergence times. As expected, the two reaction approximation yields multiple Point-Wise Adequate solutions for the adjustable parameters (β). Differences in the calculated adjustable parameter values are of little concern at this point, since only model adequacy is being checked. These results were checked by optimizing the model using the parameter values in Table 2.2. In each case the calculated optimum values for the manipulated variables (reactor temperature and flow-rate) in the two reaction approximate problem coincided exactly with the plant optimum manipulated variable values.

2.2 Fully-Constrained Point-Wise Model Adequacy

Section 2.1 examined the partially constrained case of Point-Wise Model Adequacy, where there were excess degrees of freedom for optimization available after satisfying all of the product quality and plant operating constraints. This section will examine the situation where optimal plant operation is uniquely specified by the equality and active inequality constraints. More specifically, for a (nonlinear) plant with "n" independent manipulated variables, where the optimum plant operation occurs at the intersection of "m" constraints, with independent tangent hyperplanes. The fully constrained case occurs when $m = n$ and the reduced operating space has zero dimension (a point). As mentioned in the preamble to Section 2.1, there may be more than "m" active constraints at the process optimum, that do not have more than "m" independent tangent hyperplanes. Again, the choice of which independent subset of the constraints to use for adequacy testing is arbitrary and may be based on considerations other than those which are the considered in this work.

In this section, discussions will concentrate on the determination of model adequacy when the optimum operations policy is uniquely determined by the model equations, product quality and process equipment constraints. This situation is of particular interest since it often occurs when the plant is approximated by linear models. Common examples are Linear Programming and Quadratic Programming for operations optimization, such as are found in modern constraint-handling control systems [Yousfi and Tournier, 1991].

2.2.1 Theoretical Development

Throughout this chapter model adequacy has been defined as the ability of the model-based optimization system to match the optimal manipulated variable values for the plant (Definition 2.1). Since model adequacy is framed solely in terms of the manipulated variables, adequacy testing is more simply performed in the Reduced Space [Avriel, 1976] of these manipulated variables. Reduced Space techniques utilize equality, and in some instances active inequality, constraints to eliminate dependent process variables from the optimization problem. For the partially-constrained case of model adequacy (Section 2.1) both the equality and active inequality constraints were used to reduce the dimension of the optimization space. If this approach were adopted in the fully-constrained case, the dimension of the reduced space would be zero and adequacy testing would be framed in terms of ensuring that the appropriate constraint set was active and intersected at the plant optimum manipulated variable values. Although this approach would be viable, it would not provide the interpretive characteristics of the approach used in this section. These interpretive characteristics are exploited in Chapter 3 to explore the robustness of model-based optimization systems using bias updating to modelling errors.

For the purposes of developing a Point-Wise Model Adequacy test for fully-constrained systems, the optimization space is reduced using only the equality constraints in the process model. This eliminates dependent process variables from the model equations and inequality constraints, allowing adequacy testing to be framed in terms of the manipulated process variables alone. In this Reduced Space, the Karush-Kuhn-Tucker (KKT) conditions [Edgar and Himmelblau, 1988] can be used directly to yield criteria for Point-Wise Model Adequacy:

Criteria 2.2: **Point-Wise Model Adequacy (Fully-Constrained Case)**

Given a unique process optimum x_p^**, the candidate process model, of the form given in Problem 2.1, is Point-Wise Adequate only if there is at least one set of values for the adjustable parameter* $\beta \in B$ *such that:*

$$\nabla_r P - \mu^T \nabla_r g_A = 0 \tag{2.11}$$

where:

$$\mu_i \geq 0 \quad \forall \; i = 1, \ldots, m \tag{2.12}$$

and:

$$\begin{aligned} f(x_p^*, u_m^*, \alpha, \beta) &= 0 \\ g_A(x_p^*, u_m^*, \alpha, \beta) &= 0 \\ g_I(x_p^*, u_m^*, \alpha, \beta) &> 0 \end{aligned} \tag{2.13}$$

The derivation of these expressions is presented in Appendix A. Notice that in this formulation the Lagrange (or KKT) multipliers for the active inequality constraints have been reintroduced into the adequacy problem. The addition of these variables to the adequacy problem slightly increases the complexity of the testing procedures; however, any increase in complexity is off-set by the usefulness of the formulation, as will be illustrated in Chapter 3. Further, no direct correspondence is assumed between the multipliers for the plant and model constraints, other than their signs.

As explained in Section 2.1.2 for the partially-constrained case of Point-Wise Model Adequacy, there may exist multiple solutions for the adjustable parameters (β) which ensure an adequate model. These excess degrees of freedom can be used, as in Section 2.1.2, for solving the model adequacy problem while simultaneously matching the dependent process variables as closely as possible. For the fully-constrained model adequacy case the problem can be formulated as:

$$\min_{\beta} \quad (u_m^* - Tu_p^*)^T W (u_m^* - Tu_p^*)$$

subject to:

$$\begin{aligned} \nabla_r P - \mu^T \nabla_r g_A &= 0 \\ \mu &\geq 0 \\ f(x_p^*, u_m^*, \alpha, \beta) &= 0 \\ g_A(x_p^*, u_m^*, \alpha, \beta) &= 0 \\ g_I(x_p^*, u_m^*, \alpha, \beta) &> 0 \end{aligned} \qquad 2.14$$

As discussed previously in Section 2.1.2, Problem 2.14 can be further refined by the addition of bounds on the adjustable parameters and the dependent process variables when they have physical significance.

The fully-constrained Point-Wise Model Adequacy criteria can be illustrated with the following simple example.

2.2.2 Fully-Constrained Model Adequacy Example

In this example we will examine the Point-Wise Adequacy of a process model for several proposed values of the fixed parameter (α). Consider the model-based optimization problem of the form:

$$\underset{\mathbf{x}}{\text{maximize}} \quad [1 \;\; 0.51]\,\mathbf{x}$$

subject to:

$$\begin{bmatrix} 2 & 4 \\ 4 & \alpha \end{bmatrix} \mathbf{x} \leq \boldsymbol{\beta}$$

where $\boldsymbol{\beta}$ is the set of adjustable model parameters. Since the adjustable model parameters all appear in the "bias" term of the constraints, any optimization system of this form is said to use bias model updating. Such systems will be dealt with in detail in Chapter 3 of this work.

In the design phase of the optimization system, the value of the manipulated variables at the process optimum were determined to be $\mathbf{x}^*_p = [1.67 \quad 1.67]^T$, using a detailed nonlinear model. The coefficient matrix in the problem contains some error-free known values (such as stoichiometric coefficients, etc.) and a fixed parameter. The fixed model parameter (α) is estimated infrequently (eg. daily or weekly), compared to the execution frequency of the optimizing controller and is therefore considered "fixed". In this case, the estimated "nominal" value for α is 2. Then, the solution to the model adequacy problem of Equations 2.11 and 2.13 in Criteria 2.2 yields:

$$\boldsymbol{\beta} = [10 \quad 10]^T, \quad \mu = [0.0033 \quad 0.2483]^T.$$

As both elements of μ are positive, the given values of the manipulated variables ($\mathbf{x}^*_p$) are an optimum of the model-based problem, and the process model can be considered Point-Wise Adequate.

Although α is fixed there is some uncertainty associated with its value. Suppose, because of this uncertainty, α were to have a value of 2.05, then the only value of the adjustable parameters for which $\mathbf{x}^*_p$ can be made a solution of Equations 2.13 of the model adequacy problem is:

$$\boldsymbol{\beta} = [10 \; 10.083]^T.$$

However, for this value of α, the solution to Equation 2.11 of the adequacy problem yields:

$$\mu = [-0.00084 \quad 0.2504]^T$$

and according to the Point-Wise Model Adequacy Criteria, the process model cannot be considered adequate. This conclusion can be confirmed by substituting $\alpha = 2.05$ and the calculated value of $\boldsymbol{\beta}$ into the example, and solving. In this case the optimum of the model-based problem is at $\mathbf{x}^*_m = [2.5 \; 0]^T$, which does not coincide with the given process optimum. Thus for this bias update case, there are values of β for which the given x^*_p is a feasible point, there is no way to update β to yield the plant optimum.

From this example, it is apparent that model adequacy can be very sensitive to the values assigned the fixed model parameters, which motivates our desire for a method to determine permissible ranges of variation in α for which the model will remain Point-Wise Adequate. This is investigated in Chapter 3.

2.3 Discussions

Previous work has shown that the success of a model-based Real-Time Optimization system is dependent upon the quality of the process model embedded within it; however, currently available methods have not provided a way to test the adequacy of a candidate process model. This chapter has presented local, necessary conditions for the success of a model-based RTO system, in the form of Point-Wise Model Adequacy Criteria, where model adequacy has been defined as the ability of the model to have optimum operating conditions coincident with the plant optimum, through the adjustment of selected parameters. From this criterion, methods were developed for determining the Point-Wise Adequacy of a model-based optimization system. Such methods will allow the system designer to investigate the suitability of a process model for use in an optimization system prior to implementation.

The main weakness of the Point-Wise Model Adequacy methods presented in this chapter is that the values of the manipulated variables, as well as the active constraint set, must be known at the process optimum. Such knowledge can be developed through direct plant experimentation, process experience, or using highly complex process models that may be unsuitable for use in a Real-Time Optimization system. A further disadvantage of the adequacy testing methods is that results are only locally valid, for the postulated active constraint set. Then to ensure a process model can adequately reflect many possible plant operation modes, the adequacy tests must be run for each of these operating points. Unknown or unexpected changes in the process equipment or active constraint sets can render an otherwise adequate process model inadequate, regardless of the extensiveness of adequacy testing during system design, since testing a large number of points does not ensure adequacy throughout a region.

Despite the possible shortcomings of the model adequacy testing methods presented here, they allow candidate process models to be evaluated using the best available process knowledge. As a result, inadequate formulations can be eliminated without extensive simulation testing of the integrated model update / optimization system. In addition, the Point-Wise Adequacy checks provide insight for model building and updating, since some adjustable parameters should appear in the expressions for the reduced properties of the objective function to affect the success of the operations optimization system.

3. Model Accuracy & Bias Update Systems

Chapter 2 presented a general set of Point-Wise Model Adequacy tests, which could be used for any operations optimization systems, of the form in Figure 1.1, to determine whether a given model-based optimization system is capable of having an optimum coincident with the plant optimum. In this chapter, model adequacy is used to investigate optimization systems which use the bias update technique for process model updating.

Figure 3.1 depicts one of the simplest forms of model-based optimization systems. In this configuration the optimizer calculates the optimal steady-state values of the manipulated variables, based on process economics, which are fed directly to the plant. Often there is a model predictive controller between the optimizer and the plant, which achieves the final steady-state operation determined by the optimizer [Brosilow and Zhao (1988), Cutler and Ramaker (1979), Yousfi and Tournier (1991)]; however, since this chapter considers the ability of the optimization system to determine the steady-state optimum operations of the plant, with respect to economics, these discussions are limited to the case of direct online optimization, without any loss of generality.

In the system of Figure 3.1, plant outputs are compared with those predicted by the process model. The difference between the actual and predicted plant outputs is used to update a "bias" or constant term appearing in the constraints of the model used by the optimizer. (The "raw" updates may be filtered to modify the dynamic behaviour of the RTO system, providing the steady-state gain of the filter is unity). Then, the updated process model is used to calculate the optimal steady-state manipulated variable values.

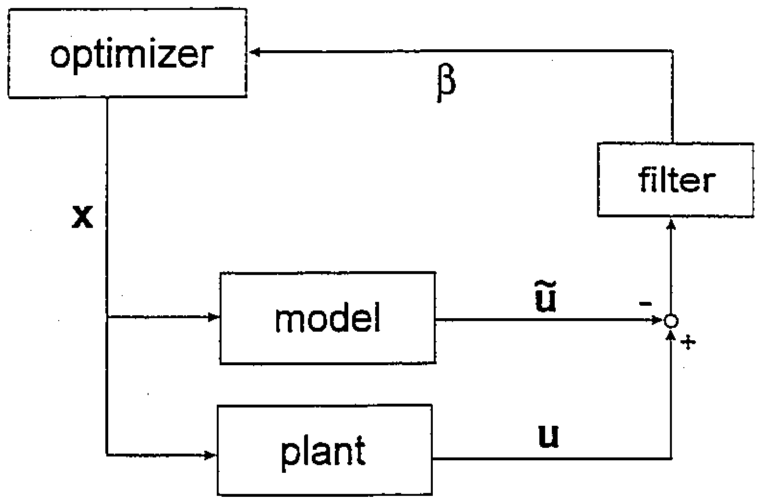

Figure 3.1: Simple RTO System with "Bias" Update.

Model predictive control (MPC) systems make extensive use of the bias updating method [Garcia, Prett and Morari, (1989)]. It has been shown that for linear systems with model updating at the control frequency, MPC systems yield zero steady-state offset for step-like disturbances in processes where the number of manipulated variables is equal to the number of setpoints. The success of the bias update method within the MPC structure has motivated control practitioners to incorporate it into the steady-state economic optimization layer [Brosilow and Zhao (1988), Stadnicki and Lawler (1985), Yousfi and Tournier (1991)]. However, to date there has been no analysis of the merits of bias update in steady-state optimization.

This chapter concentrates on the steady-state, optimizing control problem presented in Figure 3.1. The model-based optimization is generally a nonlinear programming problem of the form:

$$\underset{x,u}{\text{maximize}} \quad P(x,u)$$

$$\text{subject to:} \quad \begin{aligned} f(x,u,\alpha) - \beta_1 &= 0 \\ g(x,u,\alpha) - \beta_2 &\leq 0 \end{aligned} \qquad 3.1$$

where f is the set of process model equations including mass and energy balances, thermodynamic relationships, et cetera, g is the set of operating constraints, P is the profit function, u are the dependent process variables, x are the manipulated variables, α are the fixed model parameters and β_i are the adjustable model parameters. Note that in this expression of the optimizing control problem, all adjustable model parameters appear in the bias terms (β_i).

This chapter is restricted to the problem where there are as many independent, active constraints as manipulated variables at the process optimum (x^*_p). This situation merits special attention due to the widespread use of Linear Program (LP) and Quadratic Program (QP) based optimization systems [Brosilow and Zhao (1988), Garcia and Morshedi (1986), Morshedi et al. (1985), Yousfi and Tournier (1991)]. Although this formulation is specific, it is commonly used in optimal, model-based, predictive control systems and as such has considerable industrial relevance. Re-writing Problem 3.1 to explicitly show the active and inactive inequality constraints yields:

$$\underset{x,u}{\text{maximize}} \quad P(x,u)$$

$$\text{subject to:} \quad \begin{aligned} f(x,u,\alpha) - \beta_1 &= 0 \\ g_A(x,u,\alpha) - \beta_{2,A} &= 0 \\ g_I(x,u,\alpha) - \beta_{2,I} &< 0 \end{aligned} \qquad 3.2$$

As discussed in Chapter 2, the constraints which are active at the process optimum will usually be identified by detailed process knowledge, case study or plant experience.

In this chapter, for the bias update case, methods are developed to determine the process model's adequacy, (i.e. the ability of the updated model to sufficiently represent the process geometry so that the plant and model optima coincide) and to determine the accuracy of the process model, (i.e. its ability to yield the plant optimum despite uncertainty in the fixed model parameters). These methods are developed for the general non-linear RTO system using bias update; however, they are also applicable to the linear case. Since many industrial applications involve linear process models and constraints (e.g. Yousfi and Tournier [1991]), an analytical method for determining the effects of uncertainty in the fixed parameters of such linear constraints is presented and the method's relationship to post-optimal sensitivity analysis discussed. Finally, all of the methods are illustrated with an example built around a gasoline blending optimization and control system.

3.1 Point-Wise Model Adequacy & Bias Update

As discussed in Chapter 2, process model selection is an important step in the design of an optimization system. Even within the bias update framework, there are many modelling alternatives, and a criterion is needed to distinguish models which are adequate for use in a Real-Time Optimization system from those which are not. Chapter 2 defined an adequate process model as one which would enable the optimization system to predict the manipulated variable values which give the location of the plant optimum, regardless of the model's accuracy in predicting the process outputs or profit measure. This idea is the central concept on which model adequacy is tested and is the basis of Definition 2.1.

This chapter examines optimization systems where there are no degrees of freedom for optimization once the product quality and process operating constraints are met. In such cases, the optimum is uniquely specified by the equality and active inequality constraints (see Section 2.2). Thus, the Point-Wise Model Adequacy Criteria 2.2 for the fully-constrained case is specialized to optimization problems utilizing bias update. Then model adequacy can be stated in terms of the reduced properties of the optimization problem as:

Criteria 3.1: **Point-Wise Model Adequacy (Bias Update Case)**

Given a unique process optimum x^*_p, *the candidate process model, of the form given in Problem 3.2, is Point-Wise Adequate only if there is at least one adjustable parameter set* $\beta^* \in B$ *such that:*

$$\nabla_r P - \mu^T \nabla_r g_A = 0 \qquad 3.3$$

where:

$$\mu_i \geq 0 \quad \forall \; i = 1, \ldots, m \qquad 3.4$$

and:

$$\begin{aligned} f(x^*_p, u^*_m, \alpha) - \beta^*_1 &= 0 \\ g_A(x^*_p, u^*_m, \alpha) - \beta^*_{2,A} &= 0 \\ g_I(x^*_p, u^*_m, \alpha) - \beta^*_{2,I} &> 0 \end{aligned} \qquad 3.5$$

Notice that in the bias update formulation, the adjustable model parameters $\{\beta_i\}$ are used only to ensure feasibility and to satisfy the active status of the appropriate inequality constraints, in Equations 3.5. They do not enter directly into the optimality conditions of Equations 3.3 and 3.4. Thus, for the process model form under consideration and the specific constraints active at the process optimum, the optimality of the given point in the model-based problem depends entirely on the fixed model parameters (α). This is a particular weakness of the bias updating strategy (recall that only β is adjusted). Example 2.2 illustrated some of the difficulties of providing an adequate model within the bias update structure.

3.2 Model Accuracy Testing

In general, the plant optimum is unknown and the system designer must make process modelling choices based on the results of detailed simulations, coupled with knowledge of likely process variation and modelling errors. One of the decisions in the design of Real-Time Optimization systems is the segregation of the model parameters into adjustable and fixed sets. Selection of the bias updating method dictates which parameters will be fixed and which are adjustable. Given that all model parameters are subject to some uncertainty, Section 3.1 and Example 2.2 clearly showed that bias updating will not guarantee that the model-based optimization will find the plant optimum when there are errors in the fixed parameter; however, optimization system performance would be good over a wide range of operation if results of model-based optimization are robust to expected errors in the fixed parameters.

Friedman and Reklaitis [1975 (a) & (b)] studied a related problem in which they examined the possible set of solutions to a linear programming problem, given the presence of parametric errors. However, their interest was in determining the space of possible solutions given a pre-specified uncertainty in the model parameters and then choosing process operations which would provide the appropriate flexibility to ensure feasible operation throughout the possible range of model parameter values. In Point-Wise Model Accuracy testing we are interested in determining whether the plant optimum will remain the solution to the model-based optimization problem throughout the range of possible parameter errors. Or alternatively, accuracy testing can be used to determine the maximum amount of parameter error for which the plant optimum remains the solution to the model-based optimization problem.

Consider the two-dimensional optimization problem illustrated in Figure 3.2. In this situation the optimum is found at the intersection of two constraints (g_1 and g_2). When such a point is an optimum, the reduced gradient of the performance function ($\nabla_r P$) is contained within the cone bounded by the most limiting reduced gradients of the active constraint set ($\nabla_r g_A$), or equivalently all of the Lagrange multipliers (μ_i) are positive [Edgar and Himmelblau (1988)]. Then by definition this model is adequate, if the point of intersection of g_1 and g_2 can be made to be the process optimum (x^*_p) by an appropriate choice of values for the adjustable parameters.

Given that the process model is of the form in Problem 3.1 for which there are as many independent active constraints at the plant optimum as manipulated variables, uncertainty in the fixed parameters is interpreted as uncertainty in the slopes of the inequality constraints in the reduced space or the reduced gradient of the profit function. Figure 3.2 shows the case where there is uncertainty in a fixed parameter on which g_2 depends. The region through which the fixed parameter is expected to vary can be represented by an angle of rotation (θ) of g_2 about the plant optimum (x^*_p), assuming the corresponding bias term can be adjusted so that the constraints intersect at x^*_p throughout the range of possible values for the fixed parameters. The reduced gradient of the constraint will rotate through the same angle. If θ is large enough then $\nabla_r g_2$ will cross over $\nabla_r P$, moving $\nabla_r P$ outside of the cone of the constraints, as shown be the dashed line in Figure 3.2. In such a case x^*_p would no longer be an optimum of the model-based problem, as one of the Lagrange multipliers would become negative.

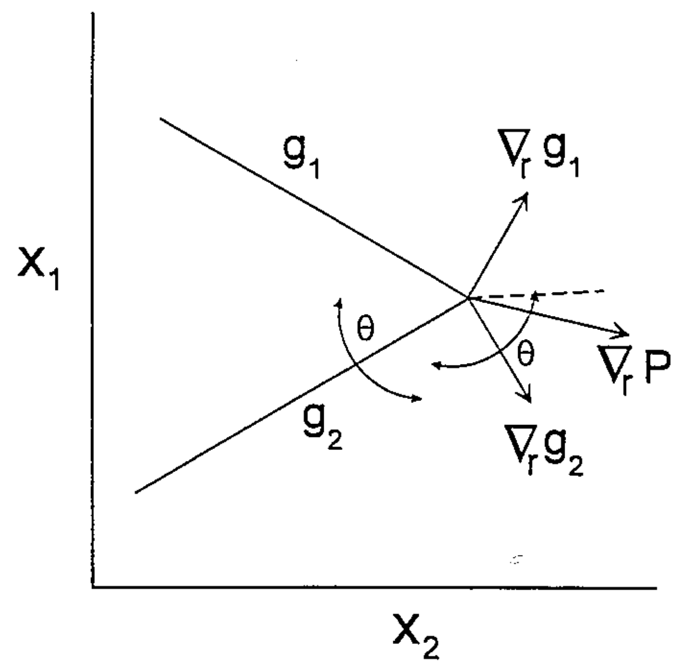

Figure 3.2: Model Accuracy in 2 Dimensions

In the preceding discussions, uncertainty in the fixed parameters associated with a single constraint has been considered. Typically there is uncertainty in many of the fixed parameters on which the reduced gradients of the constraints and profit function depend. Thus, associated with each constraint gradient (and possibly the gradient of the profit function) are angles of rotation which depend upon the uncertainty in the fixed parameters. Clearly, there are many ways in which the reduced gradient of the profit function may be rotated outside of the cone of reduced gradients of the active constraints, due to uncertainty in the fixed parameters.

Ideally, the model-based optimization problem should be posed in such a fashion and the fixed model parameters known to the degree of accuracy, that x^*_p will remain the optimum of the model-based problem for all values of the fixed parameters within the defined region of likely variation (or mismatch from the plant). Based on these ideas Point-Wise Model Accuracy can be defined as:

Definition 3.1: Point-Wise Model Accuracy

If the model-based optimization recognizes the true process optimum (x^*_p) as an optimum for every value of the fixed parameters (α) within the expected region of variation for the estimates of α, then the model is Point-Wise Accurate.

Stating that all μ_i must remain positive within the allowable region of variation for the fixed parameter estimates is equivalent to $\nabla_r P$ remaining within the cone of the constraints, for all values of α within this region. Then, the Point-Wise Accuracy of a process model-based optimization, with respect to an expected range of errors in the fixed model parameters, can be determined by solving the optimization problem:

$$\underset{\alpha}{\text{minimize}} \quad \delta$$

subject to:

$$\nabla_r P - \boldsymbol{\mu}^T \nabla_r g_A = \mathbf{0} \qquad 3.6$$

$$\delta = \min(\mu_i)$$

$$\alpha_l \le \alpha \le \alpha_u$$

Also, if the adjustable parameters have a fixed range then both upper and lower bounds on β, as well as the feasibility conditions of Equations 3.5 should be included in the accuracy test. Since both the process model and constraint equations can be nonlinear, it is possible that the permissible range of values for α contain singularities of these equations. In such cases, care should be taken to ensure that such values of the fixed parameters, which lead to such singularities, are physically meaningful and the specific values excluded from the problem where appropriate.

Problem 3.6 may not be solvable using conventional nonlinear programming (NLP) codes, since δ could be nonsmooth. In such cases mixed integer nonlinear programming (MINLP) can be used to solve the accuracy problem [Balakrishnan and Boyd (1992), Duran and Grossman (1986), Arkun and Stephanopoulos (1981)]. Alternatively Problem 3.6 could be reformulated to minimize each individual Lagrange multiplier in turn and the select the smallest of these minimum values. This could be written:

$$\delta = \min_i \left\{ \begin{array}{l} \min_{\alpha} \ \mu_i \\ \text{subject to:} \\ \qquad \nabla_r P - \mu^T \nabla_r g_A = \mathbf{0} \\ \qquad \boldsymbol{\alpha}_l \le \boldsymbol{\alpha} \le \boldsymbol{\alpha}_u \end{array} \right\} \qquad 3.6a$$

Solving the model accuracy problem in the form of Problem 3.6a requires the solution of as many individual optimization problems as there are manipulated variables or independent active constraints at the plant optimum. Typically the set manipulated variables are a small subset of the plant variables, so Problem 3.6a should be tractable in the design phase.

Should the solution to Problem 3.6 yield a negative value for δ, $\nabla_r P$ lies outside of the constraint cone for some possible values of the fixed parameters, and the bias updating method will result in incorrect operating conditions for these fixed parameter values. If the model is Point-Wise Accurate, the minimum value of δ will be positive. When the constraints of the optimization problem are linear and the problem is Point-Wise Accurate, it can be shown that the bias updating method (only β_i adjustable in Problem 3.2) leads to the true process optimum for all expected values of the fixed parameters. Proof of this is presented in Appendix C.

If a model-based optimization system fails the Point-Wise Accuracy test, the accuracy of the fixed parameter estimates must be improved. Alternatively, the offending fixed parameters can be added to the set of adjustable parameters and a model updating strategy more complex than bias updating used. Selection of alternative model updating schemes is not addressed in this work.

Example 3.1

Using the same model-based optimization problem as in Example 2.2:

$$\underset{x}{\text{maximize}} \qquad [1 \;\; 0.51]\,\mathbf{x}$$

subject to:

$$\begin{bmatrix} 2 & 4 \\ 4 & \alpha \end{bmatrix} \mathbf{x} \le \boldsymbol{\beta}$$

which was shown to be Point-Wise Adequate at the "nominal" value of $\alpha = 2$. If α is known with accuracy 2.0 ± 0.1, is this system model accurate?

Solving the minimization problem posed in Problem 3.6, with the given range of variation in the fixed parameters, yields the minimum value of δ = -0.0051, corresponding to α = 2.1. In order that the process model be considered Point-Wise Accurate, δ must remain positive. Thus, for this expected range of α the model is not Point-Wise Accurate and there is a possibility that the model-based optimization system will not yield the plant optimum.

This model can be made Point-Wise Accurate by increasing the accuracy of the estimate of α to 2.0$\pm$0.04. Yielding the minimum value of δ as 0.0, which indicates multiple optima. Thus, the uncertainty in α must be less than $\pm$0.04 for the process model to be Point-Wise Accurate, when the uncertainty is symmetric about the nominal value for α.

3.3 Model Accuracy & Sensitivity Analysis

As discussed in the previous section, fixed model parameters are often estimated and therefore contain some uncertainty. The Point-Wise Model Accuracy method of Problem 3.6 deals only with whether or not the model is capable of yielding the same optimal manipulated variable values throughout the possible range of fixed parameter values. Should a particular model, containing many fixed parameters, fail the accuracy test, little information is provided as to which parameters caused the failure. The Point-Wise Model Accuracy test can be re-run on a trial-and-error basis to determine the permissible errors in the fixed parameters for which the model is accurate. However, when a process model and constraint set fails the Point-Wise Accuracy test, it would be valuable to be able to directly determine the maximum permissible uncertainty bounds for the fixed parameters. Such information could be used to refine the fixed parameter estimates.

Post-optimality analysis methods such as Parametric Programming [Gal (1979)] or Parametric Sensitivity Analysis [Fiacco (1981)] provide insight into the effects of variation in the model parameters on the optimum of a given problem. For the model accuracy problem, such methods can be extended to yield bounds on the permissible variation of the fixed parameters. The development of Gal [1979] can be extended to all systems which are linear in the fixed parameters. Although the following developments cannot treat the general nonlinear problem, they are applicable to models containing linear combinations of functions which may be nonlinear in the process variables. This analysis could be applied to optimization systems which contain linear, quadratic or nonlinear programming problems, that have constraints which are linear in the fixed parameters (α). (Examples of such constraints are polynomials in x). Consider the optimizing control problem:

$$\begin{aligned} &\underset{x}{\text{maximize}} \quad P(x) \\ &\text{subject to:} \\ &\qquad g(x,\alpha) - \beta \le 0 \end{aligned} \tag{3.7}$$

where the constraints are linear in the fixed parameters (α). At the optimum:

$$\nabla_r P\big|_{x_p^*} - (\mu^*)^T A_o = 0 \tag{3.8}$$

where:

$$A_o = \nabla_r g_A\big|_{x_p^*} \tag{3.9}$$

In this chapter discussions have been limited to problems where there are as many independent active constraints as manipulated variables; therefore A_o is invertible and:

$$\mu^* = \left[\nabla_r P\big|_{x_p^*} (A_o)^{-1}\right]^T \tag{3.10}$$

Note that μ^* are the Lagrange multipliers of the model-based optimization problem at the plant optimum, and not the multipliers for the plant. In general, each element of A_o is not a parameter that is subject to error, since the model can contain known physical relationships such as stoichiometry and so forth. Hence, perturbations in the selected fixed parameters can be considered as a low rank correction to A_o [Golub and Van Loan (1989)] and the dependence of the Lagrange multipliers on these perturbations can be written as:

$$\mu = \left[\nabla_r P\big|_{x_p^*} (A_o + V E^T)^{-1}\right]^T \qquad 3.11$$

where E contains the errors in the fixed parameters and V is a matrix (containing 1's and 0's) which places these errors in the correct positions in A_o. This expression can be expanded using the Sherman-Morrison-Woodbury formula [Ortega, 1987] to yield:

$$\mu = \left[I - V(I + E^T A_o^{-1} V)^{-1} E^T A_o^{-1}\right]^T \left[\nabla_r P\big|_{x_p^*} (A_o)^{-1}\right]^T \qquad 3.12$$

Simplifying using Equation 3.10 gives :

$$\mu = \left[I - V(I + E^T A_o^{-1} V)^{-1} E^T A_o^{-1}\right]^T \mu^* \qquad 3.13$$

Equation 3.13 will allow the changes in the Lagrange multipliers to be directly calculated as a function of specific perturbations in the fixed parameters, which in turn provides a basis for investigation of model accuracy. It would be particularly valuable if Equation 3.13 could be used in conjunction with the non-negativity requirements on the Lagrange multipliers to yield a simple model accuracy criterion. However, Equation 3.13 is non-linear in the perturbations to the fixed parameters and little further refinement is possible except when the fixed parameter errors occur in a single constraint. In this situation Equation 3.13 can be expressed as:

$$\mu = \left[I - \frac{ve^T A_o^{-1}}{(1 + e^T A_o^{-1} v)^{-1}} \right]^T \mu^* \qquad 3.14$$

where e is the vector containing the perturbations in the fixed parameters of a single constraint and v is the vector of (1's and 0's) which places these perturbations in the correct row of A_o.

These developments are framed as perturbations to a row of the parameter matrix A_o, since in general the rows of A_o represent individual constraints. In situations where perturbations to columns of A_o are of interest, such as when a parameter appears in several constraints, the following developments can be reformulated by substituting ev^T for ve^T and performing the appropriate algebra.

In order that x^*_p remain the optimum value for the manipulated variables, optimality theory requires that $\mu \geq \mathbf{0}$ for all permissible values of e. This optimality condition can be re-written:

$$\left[(1 + e^T A_o^{-1} v)\, I - ve^T A_o^{-1} \right]^T \mu^* \geq \mathbf{0} \qquad 3.15$$

when $(1 + e^T A_o^{-1} v) > 0$, which will generally be the case when the errors in the fixed parameters are much smaller in magnitude than the parameters themselves. (If $(1 + e^T A_o^{-1} v) < 0$ then the inequality sign would be reversed.) For this work we will assume $(1 + e^T A_o^{-1} v) > 0$, and Inequality 3.15 can be simplified to:

$$\left[v^T \mu^* I - \mu^* v^T \right] (A_o^T)^{-1} e \leq \mu^* \qquad 3.16$$

Since A_o, v and μ^* are known and constant, the set of simultaneous linear Inequalities 3.16 can be used to directly calculate the maximum (or minimum) permissible perturbation (e) to the fixed parameters (α) for which the process model and constraint equations will remain Point-Wise Adequate. This method allows the Point-Wise Accuracy of a problem to be analyzed on a constraint-by-constraint basis.

Example 3.2

Consider the model-based optimization system of Example 2.2 which was shown in Example 3.1 to be Point-Wise Accurate for $\alpha = 2.00 \pm 0.04$ by trial and error. To directly determine the allowable range of values for α define:

$$v = [0\ 1]^T,$$

since the fixed parameter under consideration is in the second row of the constraint matrix, and $e = [0 \quad e_2]^T$. Recalling that $\mu^* = [0.0033 \quad 0.2483]^T$, Inequality 3.16 becomes:

$$\left\{ \begin{bmatrix} 0.2483 & 0 \\ 0 & 0.2483 \end{bmatrix} - \begin{bmatrix} 0 & 0.0033 \\ 0 & 0.2483 \end{bmatrix} \right\} \begin{bmatrix} 2 & 4 \\ 4 & 2 \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ e_2 \end{bmatrix} \leq \begin{bmatrix} 0.0033 \\ 0.2483 \end{bmatrix}$$

which simplifies to:

$$0.0833\, e_2 \ \leq 0.0033$$

or the permissible bounds on the fixed parameter are $-\infty \leq \alpha \leq 2.04$, which agrees with the results from the numerical solution of the mathematical programming accuracy test.

3.4 Gasoline Blending Case Study

This case study is taken from Crowe et al. [1989], in which two types of automotive gasoline are blended from feedstocks with the objective of maximizing profit. Real-Time Optimization for gasoline blending is of particular interest due to the widespread use linear programming in solving such blending problems [Leung(1985), MacDonald et al. (1991)] and the common use of the bias update technique (e.g. Stadnicki and Lawler [1985]) in the real-time control and optimization of these systems. The process model was written in the bias update form of Problem 3.1. In the case study, the model consisted of inequality constraints on maximum and minimum production rates, feedstock availability, octane and Reid Vapour Pressure (RVP). Product octane and RVP were calculated as weighted averages of the feedstock properties, with RVP's represented by their blending indices to yield linear blending correlations [Gary and Handwerk, (1984)]. Using the product and feedstock data given in Tables 3.1, 3.2 and 3.3., the formulation of the steady-state, economic optimizing control problem is:

$$\underset{F_{i,j}}{\text{maximize}} \quad \sum_j \sum_i (p_j - c_i) F_{i,j}$$

subject to:

$$\sum_i Q_i F_{i,j} \leq S_{j,max} \sum_i F_{i,j} + \beta_1 \qquad \textit{maximum quality limits}$$

$$\sum_i Q_i F_{i,j} \geq S_{j,min} \sum_i F_{i,j} + \beta_2 \qquad \textit{minimum quality limits}$$

$$\sum_i F_{i,j} \leq D_{j,max} + \beta_3 \qquad \textit{maximum demand limits}$$

$$\sum_i F_{i,j} \geq D_{j,min} + \beta_4 \qquad \textit{minimum demand limits}$$

$$\sum_j F_{i,j} \leq R_{i,max} + \beta_5 \qquad \textit{maximum feed availabilities}$$

$$\sum_j F_{i,j} \geq R_{i,min} + \beta_6 \qquad \textit{minimum feed availablilities}$$

where: c_i are the feedstock costs, D_j are the production limits for product "j" (regular or premium gasoline), $F_{i,j}$ is the flow of feedstock "i" to product "j", p_j are the product values, Q_i are the feedstock qualities (octane or Reid Vapour Pressure), R_i are the availability limits for the feedstocks, S_j are the product quality specifications.

This case study will deal with the effects of mismatch in the fixed parameters on the ability of the optimization system, using bias update, to successfully match the plant optimum operations. The plant optimum will be taken as the solution of nominal optimization problem with the bias terms set to zero, using the data in Tables 3.1, 3.2 and 3.3.

Table 3.1: Gasoline Blending Production Requirements

		Regular	Premium
Value (\$/bbl)	(p_j)	33.00	37.00
Max. bbls/day	($D_{j,max}$)	8000	10000
Min. bbls/day	($D_{j,min}$)	7000	10000
Min. Octane	($S_{j,min}$)	88.5	91.5
Max. RVP (psi)	($S_{j,max}$)	10.8	10.8

Table 3.2: Gasoline Blending Feedstock Availability (R_i) and Cost (c_i)

	Available (bbls/day)	Cost (\$/bbl)
Reformate	12000	34.00
LSR Naphtha	6500	26.00
N-Butane	3000	10.30
FCC Gasoline	4500	31.30
Alkylate	7000	37.00

Table 3.3: Gasoline Blending Feedstock Quality Data (Q_i)

	Octane	RVP (psi)
Reformate	91.8	4.0
LSR Naphtha	64.5	12.0
N-Butane	92.5	138.0
FCC Gasoline	78.0	6.0
Alkylate	96.5	7.0

Table 3.4: Gasoline Blending Plant Optimum (x^*_p)

	Regular (bbls/day)	Premium (bbls/day)
Reformate	2747	9253
LSR Naphtha	0	0
N-Butane	283	504
FCC Gasoline	2268	243
Alkylate	1702	0

The optimum plant operating conditions are given in Table 3.4. At the plant optimum of the problem the active constraints are:

1) minimum production of regular,

2) maximum production of premium,

3) all available reformate used,

4) no LSR naphtha in either blend,

5) no alkylate in premium gasoline,

6) maximum RVP for both products,

7) minimum octane for both products.

Since there are 10 active constraints and 10 manipulated variables, the RTO problem is fully constrained.

The fixed parameters in the process model are the feedstock qualities (octane and RVP). These qualities are infrequently measured by laboratory testing and can change frequently since the feedstocks are intermediate products in a refinery, whose qualities depend on upstream plant operations. Thus, the range of variation in feedstock qualities is due to a combination of measurement error and upstream process variation. As a result the errors in octane and RVP are estimated to be no more than ± 0.5 octane number and ± 0.3 psi, respectively. Solving the optimization problems as posed in Problem 3.6a, using these expected errors for the feedstock qualities, gave a negative value for δ. (Further analysis using the fixed parameter values of this solution revealed negative μ_i's associated with the minimum use of LSR Naphtha). Such negative values indicate the process model is not Point-Wise Accurate for these levels of uncertainty in the feedstock qualities. Thus, there are some possible values of the fixed parameters (or some true process conditions) for which an optimizing controller using bias updating will not converge to the plant optimum.

By reducing the expected error regions for the product qualities to ± 0.1 octane number and ± 0.1 psi for feedstock octane and RVP, respectively, the solution to Problem 3.6a yields a $\delta > 0$ and therefore the process model becomes Point-Wise Accurate. Thus, a model-based optimization system using bias updating can only be successful throughout the range of expected uncertainty in the fixed parameters, if the accuracy of the laboratory tests are significantly improved or the frequency of feedstock quality measurement increased. Should such improvements not be possible another updating strategy should be considered.

To illustrate the dangers of using an inaccurate process model, simulations were run with fixed errors in the octane numbers and RVP of the feedstocks. As was previously stated, the plant was simulated using the equations in the nominal optimization problem with the bias terms set to zero and feedstock data given in Table 3.3. The fixed parameter errors used in the optimizing controller are given in Table 3.5. No noise was added to the process measurements. For the first set of errors (labelled Inadequate Model in Table 3.5), the plant-model mismatch in the fixed parameters was sufficient to yield an inadequate model, at the plant optimum given in Table 3.4. The second set of fixed parameter errors (labelled Adequate Model in Table 3.5) were sufficiently small so as to yield an adequate model at the plant optimum. In both cases a bias update was used, as in Figure 3.1, with no filter.

Table 3.5: Fixed Parameter Errors for Gasoline Blending Closed-Loop Simulations

	Inadequate Model	Adequate Model
LSR Naphtha	octane +0.5 RVP -0.3	octane +0.1 RVP -0.1
FCC Gasoline	octane -0.5 RVP +0.3	octane -0.1 RVP +0.1

The simulation results for the regular gasoline blend are given in Figures 3.3 through 3.6. Figures 3.3 and 3.4 clearly show that both optimization systems controllers adjusted the manipulated variables to quickly and successfully satisfy product quality constraints. In this case, the inadequate model was in violation of both the minimum octane and maximum RVP specifications for the first RTO step.

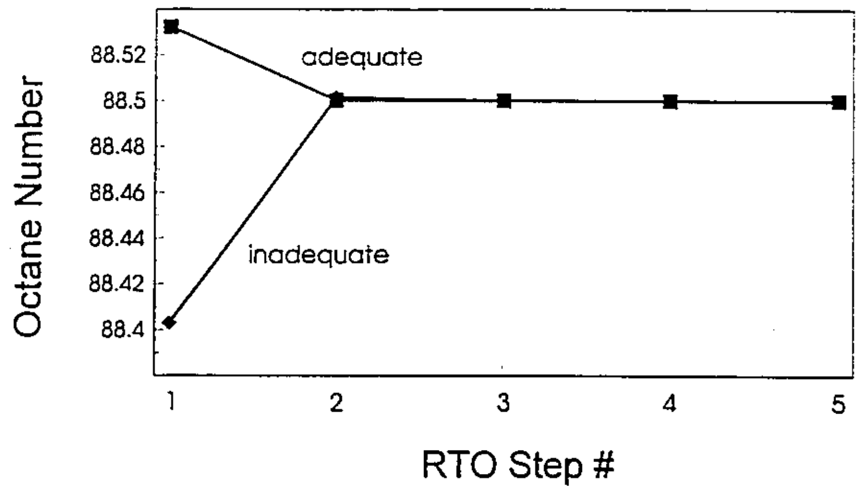

Figure 3.3: Regular Gasoline Octane Trajectory.

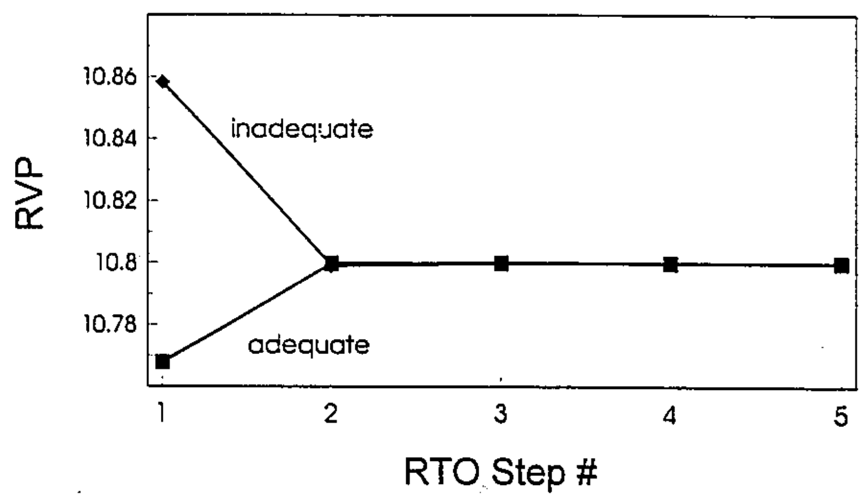

Figure 3.4: Regular Gasoline RVP Trajectory.

Figure 3.5 presents the deviation of the feedstock flows from their optimal values (x^*_p), as given in Table 3.4, for the inadequate model. Note that all flows exhibit offset. The major feature of the solution to the model-based optimization using the inadequate model is that FCC Gasoline is dropped from the solution basis and LSR Naphtha is added to the basis. Finally Figure 3.6 shows that the adequate model-based optimization system quickly converges to the optimal solution.

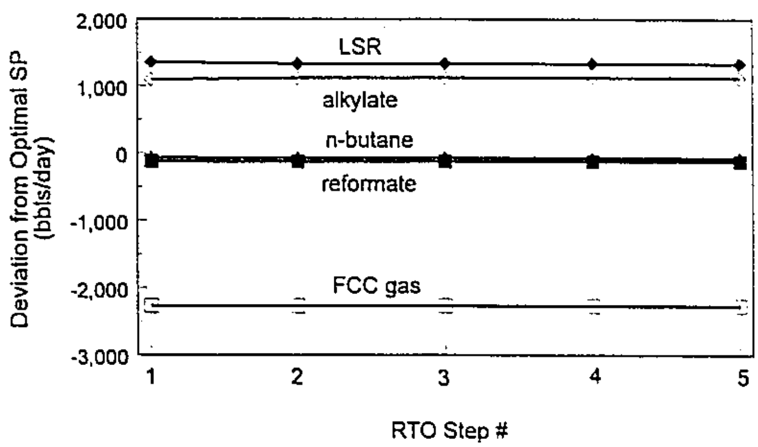

Figure 3.5: Regular Gasoline Feedstock Flows (Inadequate Model)

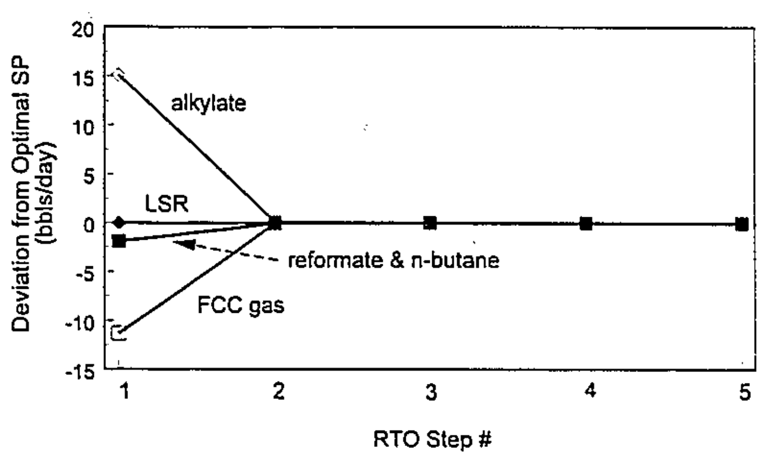

Figure 3.6: Regular Gasoline Feedstock Flows (Adequate Model)

The results for premium gasoline are similar to those presented for the regular blend and are presented in Figures 3.7 through 3.10.

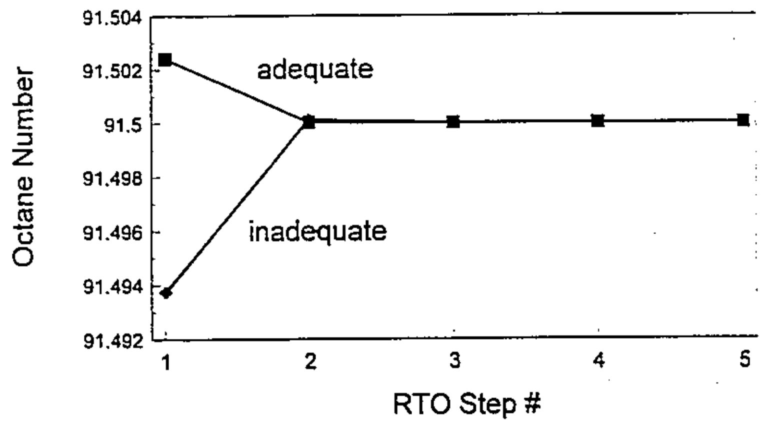

Figure 3.7: Premium Gasoline Octane Trajectory

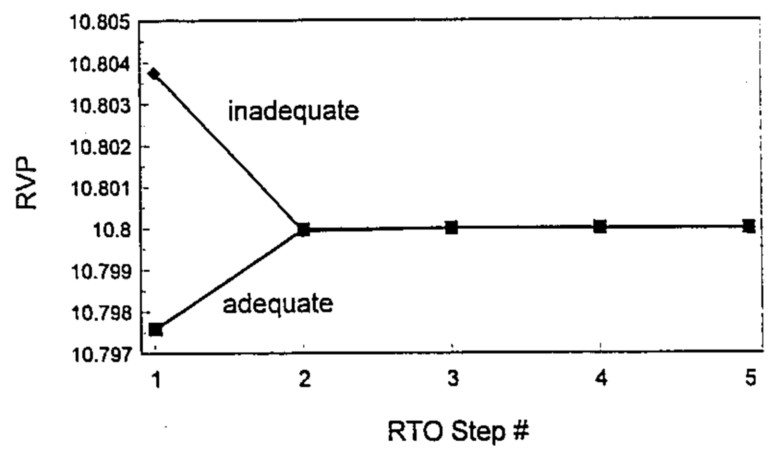

Figure 3.8: Premium Gasoline RVP Trajectory

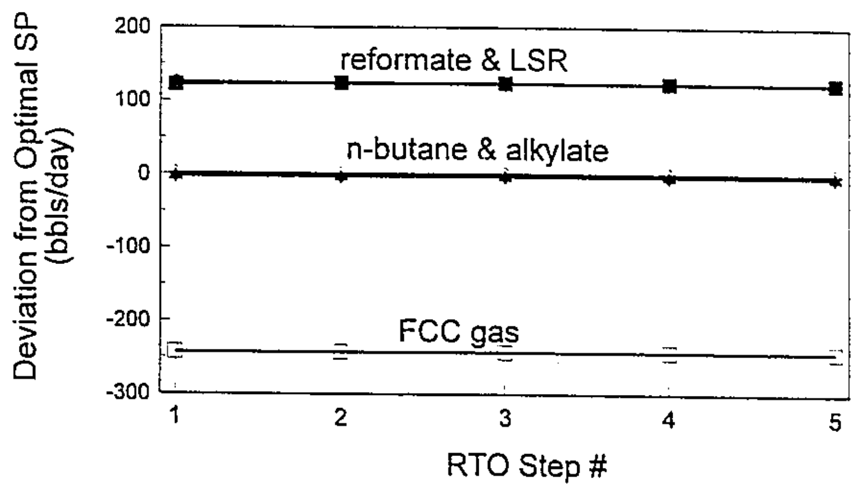

Figure 3.9: Premium Gasoline Feedstock Flows (Inadequate Model)

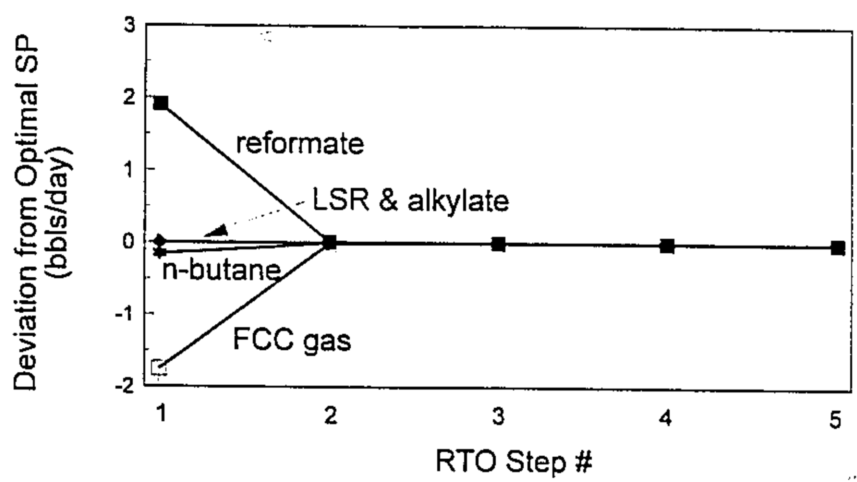

Figure 3.10: Premium Gasoline Feedstock Flows (Adequate Model)

Figure 3.11 presents the true plant profit trajectory for both the adequate and inadequate models. The inadequate model seems to exceed the optimal plant profit during the first control cycle; however, this is due to infeasible operation (see Figures 3.3 and 3.4). The adequate model quickly converges to the optimal plant profit. Care should be taken in interpreting the results in Figure 3.11, as model adequacy is not dictated by the ability of the model-based optimization to match the optimal plant profit. Recall that model adequacy is determined by the ability of the model-based optimization system to match the optimal manipulated variable values for the plant. In Chapter 2, the two reaction approximation to the Williams-Otto [1960] reactor was an example of an adequate model-based optimization which does not match the optimal plant profit level.

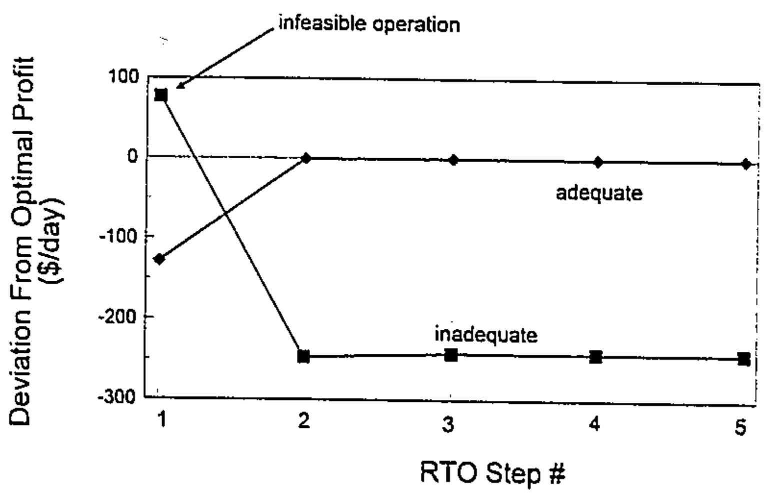

Figure 3.11: Plant Profit from Implementing RTO Results.

In the gasoline blending problem, the same feedstock qualities appear in constraints for both the premium and regular gasoline blends; thus the fixed parameters in the quality constraints are not independent of each other and a constraint-by-constraint analysis is not possible. However, consider the revised situation where the premium blend is completed (i.e., the flows for the premium blend are fixed at the values in Table 3.4). The economic optimization problem is then reduced to determining the blend for regular gasoline. For this revised sub-problem for on-line optimization of only the regular blend. the fixed parameters are now independent of one another and a constraint-by-constraint analysis is possible. In order to determine the required accuracy of the feedstock octane and RVP for which the model of the sub-problem is Point-Wise Accurate, the method of Section 3.3 can be used and Table 3.6 presents the results.

Table 3.6: Quality Perturbations (e) in Regular Blend Fixed Parameters

	Octane	RVP
Reformate	$-6.5438 \leq e \leq \infty$	$-\infty \leq e \leq 10.7417$
LSR Naphtha	$-\infty \leq e \leq 0.5198$	$-0.8533 \leq e \leq \infty$
n-Butane	$-1.785 \leq e \leq 67.5148$	$-61.0 \leq e \leq 19.05$
FCC Gasoline	$-0.3075 \leq e \leq 4.1$	$-8.767 \leq e \leq 0.4961$
Alkylate	$-18.39 \leq e \leq 0.7009$	$-1.116 \leq e \leq \infty$

Thus, for this regular gasoline blending problem, wider variation in the fixed parameters can be tolerated (see Table 3.5) while maintaining model accuracy.

3.5 Discussions

The common model-based optimization system with bias updating can be a successful tool for solving some steady-state, economic Real-Time Optimization problems. However, care must be taken in order to ensure a successful implementation. Particular attention must be paid to expected errors in the fixed model parameters, since these can dictate the ability of the optimizing controller to find the plant optimum.

Techniques have been presented for determining whether a model-based optimization system with bias update can find the plant optimum and for ensuring that the optimization results are robust to expected errors in the estimates of the fixed parameters. Finally, these methods have been used to determine the maximum permissible range of fixed parameter errors within which the optimizer will be guaranteed to successfully recognize the plant optimum.

As with the model adequacy methods of Chapter 2, testing model accuracy requires knowledge of the manipulated variable values and active constraint set at the process optimum. The methods of this chapter further require estimates of the possible error in the fixed parameters. Such information can be developed from plant experimentation, process knowledge, or from detailed process models which would not be suitable for implementation in a RTO system.

It is possible that some elements of bias vector are dependent on other elements. Since the optimality conditions of Equations 3.3 and 3.4 do not depend on the bias, they are unaffected by the situation. The bias term only appears in the feasibility portion of the accuracy test (Equation 3.5). Then, when dealing with a model-based optimization problem where the elements of the bias vector are not independent, the feasibility test of Equation 3.5 must be included in any model accuracy testing.

The discussions of this chapter have been limited to the situation where there are only as many independent active operating and product quality constraints, at the process optimum, as independent manipulated variables, or the economic optimization problem is fully-constrained. It is possible, in some constraint sets, for degeneracy to arise by having additional dependent constraints which are active at the process optimum. In such cases, it is possible to define many different fully-constrained optimization problems by appropriately interchanging various subsets of the entire active constraint set. Then, errors in the fixed parameters of the constraints may cause some of these subsets of the active constraint set to fail the accuracy test of Problem 3.6, while the active set as a whole is Point-Wise Adequate throughout the entire region of expected fixed parameter errors. A study of each possible subset of active constraints could be employed to map out the entire region of model accuracy for the active set as a whole; however, this approach would be time consuming when there are many extra constraints active at the plant optimum. Further work is required to develop direct methods for dealing with this situation.

The ideas presented in this chapter have been framed as design considerations and are important to the eventual success of an optimization system. In addition, the model accuracy methods could also be used for periodic real-time monitoring of the "robustness" of the Real-Time Optimization system to occasional changes in the process economics and in the fixed parameters (α) of the active constraint set. Problem 3.6 could be solved periodically, in real-time, as changes occur in the active set of constraints, fixed parameters or process economics to indicate the "robustness" of the current optimization system. However, further study of solution methods for Problem 3.6 is required to ensure reliability on industrial-scale problems.

4. Necessary Conditions for Zero-Offset

Elimination of offset from target values in the steady-state has been, and is, a subject of great interest to both process control researchers and practitioners, alike. Many control schemes have components included explicitly to provide offset elimination (e.g. integral action in a PID controller). Typically, such control systems have available to them a direct measure of the control variable, allowing such reset action to act directly on a measured error. In a model-based Real-Time Optimization system, plant profit (or operating cost) is the controlled variable and is usually an inferential quantity, since it is only rarely (if ever) directly measurable. As discussed in Chapter 2, any model-based Real-Time Optimization system adapts model parameters with the goal of eliminating offset from the optimum manipulated variable values ($\mathbf{x}^*_p$) of the plant and not matching the optimal profit level. As a result, traditional process control offset elimination schemes will not work. This chapter establishes rigorous criteria for the entire integrated RTO system, which can be used to evaluate whether it is possible for the RTO system to attain zero-offset from the plant optimum manipulated variable values.

Chapter 2 presented Point-Wise Model Adequacy, which was defined as the ability of the model-based optimization to have optimal values for the manipulated variables coincident with those of the plant. Figure 4.1 gives a schematic representation of Point-Wise Model Adequacy.

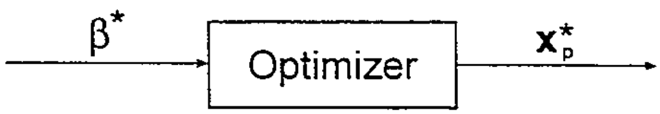

Figure 4.1: Point-Wise Model Adequacy

The model adequacy tests developed in Chapter 2 concentrated on determining whether a set values for the adjustable parameters existed (perhaps within some permissible range) which would allow the model-based optimization to predict the optimal manipulated variable values. The adequacy test had the general form:

$$\underset{\boldsymbol{\beta}}{\text{minimize}} \quad (\mathbf{u}_m^* - \mathbf{T}\mathbf{u}_p^*)^T \, \mathbf{W} \, (\mathbf{u}_m^* - \mathbf{T}\mathbf{u}_p^*)$$

subject to:

$$\begin{aligned} \mathbf{f}\,(\mathbf{x}_p^*, \mathbf{u}_m^*, \boldsymbol{\alpha}, \boldsymbol{\beta}) &= 0 \\ \mathbf{g}_L\,(\mathbf{x}_p^*, \mathbf{u}_m^*, \boldsymbol{\alpha}, \boldsymbol{\beta}) &= 0 \\ \mathbf{g}_I\,(\mathbf{x}_p^*, \mathbf{u}_m^*, \boldsymbol{\alpha}, \boldsymbol{\beta}) &> 0 \end{aligned} \qquad 4.1$$

$$\begin{aligned} \nabla_r P \big|_{\mathbf{x}_p^*} &= 0 \\ \nabla_r^2 P \big|_{\mathbf{x}_p^*} & \;\; \text{positive definite} \end{aligned} \qquad 4.2$$

where Equations 4.1 represent feasibility conditions and Conditions 4.2 are the required optimality conditions of the adequacy test. The discussions of this chapter are limited to the partially-constrained case of model adequacy, as in Section 2.1; however, the relationships in Conditions 4.2 can be replaced by those given in Equation 2.11 and Inequality 2.12 for fully-constrained optimization problems. Thus, although discussions are limited to the partially-constrained situation, the developments of this chapter are more generally applicable.

In the Point-Wise Adequacy tests of Chapter 2, model updating was not considered beyond the selection of which parameters would be adjusted. In this chapter, model updating is shown to be crucial to elimination of offset for an RTO system and methods to test the combination of model updating / model-based optimization are presented. These tests build on the model adequacy ideas of Chapter 2. In the first section of this chapter, the Point-Wise Model Adequacy tests are expanded to include the model updating system. The second section of this chapter discusses Point-Wise Stability and introduces the necessity of considering the interaction between the optimization system and the plant, in any design for offset elimination.

The combination of Point-Wise Model Adequacy, Augmented Model Adequacy and Point-Wise Stability provide three necessary conditions for zero-offset in a given RTO problem. A general sequential testing procedure of:

1) Point-Wise Model Adequacy,
2) Augmented Model Adequacy,
3) Point-Wise Stability,

is proposed, which concentrates increasing computational effort only on those designs which have passed the preceding, simpler tests.The chapter concludes with several examples and a discussion of the limitations of the proposed methods.

4.1 Augmented Model Adequacy Test

The Point-Wise Model Adequacy tests of Chapter 2 can be used to determine whether there are any possible values for the adjustable parameters which will allow the model-based optimization problem to have an optimum at the optimum manipulated variable values of the plant. These methods do not determine whether the model update system can produce such values for the adjustable parameters from available process measurements.

Figure 4.2 illustrates the necessary condition for a combined model update / model-based optimization system to predict the optimum steady-state manipulated variable values (x^*_p) from the process measurements (z^*) available at the process optimum.

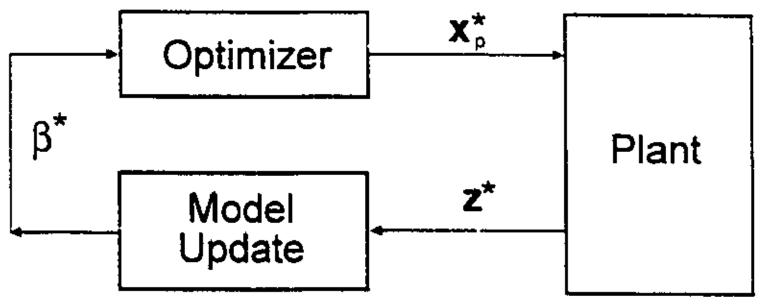

Figure 4.2: Augmented Model Adequacy

In order for the combined update / optimization system to be capable of predicting the optimal plant manipulated variables from the process measurements, the adjustable parameter values β^* must simultaneously meet the Point-Wise Model Adequacy Criteria, for the given process model, while being the result of the model updating algorithm. If such values for the adjustable parameters exist then the plant optimum (x^*_p) is an equilibrium solution (stationary point) for the model-based RTO problem.

Consider the situation where the model update problem is a parameter estimation problem of the form:

$$\begin{aligned} &\underset{\beta}{\text{minimize}} \quad \phi \\ &\text{subject to:} \\ &\qquad \mathbf{h}(\mathbf{z},\boldsymbol{\alpha},\boldsymbol{\beta}) = \mathbf{0} \end{aligned} \qquad 4.3$$

where ϕ is the objective of the parameter estimation problem and the vector **h** contains the process model equations, as appropriate for parameter estimation. Then, an Augmented Model Adequacy Criteria can be developed from a Point-Wise Model Adequacy criteria by including the optimality conditions of the parameter estimation Problem 4.3.

Criteria 4.1: **Augmented Model Adequacy (Partially-Constrained Case)**

If $\mathbf{x}^*_p$ *is an unique (local) plant minimum and* $\exists$ *at least one set of values for the adjustable parameters* ($\boldsymbol{\beta}$) *such that:*

$$\begin{aligned} \nabla_r P \big|_{\mathbf{x}^*_p} &= \mathbf{0} \\ \nabla^2_r P \big|_{\mathbf{x}^*_p} &\ \text{positive definite} \end{aligned} \qquad 4.2$$

and:

$$\begin{aligned} \nabla_r \phi \big|_{\mathbf{z}^*} &= \mathbf{0} \\ \nabla^2_r \phi \big|_{\mathbf{z}^*} &\ \text{positive definite} \end{aligned} \qquad 4.4$$

then the combined parameter estimation / model-based optimization is adequate for use in a Real-Time Optimization system.

Similarly, the Point-Wise Model Adequacy test for partially-constrained can be extended with the Conditions 4.4 to yield an Augmented Model Adequacy test:

$$\underset{\beta}{\text{minimize}} \quad (\mathbf{u}_m^* - \mathbf{T}\mathbf{u}_p^*)^T \, \mathbf{W} \, (\mathbf{u}_m^* - \mathbf{T}\mathbf{u}_p^*)$$

subject to:

$$\begin{aligned} \mathbf{f}(\mathbf{x}_p^*, \mathbf{u}_m^*, \boldsymbol{\alpha}, \boldsymbol{\beta}) &= 0 \\ \mathbf{g}_L(\mathbf{x}_p^*, \mathbf{u}_m^*, \boldsymbol{\alpha}, \boldsymbol{\beta}) &= 0 \\ \mathbf{g}_I(\mathbf{x}_p^*, \mathbf{u}_m^*, \boldsymbol{\alpha}, \boldsymbol{\beta}) &> 0 \end{aligned} \qquad 4.1$$

$$\begin{aligned} \nabla_z P \Big|_{\mathbf{x}_p^*} &= 0 \\ \nabla_z^2 P \Big|_{\mathbf{x}_p^*} & \text{ positive definite} \end{aligned} \qquad 4.2$$

$$\begin{aligned} \nabla_z \phi \Big|_{\mathbf{z}^*} &= 0 \\ \nabla_z^2 \phi \Big|_{\mathbf{z}^*} & \text{ positive definite} \end{aligned} \qquad 4.4$$

Equations 4.1 are the feasibility conditions that any candidate value of the adjustable parameters must satisfy. Conditions 4.2 and 4.4 are the requirements that β^* must meet the Point Wise Model Adequacy criteria and must be the result of the model updating algorithm, respectively. The reduced properties of the parameter estimation objective function are calculated in exactly the same fashion as those of the performance function of the model-based optimization. Details of these calculations are presented in Appendix A.

As in the case of Point-Wise Model Adequacy testing, when there are bounds on the permissible values for the adjustable parameters (or $\mathbf{u}^*_m$), the Augmented Model Adequacy problem can be suitably modified by including them. For other forms of model updating which are not optimization-based, such as the bias update method of Chapter 3, the appropriate conditions can be substituted for

Conditions 4.4 in the Augmented Model Adequacy test. The examples in Section 4.3 illustrate the use of closed-form model updating techniques.

In Chapter 2 the difficulties associated with calculating the reduced properties of the performance function were alleviated by the introduction of the grid method. A similar approach can be taken for the Augmented Model Adequacy test to yield:

$$\underset{\beta}{\text{minimize}} \quad (\mathbf{u}_m^* - \mathbf{T}\mathbf{u}_p^*)^T \, \mathbf{W} \, (\mathbf{u}_m^* - \mathbf{T}\mathbf{u}_p^*)$$

subject to:

$$\begin{aligned} \mathbf{f}(\mathbf{x}_p^*, \mathbf{u}_m^*, \boldsymbol{\alpha}, \boldsymbol{\beta}) &= 0 \\ \mathbf{g}_L(\mathbf{x}_p^*, \mathbf{u}_m^*, \boldsymbol{\alpha}, \boldsymbol{\beta}) &= 0 \\ \mathbf{g}_I(\mathbf{x}_p^*, \mathbf{u}_m^*, \boldsymbol{\alpha}, \boldsymbol{\beta}) &> 0 \end{aligned} \qquad 4.1$$

$$P(\mathbf{x}_p^*, \mathbf{u}_m^*, \boldsymbol{\alpha}, \boldsymbol{\beta}) < P(\mathbf{x}_p^*, \mathbf{u}_m^*(\mathbf{x}_p^* + \boldsymbol{\delta}\mathbf{x}_i), \boldsymbol{\alpha}, \boldsymbol{\beta}) \qquad 4.5$$

$$\phi(\mathbf{z}^*, \boldsymbol{\beta}) < \phi(\mathbf{z}^*, \boldsymbol{\beta} + \boldsymbol{\delta}\boldsymbol{\beta}_j) \qquad 4.6$$

Then, for Augmented Model Adequacy testing two grids must be selected, one in the manipulated variables $\boldsymbol{\delta}\mathbf{x}_i$ and one in the parameters $\boldsymbol{\delta}\boldsymbol{\beta}_j$. The concerns regarding grid spacing and geometry addressed in Chapter 2 also hold for the adjustable parameter grid. Also, as in the case of Point-Wise Model Adequacy testing using the grid method, care must be taken in interpreting the results of a grid-based Augmented Model Adequacy test, since the solution may not meet the analytical conditions.

The Augmented Model Adequacy test determines whether the plant optimum ($\mathbf{x}^*_p$), with the associated process measurements ($\mathbf{z}^*$), is an equilibrium solution to the

RTO problem. Specifically, this test determines whether a set of values for the adjustable parameters exist which simultaneously are the result of the model updating algorithm and allow the model-based optimization to be Point-Wise Adequate. Augmented Model Adequacy testing does not consider the stability of the closed-loop plant / model-based RTO system. This closed-loop stability is considered in the next section.

4.2 Point-Wise Stability

The Augmented Model Adequacy test determines whether $\mathbf{x}^*_p$ is an equilibrium solution to the RTO problem. Then, when RTO systems which satisfy the Augmented Model Adequacy criteria are started precisely at the plant optimum, they will remain there. Equally important to offset elimination is the manner in which the RTO systems reacts to perturbations in the manipulated variables ($\mathbf{x}$) away from the plant optimum. The adequacy tests provide no information regarding the stability of the RTO system with respect to small movements away from the optimum.

Wiggins [1990] defines stability at a fixed point of an iterated map as:

Criteria 4.2: **Point-Wise Stability**

A system of recursive algebraic equations $\{ \mathbf{x}^*_m(k) \mapsto \mathcal{F}[\mathbf{x}^*_m(k-1),k] \}$ *is said to be asymptotically stable at a fixed point* $\mathbf{x}^*$, *if it is Lyapunov stable and* $\exists$ *a constant* $b > 0$, *such that if*:

$$\|\mathbf{x}^*-\mathbf{x}^*_m(k)\| < b$$

then :

$$\lim_{k \to \infty} \| \mathbf{x}^* - \mathbf{x}_m^*(k) \| = 0$$

where k *is the iteration index.*

It follows that stability of the RTO system at the plant optimum is a characteristic of not only the system components, but also the interaction between the RTO system and the plant. Figure 4.3 illustrates the feedback nature of the plant / RTO system interaction.

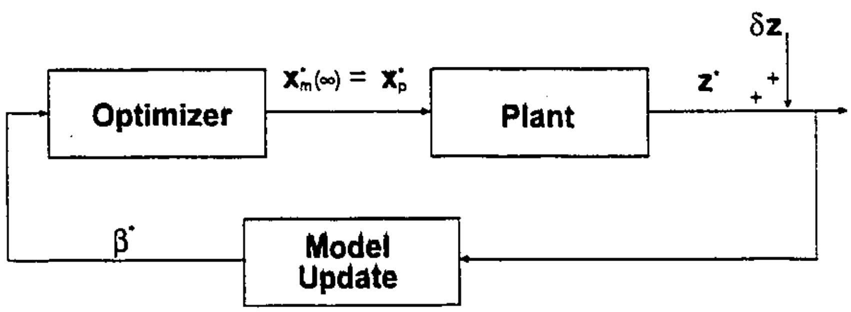

Figure 4.3: Point-Wise Stability at the Plant Optimum

Each element of Figure 4.3 can be considered a nonlinear, and not necessarily differentiable, map. The optimizer is represented by:

$$\mathbf{x}_m^* = \Xi(\boldsymbol{\beta}) \qquad 4.7$$

which predicts the optimum value of the manipulated variables given a value for the adjustable parameters. The nonlinear map for the parameter estimation problem is:

$$\beta = \Phi(z) \qquad 4.8$$

which estimates model parameters from process measurements. Finally, the plant can be considered as the map:

$$z = \Omega(x) \qquad 4.9$$

which takes manipulated variable values into the set of process measurements.

For arbitrarily small deviations from the plant optimum, the nonlinear maps of Equations 4.7, 4.8, and 4.9 can be represented by their first-order approximations:

$$\begin{aligned} \delta x_m^* &= \left.\frac{dx_m^*}{d\beta}\right|_{\beta^*} \delta\beta \\ \delta\beta &= \left.\frac{d\beta}{dz}\right|_{z^*} \delta z \\ \delta z &= \left.\frac{dz}{dx}\right|_{x_p^*} \delta x \end{aligned} \qquad 4.10$$

when the appropriate derivatives exist. (The existence of these terms is discussed later in this section). This system of linear equations can be reduced to an iterative relationship in perturbations to the predicted optimum manipulated variables (δx_m^*):

$$\delta x_m^*(k) = \left(\frac{dx_m^*}{d\beta}\frac{d\beta}{dz}\frac{dz}{dx}\right)_{x_p^*,\beta^*,z^*} \delta x_m^*(k-1) \qquad 4.11$$

The system of Figure 4.3 is stable at the plant optimum (x_p^*) for small perturbation if:

$$\left\| \left.\frac{dx_m^*}{d\beta}\right|_{\beta^*} \left.\frac{d\beta}{dz}\right|_{z^*} \left.\frac{dz}{dx}\right|_{x_p^*} \right\|_2 < 1 \qquad 4.12$$

[Wiggins (1990)].

The first term of Condition 4.12 is the parametric sensitivity of the model-based optimization problem. The second term is the sensitivity of the adjustable parameter estimates to changes in the measurements. The third term is the rate of change of the process measurements (output variables) with respect to the manipulated variables.

Ganesh and Biegler [1987] require that the solution to the model-based RTO problem strictly satisfies the necessary Karush-Kuhn-Tucker conditions, as well as the second-order sufficient condition, to ensure the existence of parametric sensitivity term at the plant optimum. They also provide a method of calculation for the parametric sensitivity using the Lagrangian of the optimization problem, which significantly decreases the required computations. Fiacco [1983] gives a more general treatment of sensitivity analysis, which allows for the relaxation of some of the conditions, and more recent results can be found in Shapiro [1987] and Rockafellar [(1988) and (1989)].

The existence of the sensitivity of the adjustable parameter estimates with respect to changes in the process measurements, in the parameter estimation problem, is an equivalent problem to the parametric sensitivity of the model-based optimization problem, when the parameter estimation has the form of Problem 4.3. The sensitivity of other possible forms of the model updating problem have to be considered on an individual basis. For the differential sensitivity of the process measurements with respect to the manipulated variables to exist, both the manipulated variables and the process measurements must be continuous. The existence of these sensitivities and derivatives is assumed for the developments of this chapter.

The Point-Wise Stability test determines whether, for arbitrarily small (differential) deviations from the plant optimum, the model-based RTO system will return to x^*_p. It should be stressed that this stability test does not guarantee convergence of the RTO system to the plant optimum and is only locally valid. Section 4.3 provides examples of the application of the Point-Wise Stability test.

4.3 Offset Elimination Examples

This section contains three examples of the sequential offset elimination testing method. The first example revisits the fully-constrained RTO system, using bias update, of Chapter 3. The second example examines the two reaction approximation to the Williams-Otto reactor kinetics used in the examples of Chapter 2. The final example investigates model-based RTO for a simple heat exchanger network.

4.3.1 Linear Constraints & Bias Update

As in Chapter 3 and Appendix C, consider the fully-constrained optimization problem:

$$\begin{aligned} &\underset{\mathbf{x}}{\text{minimize}} \quad P(\mathbf{x}) \\ &\text{subject to:} \\ &\qquad\qquad \mathbf{A}_m \mathbf{x} \geq \mathbf{b} + \boldsymbol{\beta}_k \end{aligned}$$

with the bias model update:

$$\boldsymbol{\beta}_k = \mathbf{F}(z)\ (\mathbf{A}_m - \mathbf{A}_p)\ \mathbf{x}_{k-1}$$

where: $\mathbf{F}(z)$ is a filter matrix of polynomials in the shift operator z, k is the RTO interval number, $\mathbf{x}_{k-1}$ are the measured values of the manipulated variables at time "k-1". This example is interesting since the model updating problem does not have the form of an optimization as in Problem 4.3 and the RTO problem is an example of a fully-constrained optimization where the parameter sensitivity matrix exists. Then the Augmented Model Adequacy criteria requires:

$$\boldsymbol{\mu} = (\nabla_z P\big|_{\mathbf{x}_p^*} \mathbf{A}_m)^T > 0$$

$$\boldsymbol{\beta}^* = \mathbf{F}(z)\ (\mathbf{A}_m - \mathbf{A}_p)\ \mathbf{x}_p^*$$

Notice that $\boldsymbol{\beta}$ does not appear in the Point-Wise Model Adequacy test for this system. Then, if the model-based optimization is Point-Wise Adequate and there are no constraints on the values the adjustable parameters may take, the combined optimization / bias update satisfies the Augmented Adequacy Criteria.

For an adequate model-based optimization, the parametric sensitivity is:

$$\frac{d\mathbf{x}_m^*}{d\boldsymbol{\beta}} = \mathbf{A}_m^{-1}$$

The sensitivity of the bias update with respect to the process measurements (noting that $\mathbf{z} = \mathbf{x}$) is:

$$\frac{d\boldsymbol{\beta}}{d\mathbf{x}} = \mathbf{F}(z)\ (\mathbf{A}_m - \mathbf{A}_p)$$

Then, the Point-Wise Stability Criterion requires:

$$\|\mathbf{A}_m^{-1}\mathbf{F}(z)\ (\mathbf{A}_m - \mathbf{A}_p)\|_2 < 1$$

for the RTO system / plant to be stable at the plant optimum. This is the same requirement as Condition C.8 of the convergence proof for these systems in Appendix C.

These general results can be used to revisit Example 2.2.2, which had an optimum at $x^*_p = [1.667\ 1.667]^T$. The model-based optimization had the form:

$$\underset{\mathbf{x}}{\text{maximize}} \quad [1 \quad 0.51]\,\mathbf{x}$$

$$\text{subject to:}$$

$$\mathbf{A}_m \mathbf{x} \leq \boldsymbol{\beta}_k$$

For this example, the plant coefficient matrix is assumed to be:

$$\mathbf{A}_p = \begin{bmatrix} 2 & 4 \\ 4 & 2 \end{bmatrix}$$

and the bias model update is:

$$\boldsymbol{\beta}_k = (\mathbf{A}_m - \mathbf{A}_p)\,\mathbf{x}_{k-1}$$

where the filter matrix $\mathbf{F}(z)$ is assumed to be the identity matrix.

Table 4.1 gives the coefficient matrices for three candidate process models, as well as values for the Lagrange multipliers, adjustable parameters at the plant optimum, and the point to which the RTO system ultimately converges.

Note that Model 1 does not satisfy the Point-Wise Adequacy Criteria, although there are values for the adjustable parameters which allow $\mathbf{x}^*_p$ to be a feasible point. Since both Models 2 and 3 meet the Augmented Model Adequacy Criteria, their Point-Wise Stability should be considered in the next step of the design procedure.

Table 4.1: Candidate Models and Adequacy Results

Model	A_m	μ	β	$x^*_m(\infty)$
1	$\begin{bmatrix} 2 & 4 \\ 4 & 2.1 \end{bmatrix}$	$\begin{bmatrix} -0.0051 \\ 0.2525 \end{bmatrix}$	$\begin{bmatrix} 10.00 \\ 10.17 \end{bmatrix}$	$\begin{bmatrix} 0.00 \\ 2.50 \end{bmatrix}$
2	$\begin{bmatrix} 2 & 4 \\ 4 & 1.9 \end{bmatrix}$	$\begin{bmatrix} 0.0115 \\ 0.2443 \end{bmatrix}$	$\begin{bmatrix} 10.00 \\ 9.833 \end{bmatrix}$	$\begin{bmatrix} 1.67 \\ 1.67 \end{bmatrix}$
3	$\begin{bmatrix} 8 & 4 \\ 3 & 6 \end{bmatrix}$	$\begin{bmatrix} 0.1242 \\ 0.0022 \end{bmatrix}$	$\begin{bmatrix} 20 \\ 15 \end{bmatrix}$	depends on starting point

Table 4.2 presents the results of stability testing for Models 2 and 3. From the results it is clear that Model 2 is stable, while Model 3 is not, when $F(z) = I$.

Table 4.2: Point-Wise Stability Results

Model	$\| I - A^{-1}_m A_p \|_2$
2	0.0164
3	1.554

To highlight the importance of Point-Wise Stability, closed-loop simulations were run with both Models 2 and 3, using the starting values for the adjustable parameters (β) given in Table 4.1 perturbed by -0.1 (i.e. β_0 = $[9.9\ \ 9.733]^T$ and $[19.9\ \ 14.9]^T$ for Models 2 and 3, respectively). Figures 4.4 and 4.5 present the simulation results. Figure 4.4 shows that the RTO system using Model 2 quickly converges to the plant optimum and remains there.

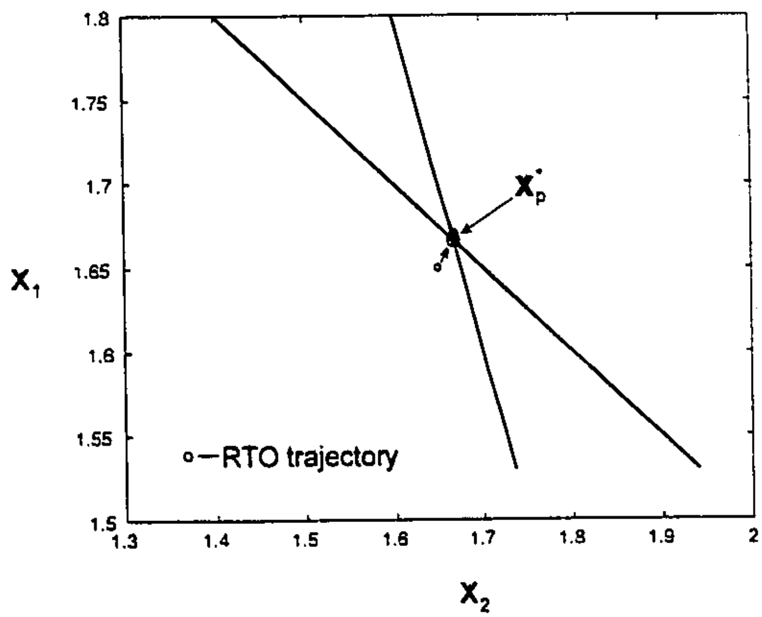

Figure 4.4: Model 2 Manipulated Variable Trajectory

Figure 4.5 shows that the RTO system using Model 3 initially moves toward the plant optimum, but after several iterations diverges from it and continues to do so. Then, of the three candidate process models, only Model 2 is acceptable for use in the proposed RTO system. In order to use Model 3, the model update procedure must be altered; for example, an RTO system using Model 3 could be stabilized by adding a filter to the bias update as shown in Appendix C.

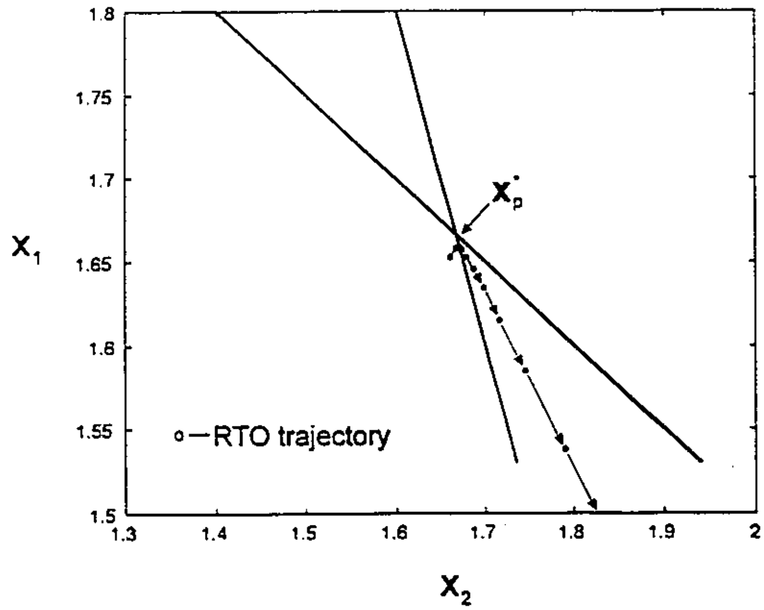

Figure 4.5: Model 3 Manipulated Variable Trajectory

4.3.2 Williams-Otto Reactor

In Section 2.1.3, a two reaction approximation to the Williams-Otto reaction sequence was shown to be Point-Wise Adequate. In this approximation all of the kinetic parameters were assumed adjustable. Values for the frequency factors and activation energies which allow the model-based optimization to have an optimum coincident with that of the plant are given in Table 2.2.

For the purposes of this example, the parameter estimation problem has the form given by Box [1970] or Sutton and MacGregor [1977]:

$$\underset{\beta}{\text{minimize}} \quad \gamma^T \gamma$$

subject to:

$$f(z^*, \alpha, \beta) = \gamma$$

where $f(z^*,\alpha,\beta)$ is the set of material balances for the two reaction approximation given in Section 2.1.3 and γ represents the amount by which these balances are non-zero. Process measurements for all compositions, flows and temperatures are assumed to be available.

The combined model-based optimization / parameter estimation system was tested using an Augmented Model Adequacy test containing Conditions 4.2 and 4.4. The closed-loop system was shown to be Point-Wise Stable at these values of the manipulated variables, with a spectral norm of 0.9164. The sensitivity matrices of the optimization and parameter estimation problems were determined by finite difference approximation, as were the plant derivatives. The details of the finite difference approximations for these terms can be found in Appendix D.
The positive definiteness of the reduced Hessians of the optimization's profit function and parameter estimation's objective function was ensured by forcing all eigenvalues of these matrices to be positive, similar to the Point-Wise Adequacy Problem 2.5. No values were found for the adjustable parameters which satisfied the Augmented Model adequacy test; thus, the combined optimization / model update is not capable of eliminating offset with respect to the plant optimum.

Closed-loop simulations were run using the combined model-based optimization and parameter estimation system. It was found that the RTO system converges to a point in the reduced space of F_B = 4.473 kg/s and T_R = 78.02°C. Figure 4.6 demonstrates a typical trajectory, starting at the plant optimum.

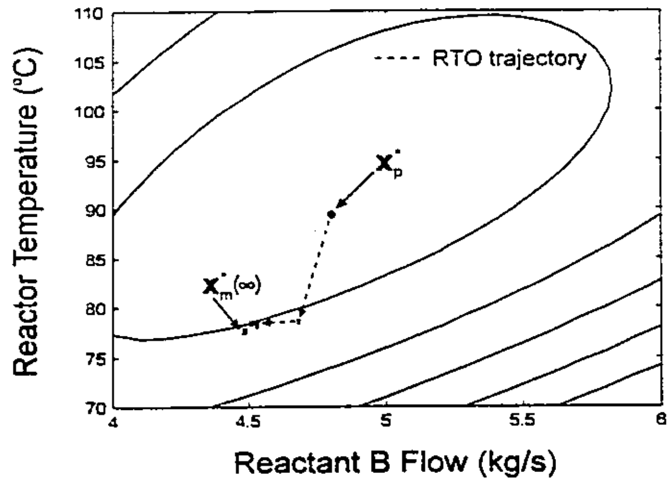

Figure 4.6: RTO Trajectory for Two Reaction Approximation to Williams-Otto Reactor

To re-design this system for zero-offset, either the model or the update technique must be changed.

4.3.3 Heat Exchanger Network

Figure 4.7 shows a simple heat exchanger network, with the streams numbered. Associated with each stream is a flow and a temperature. The only manipulated variable available is the split of the constant feed flowrate (F_1) which flows to the first heat exchanger (F_2) and the second heat exchanger (F_3). The objective in this example will be to maximize the outlet temperature T_6.

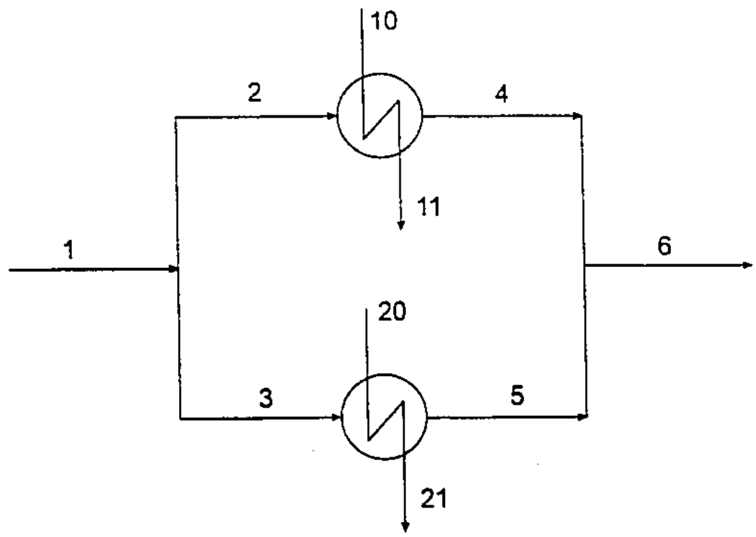

Figure 4.7: Simple Heat Exchanger Network (with stream numbers)

The plant model equations are:

$$
\begin{aligned}
F_1 &= F_2 + F_3 = 100.0 \\
F_2 &= r\,F_1 \\
F_4 &= F_2 \\
F_5 &= F_3 \\
F_{10} &= F_{11} = 50.0 \\
F_{20} &= F_{21} = 120.0
\end{aligned}
$$

$$T_1 = T_2 = T_3$$

$$T_4 = T_2 + \frac{UA_{HX1}}{F_2} \frac{(T_{11} + T_4 - T_{10} - T_2)}{\ln\left(\frac{(T_{11}-T_2)}{(T_{10}-T_4)}\right)}$$

$$T_5 = T_3 + \frac{UA_{HX2}}{F_3} \frac{(T_{21} + T_5 - T_{20} - T_3)}{\ln\left(\frac{(T_{21}-T_3)}{(T_{20}-T_5)}\right)}$$

$$T_6 = \frac{F_4 T_4 + F_5 T_5}{F_4 + F_5}$$

$$T_{10} = 320.0$$

$$T_{11} = T_{10} - \frac{UA_{HX1}}{F_{10}} \frac{(T_{11} + T_4 - T_{10} - T_2)}{\ln\left(\frac{(T_{11}-T_2)}{(T_{10}-T_4)}\right)}$$

$$T_{20} = 341.0$$

$$T_{21} = T_{20} - \frac{UA_{HX2}}{F_{20}} \frac{(T_{21} + T_5 - T_{20} - T_3)}{\ln\left(\frac{(T_{21}-T_3)}{(T_{20}-T_5)}\right)}$$

$$UA_{HX1} = \frac{1}{\frac{1}{11.7F_{10}^{0.6}} + \frac{1}{24.2F_2^{0.6}}}$$

$$UA_{HX2} = \frac{1}{\frac{1}{12.0F_{20}^{0.6}} + \frac{1}{23.2F_3^{0.6}}}$$

Heat capacities for all streams are assumed to be unity. The flow dependence of the heat transfer coefficients is derived using the methods of Holman [1972] as:

$$h_i \propto F_i^{0.6}$$

and:

$$U_{overall} = \left(\sum_i \frac{1}{h_i}\right)^{-1}$$

This example assumes that heat transfer within the fluids is controlling and neglects the resistance to heat transfer within the metal. The only manipulated variable for the optimization is the fraction (r) of constant feed flow F_1 that passes into F_2. The plant optimum is at r = 0.2904, or 29.04% of the flow in Stream 1 going to Stream 2.

The process model used by the RTO system replaced the expressions for UA_{HX1} and UA_{HX2} with adjustable parameters, thus eliminating the flow dependence of the heat transfer coefficients. Then, the model and plant equations are identical with the exception that:

$$UA_{HX1} = \beta_1$$
$$UA_{HX2} = \beta_2$$

The model update is a nonlinear least squares problem using T_4, T_5, T_{11} and T_{21} as the predictor variables. All flow and temperature measurements were available. The parameter estimation problem is:

$$\min_{\boldsymbol{\beta}} \quad (\hat{T}_4-T_4)^2 + (\hat{T}_5-T_5)^2 + (\hat{T}_{11}-T_{11})^2 + (\hat{T}_{21}-T_{21})^2$$

subject to:

$$\mathbf{f}_m(\mathbf{z}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = \mathbf{0}$$

where $\hat{T}_i$ are the predicted temperatures for stream "i" using the model equations $\mathbf{f}_m$.

This model can be made Point-Wise Adequate; however, the combination of model-based optimization and parameter estimation does not pass the Augmented Model Adequacy test. If a closed-loop simulation is run, the RTO system using the model and parameter estimation scheme converges to r = 0.30287, as is shown in Figure 4.8.

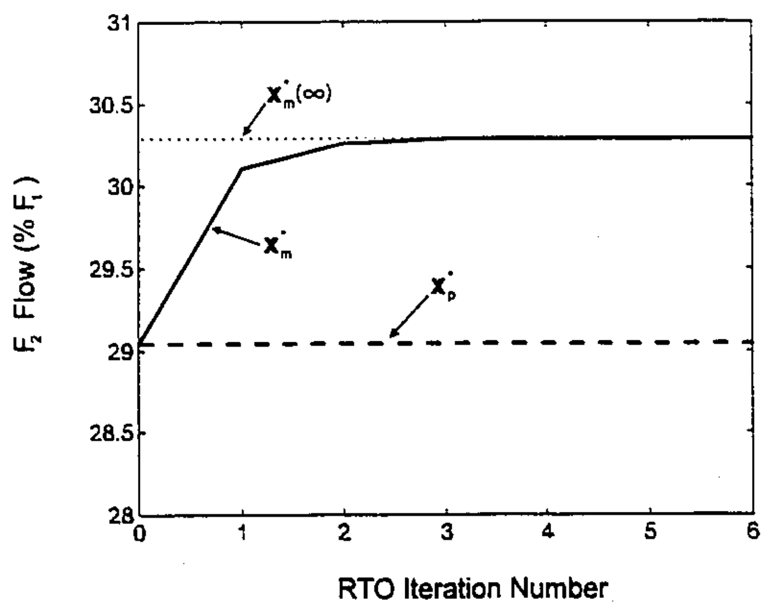

Figure 4.8: RTO Trajectory for Model with Heat Transfer Independent of Flow.

The flow dependence of the heat transfer coefficients was eliminated from the model equations by making the product of the heat transfer coefficient and the heat transfer area, an adjustable parameter. Recognizing this deficiency, a simple flow dependence was re-introduced into the model; however, the modified model equations shown below were selected to have structural mismatch with respect to the corresponding plant equations:

$$UA_{HX1} = \beta_1 F_2^{0.769}$$
$$UA_{HX2} = \beta_2 F_3^{0.596}$$

with $\boldsymbol{\beta}$ the set of adjustable parameters. The exponent values for the flowrates were determined such that the Augmented Model Adequacy criteria could be satisfied with $\beta = [5.49 \;\; 9.79]^T$. The Point-Wise Stability test yields:

$$\left\| \frac{dr_m^*}{d\beta} \frac{d\beta}{dz} \frac{dz}{dr} \right\| = 0.1741 < 1$$

Thus the closed-loop RTO system is stable, at the plant optimum.

The plant derivatives, as well as the sensitivity matrices of the model-based optimization and parameter estimation problems, were approximated by finite differences. The finite difference approximations for the plant derivatives were checked by comparison to analytically derived values. Appendix D gives the details of these calculations.

Closed-loop simulations were run and Figure 4.9 shows the results. The RTO system converges quickly to the plant optimum. Then, the modified model is suitable for implementation in a RTO system when offset elimination is the design goal. The results of this example are only applicable for the specified operating conditions (F_1, F_{10}, F_{20}, T_1, T_{10}, T_{20}); if these should change, the model may no longer be appropriate. Then, for a plant which experiences disturbances in the inlet flows or temperatures, the zero-offset tests must be performed for each expected set of disturbance values.

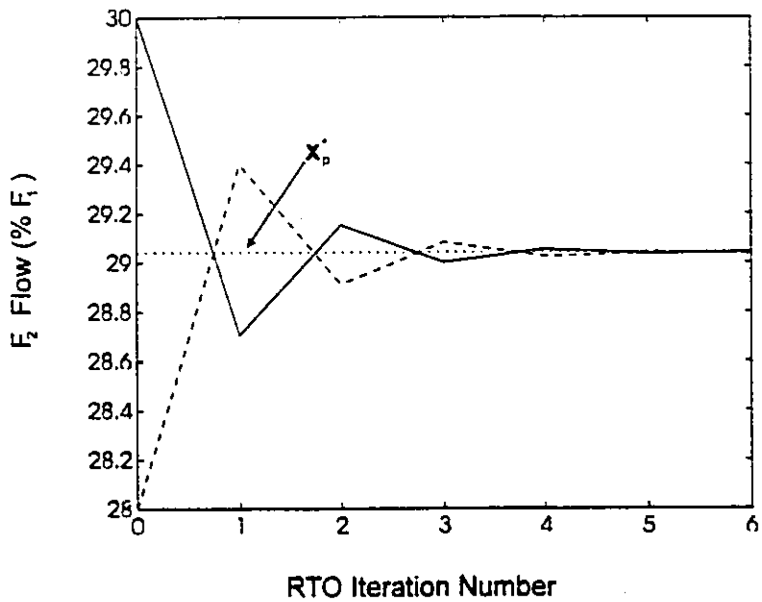

Figure 4.9: RTO Trajectories for Model with Simple Heat Transfer Flow Dependence (2 different starting points).

4.4 Discussions

This chapter has extended a set of necessary conditions which must be met for a given RTO system to be capable of exhibiting zero-offset in the manipulated variables with respect to the plant optimum. The necessary criteria are:

1) Point-Wise Model Adequacy (as developed in Chapter 2),
2) Augmented Model Adequacy,
3) Point-Wise Stability.

These three criteria are implemented as sequential tests which concentrate computational effort only on those RTO systems which have successfully passed previous, simpler tests.

The first test, Point-Wise Model Adequacy which is discussed in detail in Chapter 2, determines the ability of the model-based optimization to possess an optimum coincident with that of the plant. The second test, Augmented Model Adequacy, investigates the required steady-state behaviour of the integrated model-based optimization / parameter estimation systems. Specifically, Augmented Model Adequacy determines whether values exist for the adjustable parameters which simultaneously meet the Point-Wise Model Adequacy criteria and are also the solution to the parameter estimation problem. The final condition, Point-Wise Stability, investigates the closed-loop behaviour of the combined RTO system / plant to determine whether for differential moves away from the optimum manipulated variable values, the system will return to the plant optimum.

As discussed in Chapters 2 and 3, model adequacy testing requires knowledge of the manipulated variable values and the active constraint set at the plant optimum. The Augmented Model Adequacy criteria further requires values for the process measurements that will be used for model updating, at the plant optimum. Point-Wise Stability is determined using sensitivity information and the derivatives of the process measurements with respect to the manipulated variables. Sensitivities of the parameter estimation and model-based optimization problems are dependent upon RTO system characteristics only, and can be determined for a given design. Such sensitivities will typically be determined by finite difference approximation in industrial scale problems. Smaller problems may allow symbolic determination of the sensitivity matrices using software such as Maple [Char et al. (1991)]. The process derivatives, as for the process information required in previous chapters, must be determined directly from the plant or using a more complex model which is unsuitable for implementation within a RTO system.

As stated in the introduction, this chapter discusses necessary conditions for zero-offset. Successfully meeting all of these conditions is not sufficient to guarantee convergence to the plant optimum for finite deviations from x^*_p. Further, the tests of this chapter are point-wise in nature and any results for a specific point are valid locally only. Thus, offset elimination testing must be performed on a point-wise basis.

These offset elimination tests must be met for any RTO system design to exhibit zero-offset with respect to the optimum manipulated variables. However, the requirements placed on an RTO system design by these conditions are quite stringent and it is likely that, in many situations, zero-offset is not achievable for all the possible values of the external process variables, with the RTO system of Figure 1.1. The heat exchanger network example of Section 4.3.3 demonstrated the difficulty of attaining zero-offset from the optimum plant manipulated variable values, even for simple systems. Since this example was meant to illustrate the use of the offset elimination tests, the exponents in the flow dependence relationships were chosen so that the modified RTO system would meet the necessary conditions for zero-offset, at the nominal external variable (inlet flows and temperatures) values. In most practical situations, such "reverse engineering" of RTO systems will not be possible. Further, although the heat exchanger RTO system could eliminate offset at the nominal external variable values, it was unable to at other values of the external variables. Zero-offset is not required to achieve some, and perhaps substantial, economic benefit and a major portion of the RTO design effort can be selecting among design alternatives that do not satisfy all of the zero-offset conditions. This selection problem is the subject of the next chapter.

Chapter 5: Design Cost

The main emphasis of previous chapters has been on determining whether a Real-Time Optimization system has the ability to match the plant optimum. As was seen in Chapter 4, for offset elimination, the requirements placed on the components of a RTO system are quite stringent and may not be met in practice. When it is impractical to match the plant optimum in all situations, the design objective in any model-based RTO system design procedure should be the minimization of the cost due to deviation from the optimum values of the manipulated variables for the plant ($\mathbf{x}_p^*$).

Consider the closed-loop RTO system of Figure 5.1, consisting of model updating and model-based optimization. The examples of Chapter 4 illustrated that for a given set of external variables (such as feed qualities and process performance) and noise-free measurements, the RTO system can have a stable solution at some point $\mathbf{x}_m^*$, not necessarily the plant optimum.

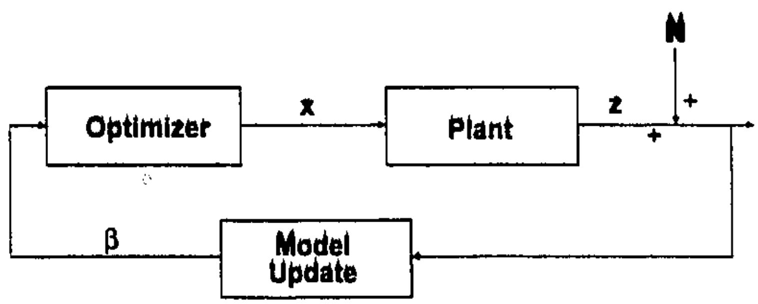

Figure 5.1: Closed-Loop RTO System Subject to Measurement Noise (**N**).

Note that in Figure 5.1 noise (N) has been added to the measurements. Such noise could be the result of random measurement errors, stochastic process disturbances and so forth. This chapter will consider only those measurement noise processes which appear to be stationary, of comparatively high frequency and not autocorrelated, with respect to the RTO cycle. The methods presented here can easily be extended to other linear measurement noise models. In general, RTO results will vary around x_m^* due to variance in the process measurements propagating through the model updating and optimization sub-systems. Figure 5.2 depicts the profit surface for some plant with constant external inputs, with an unique maximum profit at $\mathbf{x}^*_p$. In this figure, the RTO system of Figure 5.1 has converged to a point $\mathbf{x}^*_m$, which has an uncertainty region associated with it due to the presence of process noise. Then, any measure of the loss in performance of the RTO system due to imperfect optimization has two components: one for the difference between the plant optimum ($\mathbf{x}^*_p$) and the model-based optimum ($\mathbf{x}^*_m$), and one for the variance of the model-based optimum.

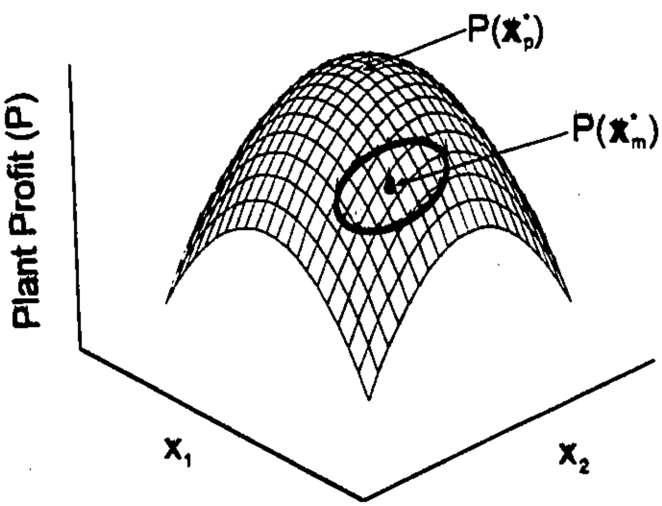

Figure 5.2: Example Plant Profit Surface Illustrating Design Cost.

This chapter defines Design Cost as the loss of economic benefits relative to perfect optimization, in terms of both offset from the plant optimum values of the manipulated variables and variance in the predicted optimum optimization variable values. The main goal of this chapter is to develop a RTO systems design metric based on such a definition of Design Cost.

For the purposes of this discussion, the goal of the optimization system will be assumed to be maximization of profit. All derivations could be reformulated for operating cost minimization with no change in the results. Further, the developments of this chapter assume that the plant has some degrees of freedom for optimization after all product quality and operating constraints are met, or that the reduced space of the plant optimization problem has dimension higher than zero. No other restrictions are assumed on the form of the model-based optimization problem.

This chapter starts by developing the Design Cost Criteria as a general approach to RTO system design. Examples serve to illustrate some specific uses of the criteria for adjustable parameter and model selection. A discussion at the end of the chapter examines some of the limitations of the method.

5.1 Design Cost Criteria

As discussed in the introduction, when there is no process noise, the RTO system of Figure 5.1 would converge to some set of manipulated variable values $\mathbf{x}^*_m$. With process noise present, the results at the end of an RTO cycle could be any point in a region which depends on the properties of the process measurement variation. Figure 5.2 illustrates such a situation. Then, the loss in RTO system performance with respect to perfect optimization should be defined in terms of the average deviation of model-based optimization results from the plant optimum. An expression for the loss in performance for the RTO system or Design Cost, at a given set of external variable values is:

$$C = P(x_p^*) - E[P(x_m^*)] \tag{5.1}$$

where C represents the portion of the theoretically attainable profit that the RTO system does not realize, E is the expectation operator, and P is the plant profit either at the plant optimum manipulated variable values (x^*_p) or the model-based optimum manipulated variable values (x^*_m). It must be stressed that P represents the actual profit the plant would produce by operating at a given set of manipulated variable values; it does not refer to any model-based prediction of profit.

The uncertainty in the predicted optimum values of the manipulated variables (x^*_m) can be described by the probability density function $f(x_m^*-\xi, Q)$, where Q is the variance-covariance matrix of the predicted optimum variable values. Although the probability density function also depends upon the higher moments of the distribution of x_m^*, these have been omitted from the notation for brevity. Providing that both of the functions P and f are Lebesgue integrable on the domain of interest, the expected profit of the RTO system is:

$$E[P(x_m^*)] = \int_{\Psi} P(\xi)\, f(x_m^* - \xi, Q)\, d\xi \tag{5.2}$$

where ξ is an integration variable defined on Ψ, the space of possible predicted optimum manipulated variable values for the given external variable values. Then, the loss in profit due to RTO system imperfections, at the point x_p^*, is:

$$C = P(x_p^*) - \int_{\Psi} P(\xi)\, f(x_m^* - \xi, Q)\, d\xi \tag{5.3}$$

The optimization problems with which this chapter is concerned have excess degrees of freedom in the manipulated variables for the maximization of plant profit and as a result the reduced space of the plant optimization problem has dimension higher than zero. If the response surface of profit is at least C^2 in the reduced space, it can be represented by the truncated Taylor series expansion:

$$\begin{aligned} P(\xi) = P(x_p^*) + \nabla_r P\big|_{x_p^*}(x_p^* - \xi) + \\ \frac{1}{2}(x_p^* - \xi)^T \nabla_r^2 P\big|_{x_p^*}(x_p^* - \xi) + o(\|x_p^* - \xi\|^3) \end{aligned} \quad 5.4$$

Noting that the reduced gradient vanishes at x_p^* and neglecting terms higher than second-order, the expansion of the profit function may be re-written:

$$P(\xi) = P(x_p^*) + \frac{1}{2}\left[(x_p^* - x_m^*) + (x_m^* - \xi)\right]^T \nabla_r^2 P\big|_{x_p^*}\left[(x_p^* - x_m^*) + (x_m^* - \xi)\right] \quad 5.5$$

which in turn can be re-arranged:

$$\begin{aligned} P(\xi) = P(x_p^*) + \frac{1}{2}(x_p^* - x_m^*)^T \nabla_r^2 P\big|_{x_p^*}(x_p^* - x_m^*) + \\ (x_p^* - x_m^*)^T \nabla_r^2 P\big|_{x_p^*}(x_m^* - \xi) + \frac{1}{2}(x_m^* - \xi)^T \nabla_r^2 P\big|_{x_p^*}(x_m^* - \xi) \end{aligned} \quad 5.6$$

Then Equation 5.6 can be substituted into the definition of Design Cost in Equation 5.3 and simplified. Consider the individual second-order terms:

$$\int_\Psi (x_p^* - x_m^*)^T \nabla_r^2 P\big|_{x_p^*}(x_m^* - \xi)\ f(x_m^* - \xi, Q)\ d\xi = 0 \quad 5.7$$

since by definition:

$$E\left[x_m^* - \xi\right] = 0 \quad 5.8$$

The second-order term in $(x_m^* - \xi)$ can be evaluated by recognizing that:

$$\int_{\Psi} (\mathbf{x}_m^* - \xi)^T \nabla_r^2 P \Big|_{\mathbf{x}_p^*} (\mathbf{x}_m^* - \xi)\; f(\mathbf{x}_m^* - \xi, \mathbf{Q})\; d\xi = \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{d^2 P}{dx_i dx_j}\Big|_{\mathbf{x}_p^*} \sigma_{ij}^2(\mathbf{x}_m^*) \qquad 5.9$$

and since:

$$\mathbf{Q} = \left[\sigma_{ij}^2\right] \qquad 5.10$$

the right hand side of Equation 5.9 can be written as a function of the Hadamard product of the reduced Hessian and the variance-covariance matrix of the predicted optimum:

$$\int_{\Psi} (\mathbf{x}_m^* - \xi)^T \nabla_r^2 P \Big|_{\mathbf{x}_p^*} (\mathbf{x}_m^* - \xi)\; f(\mathbf{x}_m^* - \xi, \mathbf{Q})\; d\xi = \mathbf{e}^T \left(\nabla_r^2 P \Big|_{\mathbf{x}_p^*} \circ \mathbf{Q} \right) \mathbf{e} \qquad 5.11$$

where $\mathbf{e} = [1\ 1\ \ldots\ 1]^T$. Recognizing that:

$$\int_{\Psi} P(\mathbf{x}_p^*)\; f(\mathbf{x}_m^* - \xi, \mathbf{Q})\; d\xi = P(\mathbf{x}_p^*) \qquad 5.12$$

since $P(\mathbf{x}^*_p)$ is a constant and by definition:

$$\int_{\Psi} f(\mathbf{x}_m^* - \xi, \mathbf{Q})\; d\xi = 1 \qquad 5.13$$

Then, combining the results of Equations 5.7 and 5.11 yields an expression for the expected profit:

$$\int_{\Psi} P(\xi)\, f(x^*_m - \xi, Q)\, d\xi \;=\; P(x^*_p) + \frac{1}{2}\,(x^*_p - x^*_m)^T\, \nabla^2_r P\big|_{x^*_p}\,(x^*_p - x^*_m) + \frac{1}{2}\, e^T \left(\nabla^2_r P\big|_{x^*_p} \circ Q \right) e \qquad 5.14$$

Then, Design Cost is given by:

$$C \;=\; -\frac{1}{2}\left[(x^*_p - x^*_m)^T\, \nabla^2_r P\big|_{x^*_p}\,(x^*_p - x^*_m) + e^T \left(\nabla^2_r P\big|_{x^*_p} \circ Q \right) e \right] \qquad 5.15$$

The objective in any RTO systems design is the minimization of Design Cost with respect to the available design choices (γ):

$$\min_{\gamma} \quad C \qquad 5.16$$

Using the Design Cost expression of Equation 5.15, an equivalent design problem is:

$$\min_{\gamma} \quad -\left[(x^*_p - x^*_m)^T\, \nabla^2_r P\big|_{x^*_p}\,(x^*_p - x^*_m) + e^T \left(\nabla^2_r P\big|_{x^*_p} \circ Q \right) e \right] \qquad 5.17$$

or:

$$\min_{\gamma} \quad (x^*_p - x^*_m)^T \left(-\nabla^2_r P\big|_{x^*_p} \right) (x^*_p - x^*_m) + e^T \left(-\nabla^2_r P\big|_{x^*_p} \circ Q \right) e \qquad 5.18$$

The objective of the RTO problem under consideration is maximization of profit. Thus, the reduced Hessian of the plant profit surface at the plant optimum manipulated variables values (x^*_p) is at worst negative semi-definite and for a RTO problem with an unique optimum the Hessian will be negative definite. Then, the negative of the reduced Hessian of the plant profit surface is positive definite. Since the variance-covariance matrix of the predicted optimum manipulated variable values is positive definite by definition and the Hadamard product of any two positive definite matrices is itself positive definite [Horn and Johnson (1991)], the minimum value Problem 5.18 may have is zero. Problem 5.18 can then be re-written:

$$\min_{\gamma} \left| (x_p^* - x_m^*)^T \left(-\nabla_r^2 P \big|_{x_p^*} \right) (x_p^* - x_m^*) + e^T \left(-\nabla_r^2 P \big|_{x_p^*} \circ Q \right) e \right| \qquad 5.19$$

The solution of Problem 5.19 requires the Hessian of the plant profit surface. Since such detailed process knowledge may not be available, the plant Hessian can be eliminated from Problem 5.19 by using an upper bound for the Design Cost. Consider only the terms inside the absolute value markers. The triangle inequality requires:

$$\begin{aligned} &\left| (x_p^* - x_m^*)^T \left(-\nabla_r^2 P \big|_{x_p^*} \right) (x_p^* - x_m^*) + e^T \left(-\nabla_r^2 P \big|_{x_p^*} \circ Q \right) e \right| \le \\ &\qquad \left| (x_p^* - x_m^*)^T \left(-\nabla_r^2 P \big|_{x_p^*} \right) (x_p^* - x_m^*) \right| + \left| e^T \left(-\nabla_r^2 P \big|_{x_p^*} \circ Q \right) e \right| \end{aligned} \qquad 5.20$$

As all of the matrices within this expression are at least positive semi-definite, the quadratic terms are positive or zero by definition and Inequality 5.20 becomes an equality. Examining each of the quadratic terms and utilizing the Cauchy-Scwharz Inequality [Ortega (1987)] yields:

$$\left| (x_p^* - x_m^*)^T \left(-\nabla_r^2 P \big|_{x_p^*} \right) (x_p^* - x_m^*) \right| \le \left\| \nabla_r^2 P \big|_{x_p^*} \right\|_2 \left\| (x_p^* - x_m^*) \right\|_2^2 \qquad 5.21$$

and:

$$\left| e^T \left(-\nabla_r^2 P \big|_{x_p^*} \circ Q \right) e \right| \le n \left\| -\nabla_r^2 P \big|_{x_p^*} \circ Q \right\|_2 \le n \left\| \nabla_r^2 P \big|_{x_p^*} \right\|_2 \left\| Q \right\|_2 \qquad 5.22$$

Inequalities 5.21 and 5.22 give upper bound for the individual terms of the design Problem 5.18 and their sum an upper bound for Design Cost:

$$C \leq \left\| \frac{d^2P}{dx^2}\Big|_{x_p^*} \right\|_2 \left(\left\| (x_p^* - x_m^*) \right\|_2^2 + n \left\| Q \right\|_2 \right) \qquad 5.23$$

In the design of a RTO system, only the offset from the plant optimum and the variance of the predicted optimum manipulated variables can be affected by system design choices. The reduced Hessian of the plant profit function is fixed for a given set of external variables. The reduced Hessian can be estimated by plant experimentation or using models which are too complex for implementation within an RTO system. Alternatively, since the reduced Hessian is generally unknown, it would be advantageous to remove any dependence of the design problem on the Hessian. This can be accomplished by minimizing the upper bound of design cost:

$$\min_{\gamma} \left\| \nabla_r^2 P\Big|_{x_p^*} \right\|_2 \left(\left\| (x_p^* - x_m^*) \right\|_2^2 + n \left\| Q \right\|_2 \right) \qquad 5.24$$

or, since the reduced Hessian is fixed, Problem 5.24 is equivalent to:

$$\min_{\gamma} \left\| (x_p^* - x_m^*) \right\|_2^2 + n \left\| Q \right\|_2 \qquad 5.25$$

The advantage of this formulation of the design problem is that it eliminates the unknown quantities from the design objective; however, in doing so it eliminates the possible solutions which take advantage of reduced Hessian properties. Such special design solutions include aligning offset with the eigenvector corresponding to the smallest eigenvalue of the reduced Hessian, and making the vector e lie within the null-space of the Hadamard product of the reduced Hessian and the variance-covariance matrix. Any such designs would require exact knowledge of the reduced Hessian of plant profit surface, which would be rarely known with the required accuracy. In the absence of such detailed plant knowledge, the solution to Problem 5.25 will best approximate the minimum Design Cost at a point.

The Design Cost Problem 5.25 represents RTO systems design at a point. In general, the plant optimum (x_p^*) is a function of some set of external process variables (w). Thus any specific plant optimum is drawn from a space **S** of all possible plant optima. There are no a priori assumptions necessary for this space; it need neither be connected nor convex. Associated with the optima in **S** is a frequency function $\varsigma(w,\upsilon)$ which describes the occurrence rate of a particular plant optimum. The total uncaptured profit due to the RTO system, for all possible plant disturbances, is:

$$C_T = \int_S \left[P(x_p^*) - \int_\Psi P(\xi)\, f(x_m^* - \xi, Q)\, d\xi \right] \varsigma(w,\upsilon)\, dx_p^* \qquad 5.26$$

where P and ς are both integrable on **S**. The maximum theoretically attainable plant profit is:

$$P_T = \int_S P(x_p^*)\, \varsigma(w,\upsilon)\, dx_p^* \qquad 5.27$$

Thus the expression for the total loss in profit can be simplified to:

$$C_T = P_T - \int_S \left[\int_\Psi P(\xi)\, f(x_m^* - \xi, Q)\, d\xi \right] \varsigma(w,\upsilon)\, dx_p^* \qquad 5.28$$

It should be noted that no relationship is necessary between the two spaces **S** and **Ψ**, except that they both must be contained in the space of feasible manipulated variable values.

For model-based RTO system design it is desirable to minimize this total loss in profit by selecting the appropriate set of design parameters γ. This is equivalent to:

$$\min_{\gamma} \quad -\int_S \left[\int_{\Psi} P(\xi)\, f(x_m^* - \xi, Q)\, d\xi \right] \varsigma(w,\upsilon)\, dx_p^* \qquad 5.29$$

Such an optimization problem may be constrained with respect to permissible values of the design choices (γ). The objective function of Problem 5.29 takes on its maximum possible value P_T when γ is chosen such that the RTO system always finds the plant optimum, with no uncertainty in the predicted optimum.

It is unlikely that the frequency function $\varsigma(w,\upsilon)$ is known at the design stage, if ever. Thus, the maximization of Problem 5.29 will have to be approximated by a sum over an expected set of values of the external variables (w). If changes in the external variables are considered to occur as steps, Problem 5.29 becomes:

$$\min_{\gamma} \sum_{w} \left[-\int_{\Psi} P(\xi)\, f(x_m^* - \xi, Q)\, d\xi \right] \varsigma(w) \qquad 5.30$$

The objective in Problem 5.30 is to minimize the weighted sum of the solutions to the point-wise Design Cost Problem 5.18, for the set of external variable values. Then using the developments for the point-wise Design Cost problem, the Total Design Cost problem is:

$$\min_{\gamma} \sum_{w} \left[\left\| (x_p^* - x_m^*) \right\|_2^2 + n \left\| Q \right\|_2 \right] \varsigma(w) \qquad 5.31$$

The solution to Problem 5.31 provides the minimum Design Cost for the expected set of external variable values. This allows the RTO designer to compare design alternatives for the entire range of expected operations, rather than one point at a time.

5.2 Covariance Matrix Approximation

Each of the Design Cost Problems 5.25 and 5.31 contains the variance-covariance matrix (Q) for the predicted optimal manipulated variables (x^*_m). This covariance matrix is generally unknown; however, for given values of the external variables, variation in these predicted optimal manipulated variables is primarily due to process measurement noise propagating throughout the optimization system.

This section will develop approximate expressions for **Q** based on properties of the RTO system components and the plant. As discussed in Section 4.2, the closed-loop RTO system in Figure 5.1 can be considered a system of nonlinear maps:

$$\begin{aligned} \mathbf{x}^*_m &= \boldsymbol{\Xi}(\boldsymbol{\beta}) \\ \boldsymbol{\beta} &= \boldsymbol{\Phi}(\mathbf{z}) \\ \mathbf{z} &= \boldsymbol{\Omega}(\mathbf{x}) \end{aligned} \qquad 5.32$$

which can be represented by linearizations for sufficiently small deviations from the plant optimum. Then, as discussed in Chapter 4, the linear approximation of the closed-loop system is the iterated map:

$$\boldsymbol{\delta}\mathbf{x}^*_m(k) = \left(\frac{d\mathbf{x}^*_m}{d\boldsymbol{\beta}} \frac{d\boldsymbol{\beta}}{d\mathbf{z}} \frac{d\mathbf{z}}{d\mathbf{x}} \right)_{\mathbf{x}^*_p,\boldsymbol{\beta}^*,\mathbf{z}^*} \boldsymbol{\delta}\mathbf{x}^*_m(k-1) + \left(\frac{d\mathbf{x}^*_m}{d\boldsymbol{\beta}} \frac{d\boldsymbol{\beta}}{d\mathbf{z}} \right)_{\boldsymbol{\beta}^*,\mathbf{z}^*} \mathbf{N}(k) \qquad 5.33$$

For Point-Wise Stable systems excited by process noise and with $\boldsymbol{\delta}\mathbf{x}^*_m(0) = \mathbf{0}$, Equation 5.33 can be re-written as the infinite sum:

$$\boldsymbol{\delta}\mathbf{x}^*_m(k) = \sum_{i=0}^{\infty} \left(\frac{d\mathbf{x}^*_m}{d\boldsymbol{\beta}} \frac{d\boldsymbol{\beta}}{d\mathbf{z}} \frac{d\mathbf{z}}{d\mathbf{x}} \right)^i_{\mathbf{x}^*_m,\boldsymbol{\beta}^*,\mathbf{z}^*} \left(\frac{d\mathbf{x}^*_m}{d\boldsymbol{\beta}} \frac{d\boldsymbol{\beta}}{d\mathbf{z}} \right)_{\boldsymbol{\beta}^*,\mathbf{z}^*} \mathbf{N}(k-i) \qquad 5.34$$

Then, the expectation (E) of the deviations from the plant optimum due to process noise is:

$$E\left[\delta x_m^*(k)\right] = \sum_{i=0}^{\infty} \left(\frac{dx_m^*}{d\beta}\frac{d\beta}{dz}\frac{dz}{dx}\right)^i_{x_m^*,\beta^*,z^*} \left(\frac{dx_m^*}{d\beta}\frac{d\beta}{dz}\right)_{\beta^*,z^*} E\left[N(k-i)\right] \qquad 5.35$$

and the expectation of the sum of squared deviations is:

$$\begin{aligned} E\left[\delta \mathbf{x}_m^*(k)(\delta \mathbf{x}_m^*(k))^T\right] = \sum_{i=0}^{\infty} & \left(\frac{d\mathbf{x}_m^*}{d\boldsymbol{\beta}}\frac{d\boldsymbol{\beta}}{d\mathbf{z}}\frac{d\mathbf{z}}{d\mathbf{x}}\right)^i_{\mathbf{x}_m^*,\boldsymbol{\beta}^*,\mathbf{z}^*} \left(\frac{d\mathbf{x}_m^*}{d\boldsymbol{\beta}}\frac{d\boldsymbol{\beta}}{d\mathbf{z}}\right)_{\boldsymbol{\beta}^*,\mathbf{z}^*} \bullet \\ & E\left[\mathbf{N}(k-i)(\mathbf{N}(k-i))^T\right] \bullet \qquad 5.36 \\ & \left[\left(\frac{d\mathbf{x}_m^*}{d\boldsymbol{\beta}}\frac{d\boldsymbol{\beta}}{d\mathbf{z}}\frac{d\mathbf{z}}{d\mathbf{x}}\right)^i_{\mathbf{x}_m^*,\boldsymbol{\beta}^*,\mathbf{z}^*} \left(\frac{d\mathbf{x}_m^*}{d\boldsymbol{\beta}}\frac{d\boldsymbol{\beta}}{d\mathbf{z}}\right)_{\boldsymbol{\beta}^*,\mathbf{z}^*}\right]^T \end{aligned}$$

Chatfield and Collins [1980].

In this work the process noise (**N**) is assumed to be a random variable sampled from a Gaussian distribution with zero mean, no serial correlation in time and a covariance matrix **U**. Such situations occur when process disturbances are stationary, approximately normally distributed and occur at a high frequency with respect to the RTO cycle.

Since by definition:

$$Q = E\left[\delta x_m^*(\delta x_m^*)^T\right] - E\left[\delta x_m^*\right]\left(E\left[\delta x_m^*\right]\right)^T \qquad 5.37$$

and $E[\delta x^*_m] = \mathbf{0}$, the covariance matrix of the deviations from the optimum manipulated variable values is given by:

$$\mathbf{Q} = \sum_{i=0}^{\infty} \left(\frac{dx_m^*}{d\beta}\frac{d\beta}{dz}\frac{dz}{dx}\right)^i_{x_m^*,\beta^*,z^*} \left(\frac{dx_m^*}{d\beta}\frac{d\beta}{dz}\right)_{\beta^*,z^*} \mathbf{U} \bullet \left[\left(\frac{dx_m^*}{d\beta}\frac{d\beta}{dz}\frac{dz}{dx}\right)^i_{x_m^*,\beta^*,z^*} \left(\frac{dx_m^*}{d\beta}\frac{d\beta}{dz}\right)_{\beta^*,z^*}\right]^T \qquad 5.38$$

Equation 5.38 gives **Q** as an infinite weighted sum in the powers of the products of various RTO subsystem sensitivities and the process derivatives. For Point-Wise Stable systems the effects of higher powers of these products can die out quickly, allowing **Q** to be approximated with a small number of terms. However, as the spectral norm of this product approaches unity, more terms must be included in the sum to approximate **Q** closely, which complicates design cost calculations. When such higher power terms must be included to closely approximate **Q** in Equation 5.38, and since Problems 5.25 and 5.31 are based on an upper bound for Design Cost, an alternative is to frame the Design Cost problem using the upper bound for the spectral norm of the covariance matrix **Q**:

$$\|\mathbf{Q}\|_2 \leq \sum_{i=0}^{\infty} \left\|\frac{dx_m^*}{d\beta}\frac{d\beta}{dz}\frac{dz}{dx}\right\|_2^{2i} \left\|\frac{dx_m^*}{d\beta}\frac{d\beta}{dz}\mathbf{U}\left(\frac{dx_m^*}{d\beta}\frac{d\beta}{dz}\right)^T\right\|_2 \qquad 5.39$$

or for Point-Wise Stable systems:

$$\|\mathbf{Q}\|_2 \leq \frac{\left\| \frac{dx_m^*}{d\beta} \frac{d\beta}{dz} U \left(\frac{dx_m^*}{d\beta} \frac{d\beta}{dz} \right)^T \right\|_2}{1 - \left\| \frac{dx_m^*}{d\beta} \frac{d\beta}{dz} \frac{dz}{dx} \right\|_2^2} \qquad 5.40$$

Using any symmetric decomposition of the covariance matrix of the measurement noise **U**, such as a Cholesky Decomposition [Golub and Van Loan (1989)]:

$$\mathbf{U} = \mathbf{L}\mathbf{L}^T \qquad 5.41$$

the upper bound on **Q** becomes:

$$\|\mathbf{Q}\|_2 \leq \frac{\left\| \frac{d\mathbf{x}_m^*}{d\boldsymbol{\beta}} \frac{d\boldsymbol{\beta}}{dz} \mathbf{L} \right\|_2^2}{1 - \left\| \frac{d\mathbf{x}_m^*}{d\boldsymbol{\beta}} \frac{d\boldsymbol{\beta}}{dz} \frac{dz}{d\mathbf{x}} \right\|_2^2} \qquad 5.42$$

and substituting into Problem 5.25 yields the closed-loop Design Cost Problem:

<u>Closed-Loop</u>

$$\min_{\gamma} \quad \left\| \mathbf{x}_p^* - \mathbf{x}_m^* \right\|_2^2 + n \frac{\left\| \frac{d\mathbf{x}_m^*}{d\boldsymbol{\beta}} \frac{d\boldsymbol{\beta}}{dz} \mathbf{L} \right\|_2^2}{1 - \left\| \frac{d\mathbf{x}_m^*}{d\boldsymbol{\beta}} \frac{d\boldsymbol{\beta}}{dz} \frac{dz}{d\mathbf{x}} \right\|_2^2} \qquad 5.43$$

Then, the Design Cost metric in Problem 5.43 is a function of properties of the RTO systems, specifically the model update and optimization, and the plant. As discussed in Chapter 4, the sensitivities of the model-based optimization and parameter estimation are dependent upon RTO system design choices and can be calculated using the methods of Fiacco [1983] or Ganesh and Biegler [1987]. The derivatives of the process measurements with respect to the manipulated variables must be determined either by plant experimentation or using the best available complex plant models, which may be inappropriate for use within the RTO system.

If the plant derivatives are not available, an alternative is to base the Design Cost metric on the step-ahead prediction of the optimal manipulated variable values. In this case an approximation to the covariance matrix of the step-ahead predictions of the optimum manipulated variables is:

$$\mathbf{Q} \approx \frac{d\mathbf{x}_m^*}{d\mathbf{z}} \mathbf{U} \frac{d\mathbf{x}_m^*}{d\mathbf{z}}^T \qquad 5.44$$

For the open-loop predictions measurement variance is only propagated through the model update and optimization; therefore, a suitable decomposition of the sensitivity of the predicted optimum manipulated variables to the process measurements is:

$$\frac{d\mathbf{x}_m^*}{d\mathbf{z}} = \frac{d\mathbf{x}_m^*}{d\boldsymbol{\beta}} \frac{d\boldsymbol{\beta}}{d\mathbf{z}} \qquad 5.45$$

yielding an approximation to the variance-covariance matrix of:

$$\mathbf{Q} = \frac{d\mathbf{x}_m^*}{d\boldsymbol{\beta}} \frac{d\boldsymbol{\beta}}{d\mathbf{z}} \mathbf{U} \left(\frac{d\mathbf{x}_m^*}{d\boldsymbol{\beta}} \frac{d\boldsymbol{\beta}}{d\mathbf{z}} \right)^T \qquad 5.46$$

Then, the spectral norm of $\mathbf{Q}$ is given by:

$$\|\mathbf{Q}\|_2 = \left\| \frac{d\mathbf{x}_m^*}{d\boldsymbol{\beta}} \frac{d\boldsymbol{\beta}}{d\mathbf{z}} \mathbf{L} \right\|_2^2 \qquad 5.47$$

where $\mathbf{L}$ is any symmetric decomposition of the process measurement covariance matrix U. Substituting into Equation 5.47 into Problem 5.25 yields the open-loop Design Cost Problem:

One Step-Ahead

$$\min_{\gamma} \quad \left\| x_p^* - x_m^* \right\|_2^2 + n \left\| \frac{dx_m^*}{d\beta} \frac{d\beta}{dz} L \right\|_2^2 \qquad 5.48$$

An important concern when designing RTO systems using the open-loop Design Cost problem, is system stability. Point-Wise Stability is an integral part of closed-loop design Problem 5.43; however, there are no such guarantees with the open-loop problem. Also, by comparing Problems 5.31 and 5.48 it is evident that, for Point-Wise Stable systems, the open-loop problem will tend to underestimate the contribution of variance to the design metric and thus favour systems with smaller offset.

A Gaussian noise model (**N**), uncorrelated in time, is assumed for the developments of this section and used throughout the chapter. An expression for the spectral norm of the predicted optimal manipulated variable values covariance matrix (**Q**) can be developed using other noise models. In such cases, time series methods [Box and Jenkins (1976)] can be used to develop expressions for the necessary expected values, E[**N**] and E[$\mathbf{N}\mathbf{N}^T$]. Then, Equations 5.35, 5.36 and 5.37 would be used to determine the closed-loop covariance matrix, or Equation 5.46 used to determine the open-loop covariance matrix.

The Design Cost Problems 5.43 and 5.48 both address RTO system design at a single set of external variable values. When minimum Total Design Cost is the objective, expressions for **Q** have to be developed at each operating point, using the methods of this section, and Problem 5.31 solved.

Both the closed-loop Design Cost Problem 5.43 and the open-loop Design Cost Problem 5.48 approximate **Q** by decomposing the covariance matrix into independent terms which are properties of the process measurements (**L**), the model-based optimization problem ($d\mathbf{x}^*_m/d\boldsymbol{\beta}$) and the parameter estimation problem ($d\boldsymbol{\beta}/d\mathbf{z}$). In either Design Cost problem, the spectral norm of the covariance matrix **Q** can be minimized by designing the model-based optimization subsystem so that the optimization problem is insensitive to changes in the adjustable parameters. Similarly, the spectral norm of **Q** can also be minimized by designing the model updating sub-system such that the parameter estimates are least sensitive to changes in the process measurements. Alternatively, the norm of **Q** can be minimized by making the rows of the parameter sensitivity matrix for the model-based optimization orthogonal to the columns of the measurement sensitivity matrix of the parameter estimation problem, through appropriate design choices. None of these design objectives is recommended as the resulting RTO system will be de-sensitized to systematic changes in the process measurements due to non-stationary process disturbances, resulting in potentially large offsets from the plant optimum. Thus, RTO system design will require a trade-off between disturbance tracking and variance of the predicted optimum manipulated variable values.

A final alternative for minimizing the spectral norm of **Q** is to select those process measurements, for use by the RTO system, which have the smallest variance / covariance or to design the RTO system such that the product of the sensitivities of the optimization problems and the parameter estimation problem ($[d\mathbf{x}^*_m/d\boldsymbol{\beta}]\cdot[d\boldsymbol{\beta}/d\mathbf{z}]$) is orthogonal to the directions of variation in the selected process measurements (the eigenvectors of the covariance matrix **Q**). Regardless of which design objective is chosen, care must be exercised to ensure that the RTO system remains responsive to process changes.

5.3 Key Parameter Selection Example

Selection of model parameters for updating is crucial to the success of a model-based Real-Time Optimization system. This section presents an illustration of the use of Design Cost in a systematic method for determining which model parameters should be updated in real-time and illustrates the inter-dependence of the modelling and adjustable parameter selection decisions. The method, which is applied at the design stage and not within the real-time implementation, involves sequential tests for parameter observability, offset elimination, and Design Cost. The section concludes with a small example built around the Williams-Otto reactor [1960].

Step 1: Parameter Observability

Parameter observability determines which sub-set, if any, of the model parameters are observable with respect to the available process measurements. This test was developed by Krishnan [1990] as an extension of the work of Stanley and Mah [1981] on state observability for nonlinear, steady-state systems. Consider a nonlinear plant model consisting of a set of material / energy balances ($\mathbf{f}$), active constraints ($\mathbf{g}_L$) and output equations ($\mathbf{h}$) :

$$\begin{bmatrix} \mathbf{f}(\mathbf{x},\mathbf{u},\boldsymbol{\alpha},\boldsymbol{\beta}) \\ \mathbf{g}_L(\mathbf{x},\mathbf{u},\boldsymbol{\alpha},\boldsymbol{\beta}) \\ \mathbf{h}(\mathbf{x},\mathbf{u}) \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{z} \end{bmatrix} \qquad 5.49$$

Linearizing these with respect to all variables and parameters within the model yields:

$$\begin{bmatrix} \nabla_x \mathbf{f} & \nabla_u \mathbf{f} & \nabla_\beta \mathbf{f} \\ \nabla_x \mathbf{g}_L & \nabla_u \mathbf{g}_L & \nabla_\beta \mathbf{g}_L \\ \nabla_x \mathbf{h} & \nabla_u \mathbf{h} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \delta \mathbf{x} \\ \delta \mathbf{u} \\ \delta \boldsymbol{\beta} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \delta \mathbf{z} \end{bmatrix} \qquad 5.50$$

Then parameter observability requires that:

$$\text{rank} \begin{bmatrix} \nabla_x \mathbf{f} & \nabla_u \mathbf{f} & \nabla_\beta \mathbf{f} \\ \nabla_x \mathbf{g}_L & \nabla_u \mathbf{g}_L & \nabla_\beta \mathbf{g}_L \\ \nabla_x \mathbf{h} & \nabla_u \mathbf{h} & \mathbf{0} \end{bmatrix} \geq m + n + p \qquad 5.49$$

where: m is the number of dependent process variables ($\mathbf{u}$) in the model, n is the number of manipulated variables ($\mathbf{x}$), p is the number of adjustable parameters ($\boldsymbol{\beta}$), $\mathbf{z}$ are the available process measurements, and $\boldsymbol{\alpha}$ are the fixed model parameters / measured external variables.

Parameter observability provides a means to determine whether effects which manifest themselves in the measured process variables, and are not attributable to changes in the manipulated variables, can be represented by the model through appropriate values of the adjustable parameters. Thus, for the RTO system of Figure 5.1, any adjustable parameter set must be observable with respect to the available process measurements to ensure that important process changes can be reflected in the model-based optimization.

<u>Step 2:</u> <u>Offset Elimination</u>

Generally, one of the main design objectives for the model-based RTO system of Figure 5.1, is that RTO results correspond to the true plant optimum manipulated variable values. Chapter 4 presented necessary conditions for zero-offset of the model-based optimum ($\mathbf{x}^*_m$) from the plant optimum ($\mathbf{x}^*_p$) manipulated variable values. The sequential set of tests provided in Chapter 4 consist of:

1) Point-Wise Model Adequacy, which tests whether there is at least one set of values for the adjustable model parameters (β) which will allow the RTO system to predict an optimum at the values of the manipulated variables which correspond to the true plant optimum,
2) Augmented Model Adequacy, which determines whether the model updating scheme can produce a set of adjustable parameter values for which the model-based optimization is Point-Wise Adequate,
3) Point-Wise Stability, which ensures that the closed-loop RTO system is stable at the plant optimum.

Although the Design Cost approach to RTO systems synthesis accommodates designs which do not achieve zero-offset, and therefore it is not necessary that any specific design meets these criteria, it is recommended that the Point-Wise Model Adequacy tests should be used to eliminate those models which produce the wrong geometry for the optimization problem, as in Section 2.1.3 for the single reaction approximation to the Williams-Otto reactor.

<u>Step 3:</u> <u>Design Cost</u>

There may be several sets of adjustable parameters (β), or none, which meet both the observability and offset elimination criteria. In selecting from among these alternative sets, the main objective should be minimizing the cost of deviations from the optimum plant manipulated variables values $\mathbf{x}_p^*$. The Design Cost methods of Section 5.1 can be used to select from among competing alternatives.

5.3.1 Williams-Otto Reactor Example

In Sections 2.1.3 and 4.3.2, a two reaction approximation to the Williams-Otto [1960] reaction sequence was examined. The reactor is an ideal CSTR with the reaction sequence:

$$\begin{aligned} A + B &\rightarrow C \\ B + C &\rightarrow P + E \\ C + P &\rightarrow G \end{aligned}$$

The reactions are all elementary and have Arrhenius temperature dependencies. As in the previous examples, the manipulated variables were chosen to be the flowrate of Reactant B (F_B) to the reactor and reactor temperature (T_R), giving a unique local optimum at: T_R = 89.647° C, F_B = 4.7836 kg/s.

The two reaction approximation to the plant kinetics is:

$$\begin{aligned} A + 2B &\rightarrow P + E \quad \ldots\ k_1 = \phi_1 e^{-\zeta_1/T_R} \\ A + B + P &\rightarrow G \quad \ldots\ k_2 = \phi_2 e^{-\zeta_2/T_R} \end{aligned}$$

Section 2.1.3 gives the complete set of equations used in the process model. In this example we compare two of the many possible adjustable parameter sets: in the first case only the frequency factors will be updated ($\beta_1 = [\phi_1\ \phi_2]^T$) and in the second case only the activation energies will be updated ($\beta_2 = [\zeta_1\ \zeta_2]^T$). As in the Section 4.3.2, all process measurements (flows, temperatures and compositions) were made available to the model updating subsystem and the parameter estimation technique which was used is given in Box [1970] or Sutton and MacGregor [1977].

Each of the adjustable parameter sets are both observable and have values for which the model-based optimization is Point-Wise Adequate. From the results of

Section 4.3.2, we known neither alternative successfully meets the Augmented Model Adequacy criteria and as a result both cases produce an off-set from the plant optimum manipulated variable values.

Table 5.1: Converged Optimum Manipulated Variables Values (no measurement noise).

	Flowrate Reactant B (kg/s)	Reactor Temperature (°C)
Activation Energies adjustable	4.829	83.20
Frequency Factors adjustable	4.829	83.19

Table 5.1 presents the manipulated variables values to which the closed-loop RTO system converges when there is no process noise present. Such manipulated variable values depend on the values assigned the fixed parameters. Typically, the fixed parameter values will be determined from detailed plant studies and / or engineering principles; however, for illustration purposes, in this case study the fixed parameter values were set so that the closed-loop RTO system converged to the same manipulated variable values for alternative adjustable parameter sets (see Table 5.1). Table 5.2 gives the fixed parameter values for each RTO problem. These fixed parameter values will allow investigation of the selection of adjustable parameters to be based solely on the covariance matrix (**Q**) of the predicted optimum manipulated variable values.

Table 5.2: Model Parameter Values at Model-Based Optimum

	Activation Energies Adjusted	Frequency Factors Adjusted
Activation Energies (K)	7307.2 10448.9	8077.6 12438.5
Frequency Factors (s^{-1})	1.2808×10^{7} 7.172×10^{10}	1.665×10^{8} 2.611×10^{13}

The Cholesky decomposition of the covariance matrix ($\mathbf{U}$) of the plant noise was chosen to be:

$$\mathbf{L} = \begin{bmatrix} 0.126 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.11 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.05 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -0.025 & 0.0433 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.05 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.025 & 0.0433 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.05 & 0 & 0 \\ 0 & 0 & 0 & -0.0173 & -0.005 & -0.00289 & 0 & 0.0465 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.126 \end{bmatrix}$$

with the process measurements organized in the vector $\mathbf{z} = [F_B \ T_R \ X_A \ X_B \ X_C \ X_E \ X_G \ X_P \ F_R]^T$. This choice of $\mathbf{L}$ reflects the situation there is covariance between composition measurements. The relative magnitudes of the assumed variances for each measurement reflects the greater uncertainty in the composition measurements than either the flow or temperature measurements. The actual values for each measurement were arbitrarily chosen, such that the standard deviation of the flow, temperature and composition measurements were approximately $2 \sim 2.5\%$, 0.3% and $12 \sim 50\%$ of the nominal values, respectively.

The process noise vector at a given instant is:

$$N_k = \mathbf{L}\ \mathrm{diag}(\sigma_i)$$

$$\sigma_i \in \mathcal{N}(0,1)$$

and the process noise was assumed uncorrelated with respect to time.

Table 5.3: Predicted Design Costs for Different Adjustable Parameter Sets.

	Activation Energies Adjustable	Frequency Factors Adjustable
open-loop $\|\mathbf{Q}\|_2$	84.3	139.3
open-loop Design Cost	211.0	321.0
$\left\| \frac{d\mathbf{x}_m^*}{d\beta} \frac{d\beta}{d\mathbf{z}} \frac{d\mathbf{z}}{d\mathbf{x}} \right\|_2$	0.2905	0.1871
closed-loop $\|\mathbf{Q}\|_2$	92.1	144.3
closed-loop Design Cost	226.5	331.0

The sensitivities and derivatives required to approximate the covariance matrix (Q) of the predicted optimum manipulated variable values were determined by finite difference approximation. These are given in Appendix D. The predicted Design Costs for the two alternative sets of adjustable parameters are presented in Table 5.3. The information in this table shows that both the open-loop Design Cost (Problem 5.48) and the closed-loop Design Cost (Problem 5.43) indicate that it is preferable to update the activation energies. Finally, both update strategies are stable at the model-based optimum.

The predictions were checked by closed-loop simulation, and Table 5.4 presents the results. The simulations consisted of three inter-connected nonlinear problems as shown in Figure 5.1: parameter estimation, model-based optimization and plant simulation using a detailed set of nonlinear equations. The open-loop covariance matrix was determined by starting the simulation at the model-based optimum given in Table 5.1 with noise added to the measurements, and executing a single RTO step. The entire procedure was repeated until the desired amount of data was collected. Calculating the closed-loop covariance matrix required starting the simulation at the model-based optimum given in Table 5.1, adding measurement noise, and allowing the RTO system to move to the new predicted optimum at each iteration. Some numerical difficulties, within the RTO system, were encountered when gathering data for the closed-loop covariance matrix while it was driven with Gaussian noise of unit variance. These difficulties arose because process noise propagating through the parameter estimation subsystem caused such wide variation in the parameter estimates that convergence problems were encountered in the model-based optimization. This was primarily due to the unusually large value assumed for the uncertainty in the composition measurements. Such difficulties would be avoided in an industrial implementation due to averaging or other smoothing of measurements, and because changes in the parameter estimates and manipulated variable predictions would be limited to some trust region. As a result, the plant noise variance was decreased by a factor of 100 or each individual innovation by a factor of 10. Thus the closed-loop results in Table 5.4 were multiplied by the same factor to compensate.

Table 5.4: Simulation Results for Spectral Norm of **Q**.

	Activation Energies Adjustable	Frequency Factors Adjustable
open-loop $\|\mathbf{Q}\|_2$	139.1	331.2
closed-loop $\|\mathbf{Q}\|_2$	71.6	199.5

Comparison of the predicted and actual spectral norms of the covariance matrix **Q** reveal that the open-loop predictions are approximately a factor of 2 lower than the simulation results, while the closed-loop predictions are quite close. Since the RTO problem in this example is nonlinear, any linear approximations are only locally valid and the predicted results in Table 5.3 would only to be accurate for small process noise variances. Then it is expected that the open-loop predictions are more accurate, for a given noise variance, since the open-loop simulation was re-started at the model-based optimum in Table 5.1 at every iteration; whereas the closed-loop simulation was allowed to move in the reduced space of the optimization problem. Despite the expected better accuracy in the open-loop case, such estimates should only be used if the plant derivatives are unavailable and the RTO system is expected to be closed-loop stable.

What is of primary importance in this example is not whether the predicted spectral norms of the covariance matrices match those observed, but whether the predictions indicate the correct choice of adjustable parameter set; although, the observed covariance matrix should approach the predicted covariance matrix in the limit, as the noise magnitude is decreased and the sample size is increased. It is worth noting that the ratio of spectral norms of the covariance matrices ($\|\mathbf{Q}\|_2$ for frequency factor update divided by $\|\mathbf{Q}\|_2$ for activation energy update) agree. The ratio is approximately 1.6 for predictions and 2.6 for observed values.

Figures 5.3 and 5.4 present the simulation results. In the open-loop simulations a sample of 30 points was collected for each alternative adjustable parameter set. For the closed-loop simulations, 50 data points were collected for each alternative adjustable parameter set. The ellipses are drawn on the figures as guides only. Recall that for closed-loop simulation purposes the variance of the process noise was decreased, thus the smaller ellipse area in Figure 5.4 than in Figure 5.3.

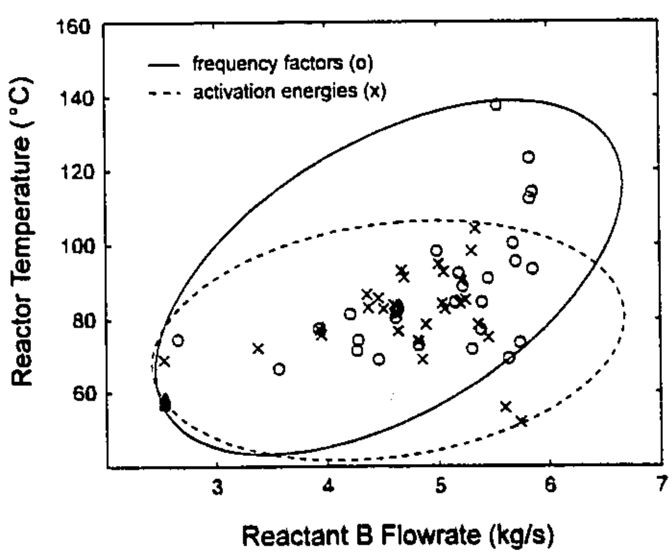

Figure 5.3: Open-Loop Simulation Results

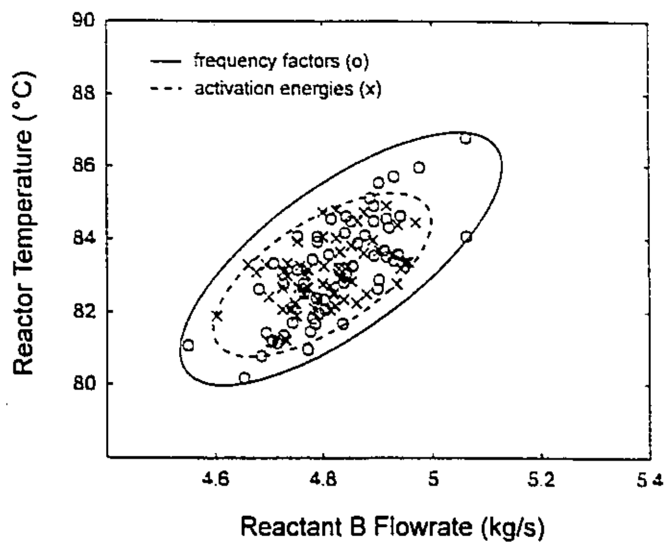

Figure 5.4: Closed-Loop Simulation Results

The design cost calculations of this example show that for the assumed measurement error covariance structure, it is better to update the activation energies than the frequency factors, in the kinetic rate expressions. For the two reaction approximation to the Williams-Otto reaction sequence, both adjustable parameter sets produce the same offset; however, updating the activation energies produces a much smaller variance in the predicted optimum. This conclusion was verified by simulation studies of the nonlinear plant.

5.3 Discussions

Design of RTO systems can be based upon fundamental principles. In this chapter, Design Cost was introduced as the loss of economic benefits due to imperfect optimization. The Design Cost method allows selection between competing design alternatives, using a metric developed from optimality and statistical theory.

The Design Cost metric in Problem 5.25 consists of two terms: one for offset from the plant optimum manipulated variable values and one for the covariance of the model-based predictions of the optimal manipulated variable values. The offset between the optimal plant and predicted manipulated variable values is dependent upon such design decisions as the process model structure and fixed parameter values, the optimization method and its tuning, the adjustable parameters, the parameter estimation technique. The second term of Problem 5.25, the covariance of the predicted optimum manipulated variable values, depends upon the manner in which process noise propagates through the integrated RTO system and the RTO system / plant interaction.

In developing the Design Cost Problem 5.25, the plant profit surface was approximated by a second-order Taylor series and the reduced Hessian of the plant profit was eliminated by minimizing an upper bound for Design Cost. Truncation of the Taylor series may cause designs to be eliminated which take advantage of the higher moments of the predicted manipulated variable's distribution, such as skewness and kurtosis. In order to take advantage of these distribution properties the third- and fourth-order derivatives of the plant profit surface would have to be known with considerable precision. Since such precision in the higher derivatives is unlikely and these derivatives would typically change with time, any design which capitalizes on some nominal value for them would be particularly susceptible to changes in the plant profit surface. If the reduced Hessian of the plant profit surface were known, then the Design Cost Problem 5.18 could be used. As with the third- and higher-order derivatives, the reduced Hessian would have to be accurately known to ensure that any design which takes advantages of its properties is an appropriate choice. Such specialized design is unlikely given some imprecision in the Hessian and changes with time.

The major difficulty encountered by eliminating the reduced Hessian of the plant profit surface from the Design Cost problem is that the problem becomes scale dependent. More precisely, by removing the reduced Hessian of the plant profit surface from the Design Cost Problem 5.18 to yield Problem 5.25, the assumption has been made that the curvature of the profit surface is approximately constant with respect to direction. It is not unusual for profit to be much less sensitive to variations in some manipulated variables than it is to others. In these cases, the advantages of aligning offset or variance of the predictions in the directions which the profit function changes slowly is lost. For such situations, when the reduced Hessian of the plant profit surface is unknown, the scaling problem can be alleviated by selecting units of measure for the manipulated variables which ensure that the curvature of the plant profit surface is approximately constant with respect to direction. Such scaling of the manipulated variables will require process knowledge or plant experimentation. Gill, Murray and Wright [1981] present a detailed discussion of scaling for optimization problems.

Two interpretations of the Design Cost problem are presented in this chapter. Closed-loop Design Cost approximates the spectral norm of the covariance matrix **Q** with an expression containing the parametric sensitivity of the model-based optimization problem, the sensitivity of the parameter estimation problem with respect to the process measurements, the derivative of the process measurements with respect to the manipulated variables from the plant and the variance structure of the process measurement noise. The open-loop Design Cost, or the Design Cost associated with the step-ahead prediction of the optimal manipulated variable values, is the product of two sensitivities and the covariance of the process measurements. These decompositions of the covariance matrix **Q** provide insight into how design decisions affect the performance of the RTO system and how such decisions are inter-dependent. For example the parametric sensitivity of the optimization problem is dependent on the objective function used in the optimization problem, the model structure and all parameter values. Whereas, the sensitivity of the parameter estimates to the process measurements is dependent on the estimation method used (Least Squares, etc.), the process model, the available measurements, the experimental design, and all fixed parameter values. The covariance matrix (U) and the process derivatives both depend on which measurements are selected for use by the RTO system. From this discussion it can easily be seen that since each RTO design decision has a potential impact on other aspects of the system, and as a result none of these decisions can be made in isolation.

The case study of Section 5.3 showed that the estimates of the spectral norm of the covariance matrix **Q** approximated the simulation results reasonably well. Both the open- and closed-loop approximations for **Q** are linear. The accuracy of these approximations could be improved by incorporating some measures of the nonlinearity of the plant, parameter estimation and optimization problems, such as the curvature measures of Bates and Watts [1988].

Section 5.3 presented a systematic method for selection of which model parameters should be adjusted by the RTO system based on Design Cost; however, since Design Cost also depends on the sensor system, estimation method, experimental design, process model, uncertainty in the fixed parameters, and so forth, it also provides a method to capture the interaction between the various RTO design decisions. Hence, Design Cost provides a general framework in which such decisions can be made. Despite the ability of the Design Cost metric for capturing the relative economic impact of a given design decision, it cannot form the sole basis of any RTO systems design. The ability of a RTO system to track unexpected non-stationary process disturbances is equally important. Thus, any good RTO design must balance Design Cost minimization and disturbance tracking for unexpected process changes.

Chapter 6: Williams-Otto Case Study

Chapters 2 through 5 introduced a variety of useful ideas for design of process operations optimization systems. These were all illustrated with examples which consisted of a relatively small number of equations, having only a few degrees of freedom available for optimization. Industrial process optimization problems often encompass integrated plants, which have process models containing sets of equations and operating constraints numbering in the thousands. Thus, although the examples presented so far were useful for illustration purposes, they are not representative of a typical industrial operations optimization problem.

The purpose of this chapter is to test the methods presented in the previous chapters, for model structure and adjustable parameter selection, on a problem more representative of those encountered in industry. The Williams-Otto [1960] was selected for this case study, since it is an integrated process which features unit operations found in many chemical industry processes. In this chapter a set of equations is used to represent the plant and a different set of model equations is used in the model-based optimization.

The chapter begins by discussing the plant and the set of equations which are used to represent it. The second section of the chapter deals with possible process model structures. These alternative model structures are examined for Point-Wise Model Adequacy and the most promising is selected for further testing. The chosen model structure, along with several alternative sets of adjustable parameters, are tested for their ability to eliminate offset and the Design Cost of each is calculated based on approximations to the covariance matrix Q of the predicted manipulated variable values. The chapter concludes with some closed-loop nonlinear simulation results, from which the covariance matrix Q can be estimated for comparison to the predicted values.

6.1 Williams-Otto Plant

The plant chosen for this case study was originally proposed by Williams and Otto [1960] as a test problem for computer control strategies and has been well studied in the optimization literature [Ray and Szekely (1973)]. Modified versions of the Williams-Otto plant have been studied by many researchers, including DiBella and Stevens [1965], McFarlane and Bacon [1989], and Roberts [1979]. Figure 6.1 is a flow diagram for the Williams-Otto plant which depicts the four main pieces of equipment: a reactor, a heat exchanger to cool the reactor effluent, a decanter to remove an unwanted reaction by-product, and a distillation column to separate the desired product. The stream naming convention shown in Figure 6.1 and used in this case study adheres to that in the original Williams and Otto [1960] paper.

Two feed streams and a recycle stream enter the reactor. The reaction vessel is a continuous stirred tank reactor in which a constant amount of material is maintained at all times. The three reactions which take place in the reactor are all exothermic and their reaction coefficients possess an Arrhenius temperature dependence. Table 6.1 gives the details for each individual reaction. Heat is provided to or removed from the reactor by heating and cooling tubes within it, as is required for a given operation. The heating tubes use steam and the cooling tubes use cooling water.

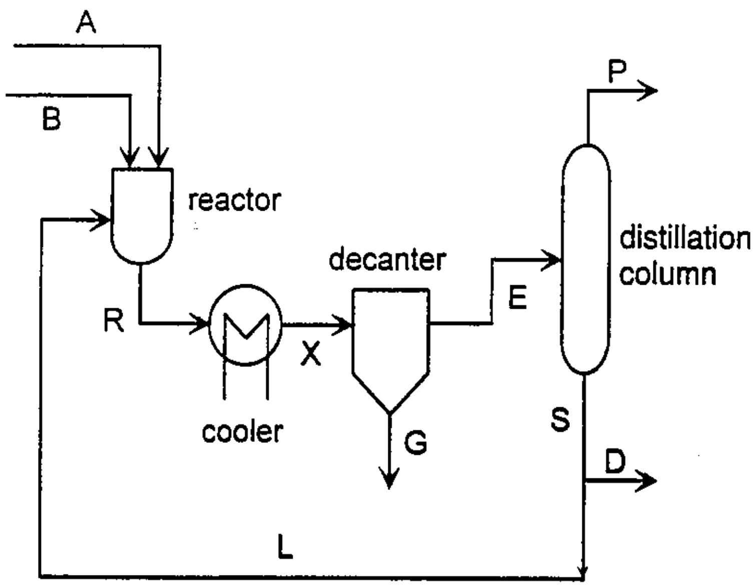

Figure 6.1: Williams-Otto Plant

Table 6.1: Williams-Otto Reaction Data

Reaction	Frequency Factor (s^{-1})	Activation Energy (K)	Heat of Reaction (kJ)	Basis
$A+B \rightarrow C$	1.6599×10^6	6,666.7	-263.8	kg. of A
$B+C \rightarrow P+E$	7.2117×10^8	8,333.3	-158.3	kg. of B
$C+P \rightarrow G$	2.6725×10^{12}	11,111	-226.3	kg. of C

The molecular weight of components A, B and P is 100, for components C and E it is 200, and for component G it is 300.

The reactor effluent is cooled in a heat exchanger, to stop the reaction and reduce the effluent temperature below the point where the undesirable by-product component G becomes insoluble (37.8°C). A decanter is used to remove all of the by-product component G from the distillation column feed. The distillation column is used to concentrate the desired product component P in the overhead stream. The bottom stream from the column is split into a recycle stream, which is returned to the reactor, and a small purge stream, which can be burned for fuel. Table 6.2 gives physical specifications for the process equipment.

The objective of Real-Time Optimization for this process is to maximize the percentage return on investment given as:

$$\begin{aligned} \text{return} = {} & 7940.77F_P + 179.991F_D - 604.32F_A - \\ & 906.480F_B - 302.160F_G - 4.57470F_R - \\ & 2.66807F_{water} - 665.961F_{steam} - 9.92806 \end{aligned} \tag{6.1}$$

where F_i are the flowrates of the indicated stream (kg/s), F_{water} and F_{steam} are the total plant cooling water and steam usage (kg/s). The main plant disturbance, as proposed in Williams and Otto [1960], consists of step-like changes to F_A, the flow of reactant A into the reactor. The plant disturbances are characterized as departures of ± 0.264670 kg/s from the nominal feed rate of reactant A to the reactor. The disturbances can occur approximately every 20 minutes.

In this study, the Williams-Otto plant was modified as follows, with respect to that proposed in the original paper:

i) simulations were performed on a steady-state basis,

ii) all heat exchange equipment was modelled using a log-mean-temperature driving force,

iii) all heat transfer coefficients were made flow dependent as in Holman [1972] with flow exponents set to 0.8,

iv) the heat transfer coefficient for the reaction cooler had to be set at

1.338 J/°C/m^2/s to match the nominal operating conditions given by Williams and Otto [1960] (Krishnan [1990] also had to make this modification),

v) the distillation column was modelled using tray-by-tray equilibrium relationships [Luyben (1973)] and assuming constant molal overflow,

vi) the separation was represented as pseudo-binary with a constant relative volatility,

vii) the relative volatility was set at 2.8 in order to simulate the nominal operating conditions given by Williams and Otto [1960],

viii) the distillation column has a total condenser, with heat transfer controlled by both cooling water flow and liquid level,

ix) the minimum acceptable concentration of product component P in the distillation column overhead stream is 95 wt% (Krishnan [1990] also made this assumption).

The plant operating constraints consist of:

1) a maximum production rate for the distillation column overhead stream of 0.600297 kg/s,

2) a minimum concentration of product component P in the distillation column overhead stream of 95 wt%,

3) a maximum available distillation column condenser heat transfer area of 458.94 m^2,

4) no by-product component G present in the distillation column feed stream and any subsequent process streams.

The manipulated variables available in the plant are: fresh feed rate of reactant B to the reactor (F_B), recycle flowrate from the distillation column bottoms (F_L), reactor operating temperature (T_R), flowrate of by-product G from the decanter bottoms (F_G), flowrate of the column overhead product stream (F_P), condenser heat transfer area, cooling water and steam flowrates in the heat exchange equipment. The fresh feed rate of reactant A to the reactor (F_A) is fixed by upstream processes and is subject to disturbances.

Table 6.2: Williams-Otto Equipment Physical Data

Equipment	Specifications	Notes
Reactor	capacity = 2,105.2 kg Area = 9.2903 m^2 U = 23.082 $F^{0.8}$ J/m^2 °Cs	an ideal continuous stirred tank.
Cooler	Area = 52.862 m^2 U = 43.794 $F^{0.8}$ J/m^2 °Cs	maximum allowable decanter feed temperature is 311.111 K.
Column	ideal stages = 21 relative volatility = 2.8	pseudo-binary distillation with constant molal overflow and constant relative volatility.
Reboiler	Area = 257.42 m^2 U = 30.378 $F^{0.8}$ J/m^2 °Cs	heating medium is hot water at fixed flowrate. Water is heated by steam injection.
Condenser	Area = 458.94 m^2 (max) U = 40.623 $F^{0.8}$ J/m^2 °Cs	total condenser with variable area.

An analysis of the plant equations for the nominal value of feed rate of reactant A (1.82749 kg/s) indicates there are three degrees of freedom available for optimization after all of the process operating constraints, thermodynamic relationships, mass and energy balances are satisfied. Then, the reduced space of the plant optimization problem has three dimensions. The three independent manipulated variables selected for this study were the fresh feed rate of reactant B to the reactor (F_B), the recycle flow rate from the column to the reactor (F_L) and the reactor operating temperature (T_R). Table 6.3 gives the plant optimum manipulated variable values and objective function value for the three disturbance values of the fresh feed rate of reactant A to the reactor (F_A).

Table 6.3: Williams-Otto Plant Optima.

F_A (kg/s)	F_B (kg/s)	F_L (kg/s)	T_R (K)	return (%)
1.56282†	3.39170	13.0966	353.737	28.5900
1.82749	3.58565	13.3940	352.748	25.8212
2.09216	3.58446	12.8837	350.778	18.5565

† in this case F_P is no longer at its maximum constrained value, (i.e. F_P = 0.567957 kg/s).

The constraints active at the plant optima are: the maximum allowable temperature at the reaction cooler exit (T_X), all by-product G removed in the decanter, the entire distillation column condenser area used for heat exchange, the maximum production rate of distillation column overhead stream (F_P) and the minimum allowable concentration of the product component P in the distillation column overhead stream.

6.2 RTO Design Alternatives

The model used in this case study contains relationships for each piece of equipment; however, the model was chosen to ensure both structural and parametric mismatch with the plant. As in Chapters 2, 4 and 5, the reactor in the Williams-Otto plant was approximated with a continuous stirred tank reactor in which the following two reactions occur:

$$A + 2B \rightarrow P + E$$

$$A + B + P \rightarrow G$$

with Arrhenius temperature dependencies for each reaction.

All heat exchange equipment was modelled with log-mean temperature driving forces and constant heat transfer coefficients. (Recall that the plant equations had heat transfer coefficients as a functions of flow through the heat exchanger).

The distillation column was represented using the modified Smoker's equation proposed by Jafarey, Douglas and McAvoy [1979]:

$$N = \frac{\ln\left[\frac{x_D(1-x_W)}{(1-x_D)x_W}\right]}{\ln\left[\frac{\alpha}{(1+\frac{1}{Rx_F})^{\frac{1}{2}}}\right]}$$

where x_D, x_F and x_W are the mole fractions of product component P not in the azeotropic mixture for the distillate, feed and bottoms streams, respectively, R is the reflux ratio and α is the relative volatility. Douglas, Jafarey and Seeman [1979] propose this equation for both process design and control.

The process model contains structural mismatch in the reactor, in the heat transfer equipment and in the distillation column equations. The model parameters available for adjustment in real-time are: the frequency factors (ϕ_i) and activation energies (ζ_i) of the Arrhenius reaction rate relationships, heats of reaction (ΔH_{rxn}), the heat transfer coefficients (U) for all heat exchange equipment, the relative volatility (α) of the mixture in the distillation column and the number of ideal trays (N) in the distillation column.

Preliminary Point-Wise Model Adequacy tests were performed on process model with all model parameters available for adjustment. The adequacy test was performed at the optimal plant operation, for the nominal disturbance value. The Point-Wise Model Adequacy test used the grid method developed in Chapter 2, with the grid spacing given in Table 6.4. Adequacy testing revealed that the process model was inadequate; thus, there are no values of the model parameters for which the manipulated variable values of the plant optimum and the model-based optimum can be made coincident.

During preliminary Point-Wise Model Adequacy testing, it was observed that the model-based optimization problems consistently under-estimated the utilities flowrates (both cooling water and steam). The objective function of the optimization problem directly costs utility flowrates rather than the heat transferred, as would usually be the case. Recall that in the plant, heat transfer coefficients are dependent upon the utility flowrates. Thus, for the plant, the incremental cost of heat transfer decreases as the process flowrates increase. The model with constant heat transfer coefficients does not contain such structure. In the model, heat transfer coefficients are constant, and as a result the costs associated with heat transfer are independent of flow. In order to more closely match the plant structure, flow dependence for the model heat transfer coefficients was re-introduced. In the modified model, the heat transfer coefficients were set to be:

$$U \propto F_i^{0.7}$$

which gives a parametric mismatch with respect to the exponent in the plant heat transfer coefficient flow dependence.

Point-Wise Model Adequacy testing was performed on the model modified to include flow dependence for the heat transfer coefficients, using the grid given in Table 6.4. The adequacy testing yielded an adequate model with the adjustable parameter values given in Table 6.5.

Table 6.4: Grid Spacing for Williams-Otto Model Adequacy Test.

	Nominal Value	**Grid Spacing**
Reactant B Flowrate (F_B)	3.58565 kg/s	±0.01891 kg/s
Recycle Flowrate (F_L)	13.3940 kg/s	±0.01891 kg/s
Reactor Temperature (T_R)	352.748 K	±0.2777 K

The remainder of the case study will examine the selection from among three alternative subsets of the possible adjustable parameters (in Table 6.5), for use in the closed-loop Real-Time Optimization system. In order to simplify discussions, the three alternatives are labelled Model1, Model2 and Model3. In Model1 the adjustable parameters are: the frequency factors (ϕ_i) in the Arrhenius reaction rate constant relationships, the heat transfer coefficients (U) and the relative volatility (α). In Model2 the adjustable parameters are: the activation energies (ζ_i) in the Arrhenius reaction rate constant relationships, the heat transfer coefficients (U) and the relative volatility (α).

Table 6.5: Adjustable Parameter Values for Point-Wise Adequate Model.

	Parameter Value	Notes
Reactor	ζ_1 = 7830.56 K ζ_2 = 10328.9 K $\phi_1 = 5.72367 \times 10^7\ s^{-1}$ $\phi_2 = 3.51404 \times 10^6\ s^{-1}$ ΔH_1 = 348.816 kJ/kg B ΔH_2 = 488.343 kJ/kg G	heats of reaction could be modified significantly without affecting the results of adequacy testing.
Reaction Cooler	U = 35.513 $F^{0.7}$ J/m^2 °Cs	
Column	α = 2.95 N = 24.0	
Condenser	U = 37.631 $F^{0.7}$ J/m^2 °Cs	
Reboiler	U = 27.679 $F^{0.7}$ J/m^2 °Cs	

The adjustable parameters were chosen for Model3 using the key parameter selection method of Krishnan [1990]. Krishnan's method uses the parametric sensitivity of the optimal value for the objective function in the model-based optimization for selecting which parameters will be adjusted on-line. Table 6.6 gives the parametric sensitivity of the objective function in the model-based optimization. For this adjustable parameter selection method, any parameters which, when varied slightly, cause an active constraint set change, are also selected for on-line adjustment. Since there were no active constraint set changes, the adjustable parameters with the largest effect on the objective function were chosen for Model3. The adjustable parameters used in Model3 are: the frequency factors (ϕ_i) and activation energies (ζ_i) in the Arrhenius reaction rate constant relationships, the number of ideal trays (N) in the distillation column and the relative volatility (α).

Table 6.6: Parametric Sensitivity of Model-Based Optimization.

	$\Delta\beta$ (%)	Δreturn (%)	Δreturn / $\Delta\beta$	rank
ϕ_1	1.066	3.289	3.085	3
ϕ_2	0.7824	-1.722	-2.201	4
ζ_1	0.0709	-1.440	-20.30	1
ζ_2	0.1076	1.301	12.097	2
ΔH_1	1.333	0.3551	0.2663	7
ΔH_2	0.9524	0.05315	0.05581	10
U_{cooler}	1.110	0.1646	0.1483	9
$U_{condenser}$	0.9937	0.1599	0.1609	8
$U_{reboiler}$	0.9752	0	0	11
α	1.017	1.274	1.253	5
N	0.8333	0.4414	0.5297	6

The parameter estimation method, used for this case study, was originally proposed by Box [1970], as well as Sutton and MacGregor [1977], and has the form:

$$\min_{\beta} \quad \epsilon^T \epsilon$$

subject to:

$$\mathbf{f}(\mathbf{z}, \boldsymbol{\beta}) = \epsilon$$

The process measurements ($\mathbf{z}$) available for parameter estimation are:

1) flowrates of Streams A, B, G, L, and P,
2) flowrates of all utility streams through each piece of equipment,
3) temperatures of Streams R and X,
4) temperature of all utility streams at the equipment exit,
5) compositions of Streams D and P.

Only the current set of measurements are used for parameter estimation.

Table 6.7 gives the variance of the measurements. The standard deviations of the measurement errors assumed for this plant correspond to approximately 0.2% to 1.0%, 0.3% and 5% of the nominal values for the flowrates, temperatures and compositions, respectively.

Table 6.7: Williams-Otto Plant Process Measurement Variance.

	Variance
flowrates of Streams A,B and L	3.57399×10^{-4} (kg/s)^2
flowrates of Streams G and P	3.57399×10^{-6} (kg/s)^2
water flowrates	3.57399×10^{-2} (kg/s)^2
steam flowrates	3.57399×10^{-6} (kg/s)^2
temperatures	7.71605×10^{-2} (°C)^2
Stream D composition	$\begin{bmatrix} 0.748 & -0.811 & 0 & 0 & 0 & 0 \\ -0.811 & 3.52 & 0 & 0 & 0 & -1.06 \\ 0 & 0 & 0.0357 & -0.177 & 0 & -0.0357 \\ 0 & 0 & -0.177 & 5.52 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.0357 & 0 \\ 0 & -1.06 & -0.0357 & 0 & 0 & 0.506 \end{bmatrix} \times 10^{-4}$
Stream P composition	$\begin{bmatrix} 0.025 & -0.025 & 0 & 0 & 0 & 0 \\ -0.025 & 0.1 & 0 & 0 & 0 & -1.42 \\ 0 & 0 & 0.001 & -0.005 & 0 & -0.0475 \\ 0 & 0 & -0.005 & 0.1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.001 & 0 \\ 0 & -1.42 & -0.0475 & 0 & 0 & 225 \end{bmatrix} \times 10^{-5}$

6.3 Zero-Offset Tests

Chapter 4 introduced a set of three necessary conditions which must be satisfied in order that a model-based real-time optimization system eliminate offset from the plant optimum manipulated variable values. These necessary conditions are implemented as a set of tests for Point-Wise Model Adequacy, Augmented Model Adequacy and Point-Wise Stability. Point-Wise Model Adequacy testing determines whether values exist for the adjustable parameters which will yield optimal manipulated variable values from the model-based optimization problem which are also optimal for the plant. Augmented Model Adequacy tests determine the ability of the model update system to produce adjustable parameter values, from available process measurements, for which the model-based optimization problem is Point-Wise Adequate. Finally, Point-Wise Stability testing ascertains whether the closed-loop RTO system will return to the optimum for arbitrarily small deviations from it.

The three modelling alternatives are Point-Wise Adequate, for the nominal disturbance value (see Table 6.5 in the previous section). As proposed in Section 4.1, Augmented Model Adequacy testing was performed using two grids: one grid for the independent manipulated variables ($\delta\mathbf{x}$) in the model-based optimization problem and one grid for the adjustable parameters ($\delta\boldsymbol{\beta}$) in the parameter estimation problem. The grid spacing for the manipulated variables is contained in Table 6.4 and Table 6.8 gives the grid spacing for the adjustable parameters.

The Augmented Adequacy tests were performed for each alternative adjustable parameter set and for all disturbance values. All three of the alternative adjustable parameter sets failed the Augmented Adequacy tests at each disturbance value, despite attempting a variety of starting points and grid spacings. Thus the combined model update / optimization system is not capable of eliminating offset with respect to the plant optimum, for any of the alternative adjustable parameter sets.

Table 6.8: Parameter Grid Spacing in Augmented Adequacy Tests.

Adjustable Parameter	Grid Spacing
frequency factor first reaction (ϕ_1)	$\pm 2.8618 \times 10^5$ s^{-1}
frequency factor second reaction (ϕ_2)	$\pm 1.7570 \times 10^4$ s^{-1}
activation energy first reaction (ζ_1)	$\pm$39.152 K
activation energy second reaction (ζ_2)	$\pm$51.645 K
cooler heat transfer coefficient (U_{cooler})	± 0.177565 $F^{0.7}$ J/m^2 °Cs
condenser heat transfer coefficient ($U_{condenser}$)	± 0.188155 $F^{0.7}$ J/m^2 °Cs
reboiler heat transfer coefficient ($U_{reboiler}$)	± 0.138395 $F^{0.7}$ J/m^2 °Cs
number of ideal column trays (N)	$\pm$0.5
relative volatility (α)	$\pm$0.1

The results of the Augmented Model Adequacy tests were confirmed by closed-loop simulation, with noise-free process measurements. The closed-loop simulations were performed for all of the alternative adjustable parameter sets and for each disturbance value. Table 6.9 gives the points, in the reduced space of the model-based optimization problem, to which each alternative converges for various values of the process disturbances. During Point-Wise testing it was found that success in solving the model-based optimization was very sensitive to initial conditions; as a result, a filter was introduced on the parameter estimates to limit the amount the closed-loop RTO system would move in a given step. The simple low-pass filter used during simulation had the form:

$$\beta_t = 0.1\ \beta_{new} + 0.9\ \beta_{t-1}$$

Alternatively, the output from the model-based optimization could have been filtered or a trust region approach employed to limit the changes in the manipulated variable values.

The closed-loop simulations showed that the model-based RTO systems all over-estimated the actual rate of return from the plant. The model-based optimization predicted rates of return in the range of 27% to 45%, while the actual rates of return for the predicted optimal variable values ranged from -10% to 6%. It should be noted that for all disturbance values, the model-based optimization problems predicted that the constraint for the maximum flowrate of the column distillate stream was active at the predicted optimum manipulated variable values; however, feasible operation of the plant at the predicted independent manipulated variable values was only possible at distillate overhead flowrates less than the maximum permissible value. Thus, the model-based optimization problems did not predict the correct active constraint set for any of the process operating points given in Table 6.9, despite model updating. Feasible plant operation was maintained at these points by a process control system which maximized the distillation column overhead product flowrate (F_P).

Table 6.9: Equilibrium Points of the Model-Based RTO System (compare with Table 6.3).

Disturbance (F_A)	**Model1**	**Model2**	**Model3**
1.56282 kg/s	F_B = 3.6049 F_L = 10.656 T_R = 353.46	F_B = 3.6208 F_L = 10.472 T_R = 353.20	F_B = 3.5842 F_L = 10.931 T_R = 352.89
1.82749 kg/s	F_B = 3.5886 F_L = 9.7299 T_R = 349.95	F_B = 3.5890 F_L = 9.7895 T_R = 349.65	F_B = 3.5706 F_L = 9.7457 T_R = 349.45
2.09216 kg/s	F_B = 3.5180 F_L = 10.444 T_R = 347.49	F_B = 3.5315 F_L = 10.529 T_R = 347.35	F_B = 3.5075 F_L = 10.528 T_R = 347.04

* the units of measure are F_B (kg/s), F_L (kg/s), T_R (K).

Although the Augmented Model Adequacy tests showed that none of the modelling alternatives was capable of eliminating offset from the plant optimum, each alternative was tested for Point-Wise Stability at all disturbance values. Point-Wise Stability testing requires the parametric sensitivity of the model-based optimization problem, the sensitivity of the parameter estimates to the process measurements in the parameter estimation problem, and the derivatives of the process measurements with respect to the independent manipulated variables. All of these derivatives were determined by finite difference approximations determined from perturbation studies of the appropriate RTO subsystem. Details of these finite difference approximations can be found in Appendix D.

Table 6.10: Point-Wise Stability Results ($\left\| \frac{dx}{d\beta} \frac{d\beta}{dz} \frac{dz}{dx} \right\|_2$).

Disturbance (F_A)	Model1	Model2	Model3
1.56282 kg/s	0.6904	0.7282	124.6
1.82749 kg/s	0.1948	0.1835	27.26
2.09216 kg/s	0.2048	0.1898	13.83

Point-Wise Stability testing showed that Model3 is unstable and would require a stabilizing filter for implementation in a RTO system. (Note that the filter used for the estimates of the adjustable parameters in the closed-loop simulations was not included in the stability tests.) Thus, Model3 was not considered in further testing. The results in Table 6.9 do not clearly identify a difference between Model1 and Model2. The Design Cost method of Chapter 5 is required to differentiate between them. Finally, if zero-offset from the plant optimum were the RTO design goal, either the model or the update strategy would have to be changed.

6.4 Design Cost Calculations

The Design Cost method developed in Chapter 5 provides a means for selecting among RTO systems design alternatives based on fundamental principles of statistics and optimization theory. The Design Cost method is framed as an optimization procedure in the form of Problem 5.31:

$$\min_{\gamma} \sum_{w} \left[\| x_p^* - x_m^* \|_2^2 + n \| Q \|_2 \right] \zeta(w)$$

where n is the number of independent manipulated variables, **Q** is the covariance matrix of the predicted optimal manipulated variable values (x^*_m), x^*_p are the optimal manipulated variable values for the plant, **w** is the set of possible plant disturbances, γ are the RTO design choices, and ζ is the frequency function for the plant disturbances.

Design Cost consists of two terms: one for the offset from the plant optimum manipulated variable values and one for the variation of the predicted optimal manipulated variable values. This variation in the predicted optimal manipulated variable values is due to measurement noise propagating through the closed-loop RTO system and is characterized by the covariance matrix **Q**. Chapter 5 provided two ways for approximating the covariance matrix **Q** from: the plant derivatives, and the sensitivities of the parameter estimation and model-based optimization problems. In this case study, the closed-loop approximation for **Q** of Inequality 5.42 is used.

Table 6.11: Closed-Loop $\| \mathbf{Q} \|_2$ Approximation for Modelling Alternatives

Disturbance (F_A)	**Model1**	**Model2**
1.56282 kg/s	47.431	61.133
1.82749 kg/s	9.2380	9.5636
2.09216 kg/s	8.6804	9.6300

Table 6.11 provides the calculated values of the closed-loop approximations to the

covariance matrix Q for the various plant disturbances. The values used for the various derivative and sensitivity matrices are given in Appendix D.

In order to calculate the Total Design Cost for a modelling alternative, a frequency function (ζ) for the possible plant disturbances (**w**) is required. In this case study the only plant disturbances are step changes in the fresh feed rate of reactant A to the reactor (F_A). The frequency function used for this case study assumed that the plant operated at the nominal disturbance value twice as often as the other disturbance values. Thus the frequency function of the plant disturbances is assumed to be :

$$\zeta(F_A=1.563) = 0.25, \quad \zeta(F_A=1.827) = 0.50, \quad \zeta(F_A=2.092) = 0.25$$

Table 6.11 summarizes the total Design Cost for the two modelling alternatives.

Table 6.12: Total Design Cost for Modelling Alternatives

	Total Design Cost (C_T)
Model1	72.277
Model2	84.841

From the results in Table 6.12, Model1 has a lower Total Design Cost than Model2. As a result, Model1 would be chosen for implementation in the model-based RTO system. Examining the results in Tables 6.9, 6.11 and 6.12 show that there was little difference between Model1 and Model2 in terms of offset from the plant optimum, and that the difference in the Design Cost for the two models was primarily due to Model2 consistently having a higher covariance among its predicted optimal manipulated variable values. Recall that the approximations used for the covariance matrix **Q** are linear and since the underlying systems are nonlinear, care must be taken in interpreting the results. The Design Cost results were checked by closed-loop simulation which incorporated measurement noise.

6.5 Simulation Results

In the Design Cost calculations of Section 6.4, the covariance matrix (**Q**) of the predicted optimal manipulated variable values was determined using numerical approximations to the required first-order derivatives. The results of such an approximation are only accurate in some small neighbourhood of the point at which the derivatives are taken, due to the nonlinearity of the equations which make up both the plant and the model in this case study. The results of the approximation of **Q** were checked by closed-loop simulation.

The closed-loop simulation of the RTO system consisted of a set of three inter-connected nonlinear problems for parameter estimation, model-based optimization, and plant simulation. The process measurements used for parameter estimation are given in Section 6.2 and had measurement noise added to them. Measurement noise was simulated by scaling innovations sampled from a $N(0,1)$ distribution using the variances given in Table 6.7, with the assumption that the measurement noise was uncorrelated with respect to time.

Preliminary attempts at closed-loop simulation encountered difficulties in solving the model-based optimization problems, associated with the adjustable parameter variation caused by the process noise. These studies showed that success in solving the model-based optimization problem is very sensitive to starting conditions, for the model structure used in this case study. Adjustable parameter variation can cause any solution from a previous model-based optimization to be sufficiently distant from the current solution, so as not to provide a sufficiently good starting point. The closed-loop simulation was designed to utilize previous solutions as starting points for the solution of the current model-based problem. This difficulty was overcome by dividing each innovation of the process noise by a factor of 5 and as a result decreasing the variance of the process measurement noise by a factor of 25.

The closed-loop simulations were performed with the reduced measurement noise variance for Model1 and Model2, as well as each of the possible disturbance values for the feed rate of Reactant A to the reactor. Each of the simulations was started at the appropriate conditions given in Table 6.9 and allowed to execute 50 complete RTO cycles. The covariance matrix **Q** was then calculated from the simulation results and multiplied by 25 to compensate for the measurement noise reduction necessary for closed-loop simulation. The spectral norms for **Q** are given in Table 6.13.

Table 6.13: Closed-Loop Simulation Results for $\| \mathbf{Q} \|_2$.

Disturbance (F_A)	**Model1**	**Model2**
1.56282 kg/s	28.857	28.384
1.82749 kg/s	11.699	13.253
2.09216 kg/s	10.534	12.505

As was shown by the approximation method for the closed-loop covariance matrix **Q**, Model1 seems to provide a smaller covariance among the predicted manipulated variable values. Comparison of the results in Tables 6.11 and 6.13, show that the results agree well, with the exception of the approximation of **Q** at the lowest disturbance value. As expected for small process noise magnitudes, the observed values for the covariance matrix spectral norms agree well with the predicted values. Differences between observed and predicted values could be due to nonlinearities, as well as the set of innovations used to simulate process measurement noise. As was discussed in Chapter 5, what is most important is that the approximation procedure for the covariance matrix **Q** indicates the correct modelling alternative. The closed-loop simulations confirm the results of the Design Cost calculations.

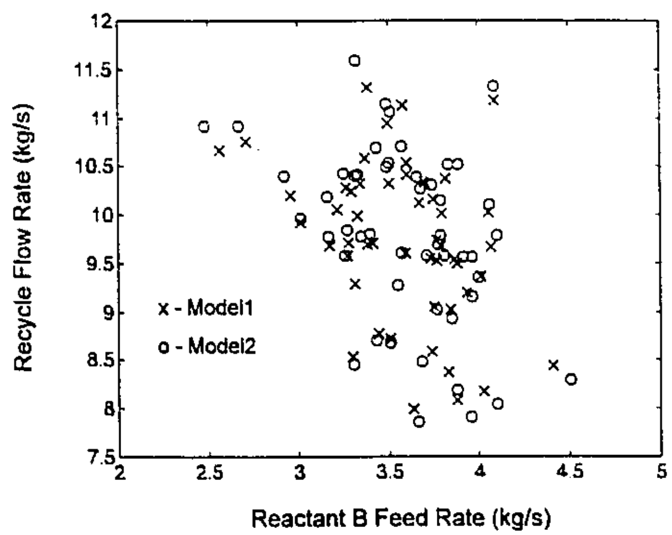

Figure 6.2: Simulation Results Comparison for F_B and F_L (nominal value for disturbance F_A).

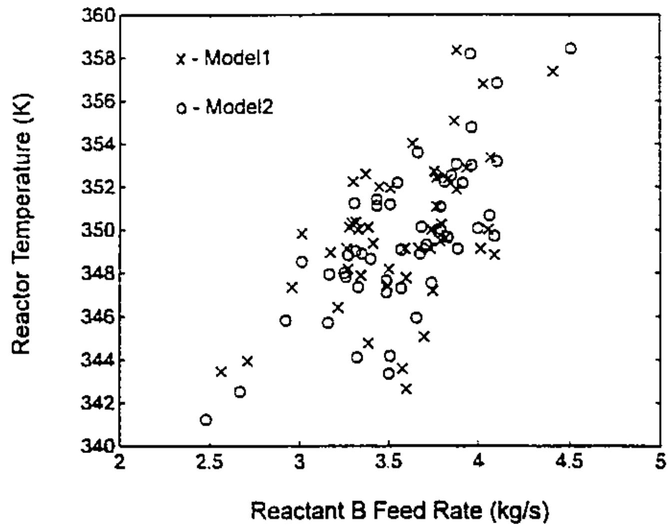

Figure 6.3: Simulation Results Comparison for F_B and T_R (nominal value for disturbance F_A).

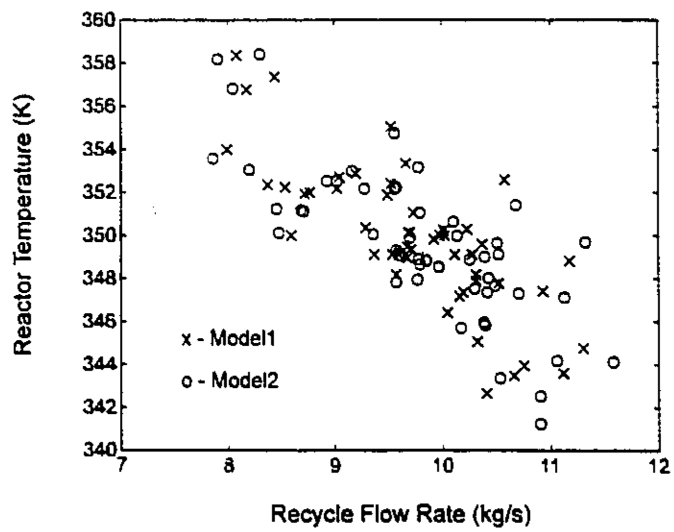

Figure 6.4: Simulation Results Comparison for F_L and T_R (nominal value for disturbance F_A).

Figures 6.2 through 6.4 present plots of the simulation results. These values were multiplied by 5 to compensate for the noise reduction necessary for successful closed-loop simulation. Note from these figures that before re-scaling, the predicted optimal operation actually varied through a range of approximately 8% to 11% of the nominal flowrate values and 1% of the nominal temperatures (or 4°C), respectively. A 4°C variation in the reactor operating temperature corresponds to a variation in the predicted reaction rates in excess of 25% of the nominal values. This range of variation should be large enough to excite some of the nonlinearities of the closed-loop system and provide a significant test of the approximations used to predict the covariance matrix **Q**.

The closed-loop simulations confirm that there is little difference between the two modelling alternatives with respect to implementation in a closed-loop RTO system. Model1 consistently has a smaller spectral norm for the covariance matrix **Q**, than does Model2; however, the differences between the two alternatives seem small when other implementation factors are considered.

The case study of this chapter provides insight into the challenges of applying the methods presented in this thesis to industrial-scale problems. As with the examples in previous chapters, the case study confirms the merits of the Design Cost of approach to RTO system design. Further, this study has illustrated the shortcomings of an existing adjustable parameter selection method (Model3).

Finally, several observations regarding the process model should be made. For the adjustable parameter sets chosen and the assumed plant disturbances, the model-based optimization had significant offsets from optimal plant operations. These offsets produced very low, and sometimes negative, rates of return. The model-based optimization problems did not identify the active constraint sets accurately. They consistently over-estimated the maximum feasible production rate for the distillate Stream P. The model-based optimization problems were much more difficult to solve than optimization problems based on the equations used to simulate the plant. As a result, while the model structure provided a useful basis for this case study, it may be inappropriate for implementation in a Real-Time Optimization system.

Chapter 7: Summary & Conclusions

Economic optimization of steady-state process operations has become increasingly important for establishing and maintaining competitive advantage in many industries. Model-based process optimization has garnered particular interest, due to the promise of faster convergence speeds and decreased amount of plant experimentation. This thesis is concerned with design of such model-based optimization systems, which include model-based Real-Time Optimization (RTO), On-Line Optimizing Control, off-line process scheduling and so forth. The available literature provides little information regarding design methods for integrated model-based optimization systems, such the system of Figure 1.1. The main objective of this work is the development of a sequential approach to integrated model-based optimization system design, based on fundamental principles of optimization and statistics. This thesis provides both insight into the model-based optimization system characteristics necessary for successful implementation, as well as useful design tools.

The importance of process model quality to the success of a model-based optimization systems has been shown by such researchers as Roberts [1979], Arkun and Stephanopoulos [1981], and Durbeck [1965]. Despite this no methods were available for determining whether a process model is adequate for use within a RTO system. Much of this work has focused on design phase process modelling issues related to model structure selection and on-line model updating.

Chapter 2 defined Point-Wise Model Adequacy as the ability of the model-based optimization to possess the same manipulated variable values as those corresponding to the plant optimum, for some value of the adjustable parameters. The Point-Wise Model Adequacy criteria focused on the manipulated variable values as the most critical match between the model and the plant, necessary for successful process optimization. In Chapter 2, design phase tests were also provided for determining the adequacy of a process model for RTO system implementation.

In Chapter 3, the Point-Wise Model adequacy methods were extended to the analysis of systems using bias updating for the process model. Such bias update systems are important since they include many of the Model Predictive Control systems used by industry. In this chapter, methods for determining the robustness of the model-based optimization system to errors in the fixed parameters were presented. For model-based optimization systems with constraints which were linear in the fixed parameters, criteria were presented which guarantee convergence to the plant optimum.

It can be readily recognized that all optimization system components in the feedback loop have an impact on the ability of the system to find the plant optimum operation. Chapter 4 presents three necessary conditions for the elimination of offset from the plant optimum, by a model-based optimization system. The three necessary conditions are Point-Wise Model Adequacy, Augmented Model Adequacy and Point-Wise Stability. Augmented model Adequacy is defined as the ability of the model updating system to provide values for the adjustable parameters, from the available process measurements, which allow the model-based optimization system to be Point-Wise Adequate. Point-Wise Stability requires that an integrated model-based optimization system return to the plant optimum for small perturbations away from it. Design phase testing procedures are presented for each of the necessary conditions.

Although much of this thesis is concerned with the ability of the model-based optimization system to find the optimal plant operation, it is recognized that zero-offset may not be the only design consideration and in many cases may not be possible using available process measurements and data. Chapter 5 presents the Design Cost approach used for making design decisions for an integrated model-based optimization system. Design Cost "trades-off" between zero-offset and the variance of the predictions for the manipulated variable values, based on statistical principles. The chapter uses Design Cost in a sequential procedure for selection of which model parameters should be adjusted on-line.

The concepts of each chapter are illustrated with small examples, containing few equations and variables. Chapter 6 provides a larger-scale case study using the Williams-Otto [1960] plant. This case study investigated both model structure and adjustable parameter selection for model-based optimization using the concepts of the Chapters 2 through 5.

This thesis serves to highlight several points regarding the design of model-based optimization systems. In general, considerable plant knowledge is required for successful implementation of the model-based optimization system Figure 1.1. Zero-offset from the plant optimum manipulated variables may not always be an attainable design goal, particularly when the process is subject to a variety of disturbances. Such disturbances could include feed grade / quality changes, equipment performance degradation and so forth. Finally, the effects of interaction between the components of an integrated model-based optimization system should be considered, to ensure a successful design.

In this thesis significant progress was made toward a systematic RTO design method; however many challenges and research opportunities remain. Much of this work was concerned with the testing of candidate design choices for model-based optimization systems. The generation of these design alternatives has been left to the system engineer. Although the tests presented in this thesis are useful for determining the ability of an optimization system to succeed, diagnosing the inadequacies of systems which fail the test has not been addressed. Since offset elimination is often desirable in a model-based optimization system, particularly for plants which experience unexpected disturbances, further work is required to develop sufficient conditions for zero-offset. Many of the testing methods used in this thesis are numerical and may not provide the most efficient methods for a given problem. Further investigation of these numerical methods should be undertaken to provide the model-based optimization system implementers with the most efficient design tools possible. Finally, the techniques presented in this thesis were applied to investigations of the inter-dependence of the model updating and model-based optimization steps of the RTO cycle shown in Figure 1.1. A comprehensive design procedure would have to consider data validation, command conditioning, the process control system, the sensor system, and so forth. The Design Cost approach can provide the framework on which such a comprehensive design procedure could be built.

Nomenclature:

A	Jacobian of active constraints.
B	space of permissible adjustable parameter values.
C	Design Cost
C^n	"n" times continuously differentiable.
c	constant vector.
c_i	cost of feedstock "i" in gasoline blending problem.
D_j	product "j" demand limits in gasoline blending problem.
E	matrix containing fixed parameter variations in decomposition of perturbations to **A**.
e	vector containing fixed parameter perturbation in a single row of **A**.
F_A	flow of reactant A to reactor in Williams-Otto plant.
F_B	flow of reactant B to reactor in Williams-Otto plant.
F_R	total outlet flow from reactor in Williams-Otto plant.
$F_{i,j}$	flow-rate of feedstock "i" to product "j" in gasoline blending problem.
F(z)	filter matrix used in Appendix C and Chapter 3.
f	equality constraints.
g	inequality constraints.
H	reduced Hessian of objective function.
L	Cholesky decomposition of the measurement covariance matrix **U**.
L	Lagrangian of optimization problem
M	number of dependent variables in true process.
m	number of dependent variables in process model.
N	process measurement noise.
N(0,1)	normal or Gaussian distribution with zero mean and unit variance.

n	number of independent (or manipulated) variables in process model.
P	objective or profit function.
p_j	product "j" pricing for gasoline blending problem.
p	number of adjustable parameters in process model.
Q	covariance matrix of predicted optimal manipulated variable values.
Q_i	feedstock "i" qualities in gasoline blending problem.
R_i	feedstock "i" availability limits in gasoline blending problem.
r	rate of reaction for single reaction approximation to Williams-Otto reaction sequence.
S	space of permissible values for manipulated variables.
S_j	product "j" quality limits in gasoline blending problem.
T	transformation matrix $(\Re^M \rightarrow \Re^m)$.
T_R	reactor temperature in Williams-Otto plant.
U	covariance matrix of process measurements (**z**).
u	dependent variables $\in \Re^m$.
V	matrix assigning position of parameter variations in decomposition of perturbations to **A**.
v	vector assigning row position in rank one decomposition of perturbations to **A**.
v	reactor volume in Williams-Otto models.
W	weighting matrix.
X_i	concentration of component "i".
x	manipulated variables $\in \Re^n$.
Z	basis vectors for null space of active constraint Jacobian.
z	process measurement vector.
z	forward shift operator.
$\boldsymbol{\alpha}$	fixed model parameters.
$\boldsymbol{\beta}$	adjustable model parameters $\in \Re^p$.
$\delta\mathbf{x}_i$	distance vector between i^{th} grid point and true process optimum.
$\boldsymbol{\varepsilon}$	distance vector between model-based optimum and process optimum.

Φ	nonlinear map representing model-based optimization problem.
η	weighting vector.
θ	angle between δx_i and ε.
κ_2	condition number of a matrix, based on L_2 norm.
λ	eigenvalues of reduced Hessian.
μ	Lagrange multiplier vector.
ν	weighting vector.
Θ	nonlinear map representing parameter estimation problem.
ς	frequency function for distribution of $\mathbf{x}^*_p$.
Ψ	nonlinear map representing the plant.

operators

∇	gradient.
∇^2	Hessian.
$\lvert \mathbf{R} \rvert$	determinant of matrix $\mathbf{R}$.
$\mathbf{R}^T$	transpose of matrix $\mathbf{R}$.
$\rho(\mathbf{R})$	spectral radius of matrix $\mathbf{R}$
$\lVert \mathbf{x} \rVert$	L_2 norm of $\mathbf{x}$.

subscripts

A	component A, Williams-Otto plant.
B	component B, Williams-Otto plant.
C	component C, Williams-Otto plant.
E	component E, Williams-Otto plant.
G	component G, Williams-Otto plant.
I	inactive.
i	feedstock index for gasoline blending problem.

j product index for gasoline blending problem.

k iteration index.

L active.

l lower limit.

m model-based property.

P component P, Williams-Otto plant.

p process property.

r reduced property.

T total.

u upper limit.

superscripts

* optimal value.

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Appendix A: Derivation of Reduced Properties for Model-Based Optimization Problems

This appendix presents the derivation of expressions for the reduced gradient and Hessian of the performance function in a model-based optimization problem. These reduced properties were used extensively in Chapters 2 and 3. The derivations are split into two main parts, which follow the discussions of Chapter 2. In the first section the reduced gradient and Hessian are derived for the partially-constrained case, where there are degrees of freedom for optimization after all of the plant operating constraints are met. The second section deals with the fully-constrained case, where the active constraint set uniquely defines the plant optimum. Both of these sections follow the reduced space conventions given in Fletcher [1987] and Gill et al. [1981]. The appendix concludes with a derivation of expressions for the reduced properties using the Implicit Function Theorem, as an alternative to the more traditional methods.

A.1 Partially-Constrained Optimization Problems

In Section 2.1, Point-Wise Model Adequacy criteria were developed around expressions for the reduced gradient and Hessian of the performance function of the model-based optimization problem. Section 2.1 dealt exclusively with the situation where there are fewer active constraints at the plant optimum that manipulated variables available for optimization. Thus, after using the active constraint set to eliminate dependent variables from the optimization problem, the reduced space of the optimization problem has a dimension higher than zero and the problem has degrees of freedom for optimization.

As a basis for the developments of this appendix section, consider the general nonlinear plant optimization problem:

$$\underset{\mathbf{x},\mathbf{u}}{\text{minimize}} \quad P(\mathbf{x},\mathbf{u})$$

$$\text{subject to:} \qquad \mathbf{f}(\mathbf{x},\mathbf{u}) = 0, \quad \mathbf{g}(\mathbf{x},\mathbf{u}) \geq 0 \qquad \text{A.1}$$

where the functions P, **f** and **g** are at least C^2 in **x** and **u**. Although the functions P, **f** and **g** may contain parameters, these have been excluded from the notation for clarity.

We assume that the problem is well posed for the plant, under any given operating policy; thus, there is a unique process optimum. This extremum will have an associated set of active operating constraints. Such active inequalities can be identified either by process knowledge or using the Karush-Kuhn-Tucker multipliers from the nominal problem. Once the active operating constraints have been identified, the equality constraint set can be reformulated as:

$$\mathbf{h}(\mathbf{x},\mathbf{u}) = \begin{bmatrix} \mathbf{f}(\mathbf{x},\mathbf{u}) \\ \mathbf{g}_L(\mathbf{x},\mathbf{u}) \end{bmatrix} = 0 \qquad \text{A.2}$$

The null space of the Jacobian of the active constraint set can be defined as [Fletcher (1987), Gill et al. (1981)]:

$$[\nabla_{\mathbf{x}}\mathbf{h} \quad \nabla_{\mathbf{u}}\mathbf{h}]\,\mathbf{Z} = 0 \qquad \text{A.3}$$

where **Z** are a set of basis vectors for the null space. Then the reduced gradient of the profit function is given by:

$$\nabla_z P = [\nabla_x P \;\; \nabla_u P]\, Z \qquad \text{A.4}$$

and the reduced Hessian of the profit function is:

$$\nabla_z^2 P = Z^T \begin{bmatrix} \nabla_x^2 L & \nabla_{x,u}^2 L \\ \nabla_{u,x}^2 L & \nabla_u^2 L \end{bmatrix} Z \qquad \text{A.5}$$

where L is the Lagrangian of the optimization Problem A.1 (i.e. $L(\mathbf{x},\mathbf{u},\mu) = P(\mathbf{x},\mathbf{u}) - \mu^T h(\mathbf{x},\mathbf{u})$). These developments allow expression of the reduced properties of an optimization problem in terms of the partial derivatives of the active constraints and the objective function. Such expressions provide a basis for determining the adequacy of a process model in terms of reduced space optimality conditions.

Sufficient conditions for a minimum require:

$$\nabla_z P = 0$$

and

$$\nabla_z^2 P \quad \text{positive definite.}$$

The reduced Hessian must be negative definite for an unique maximum.

A.2 Fully-Constrained Optimization Problems

Section 2.2 presented Point-Wise Model Adequacy criteria for the fully-constrained situation, where there are as many independent active constraints at the optimum as manipulated variables. In this case the equality constraints and active inequality constraints uniquely determine the optimum. Thus, if the optimization space were reduced using the active constraint set, the resulting reduced space would have zero dimension (a point) and model adequacy testing would require ensuring the intersection of the active set at the plant optimum. An alternative approach which provides more interpretive capability, uses the equality constraints to reduce the dimension of the optimization space to concentrate only on the manipulated variables. Then, the approach of this section requires the elimination of the dependent variables from the active constraint set.

For the purposes of this section, consider the optimization problem:

$$\begin{aligned} &\underset{\mathbf{x},\mathbf{u}}{\text{minimize}} \quad P(\mathbf{x},\mathbf{u}) \\ &\text{subject to:} \\ &\qquad f(\mathbf{x},\mathbf{u}) = 0 \\ &\qquad g_L(\mathbf{x},\mathbf{u}) = 0 \\ &\qquad g_I(\mathbf{x},\mathbf{u}) > 0 \end{aligned} \qquad \text{A.6}$$

As in the previous section, the model parameters have been eliminated from the notation for clarity.

Section A.1 defined the reduced gradients of the profit function as:

$$\nabla_r P = [\nabla_x P \quad \nabla_u P]\, \mathbf{Z} \qquad \text{A.4}$$

Elimination of the dependent variables from the active inequality constraints gives:

$$\nabla_r g_L = [\nabla_x g_L \quad \nabla_u g_L]\, \mathbf{Z} \qquad \text{A.7}$$

where **Z** is a matrix containing the set of vectors which form a basis for the null space of the Jacobian of the equality constraint set. Specifically, for a set of nonlinear model equations:

$$f(x,u) = 0 \qquad \text{A.8}$$

the matrix Z must satisfy:

$$\left[\nabla_x f \quad \nabla_u f\right] Z = 0 \qquad \text{A.9}$$

At the optimum, the Karush-Kuhn-Tucker conditions [Edgar and Himmelblau (1988)] require stationarity of the Lagrangian or:

$$\nabla_r P - \mu^T \nabla_r g_L = 0 \qquad \text{A.10}$$

which define μ in the reduced space as a function of **x** alone. The optimality conditions further require that the Lagrange multipliers associated with the active inequality constraints be non-negative or:

$$\mu \geq 0 \qquad \text{A.11}$$

where μ is defined in Equation A.10. Finally, any candidate optimal values for the variables also must be feasible:

$$\begin{aligned} f(x,u) &= 0 \\ g_L(x,u) &= 0 \\ g_I(x,u) &< 0 \end{aligned} \qquad \text{A.12}$$

Then Expressions A.10, A.11 and A.12 are the basis for determining Point-Wise Adequacy in fully-constrained optimization problems.

A.3 An Implicit Function Theorem Approach to Reduced Properties

In this section an alternative approach to eliminating the dependent variables from the optimization problem is examined. Expressions for the reduced gradient and Hessian of the performance function are derived using the Implicit Function

Theorem. The derivations will be posed for the partially-constrained optimization problem of Section A.1; however, they can easily be modified for use in the fully-constrained case.

As in Section A.1, consider the general plant optimization problem:

$$\begin{aligned} &\underset{\mathbf{x},\mathbf{u}}{\text{minimize}} \quad P(\mathbf{x},\mathbf{u}) \\ &\text{subject to:} \\ &\qquad \mathbf{f}(\mathbf{x},\mathbf{u}) = \mathbf{0} \\ &\qquad \mathbf{g}_L(\mathbf{x},\mathbf{u}) = \mathbf{0} \\ &\qquad \mathbf{g}_I(\mathbf{x},\mathbf{u}) > \mathbf{0} \end{aligned} \qquad \text{A.13}$$

where the active operating constraint set is known. Once the active operating constraints have been identified, the equality constraint set can be reformulated as:

$$\mathbf{h}(\mathbf{x},\mathbf{u}) = \begin{bmatrix} \mathbf{f}(\mathbf{x},\mathbf{u}) \\ \mathbf{g}_L(\mathbf{x},\mathbf{u}) \end{bmatrix} = \mathbf{0} \qquad \text{A.14}$$

Since all remaining inequality constraints are inactive at the point of interest, they can be ignored. The optimization is reduced to an equality constrained problem, which in turn can be simplified to an unconstrained problem by using the active constraint set to eliminate some variables, which reduces the dimension of the optimization space by the number of independent equality constraints, $\mathbf{h}(\mathbf{x},\mathbf{u})$.

The Implicit Function Theorem (Rudin, 1976) states that the set of equality constraints can be solved for $\mathbf{u}$ as a function of $\mathbf{x}$ if:

$$\left| \frac{\partial \mathbf{h}}{\partial \mathbf{u}} \right|_{\mathbf{x}^*,\mathbf{u}^*} \neq 0 \qquad \text{A.15}$$

Note that Equation A.15 is equivalent to stating the Jacobian of the equality constraints, with respect to the dependent process variables, must be full rank and therefore invertible. More simply, these gradients must be linearly independent.

Then, the relationship between the dependent and independent process variables can be expressed as:

$$\sum_{j=1}^{m} \frac{\partial h_i}{\partial u_j} \frac{\partial u_j}{\partial x_q} + \frac{\partial h_i}{\partial x_q} = 0 \qquad \text{A.16}$$

In matrix form, this is:

$$\frac{\partial \mathbf{h}}{\partial \mathbf{u}} \frac{d\mathbf{u}}{d\mathbf{x}} + \frac{\partial \mathbf{h}}{\partial \mathbf{x}} = 0 \qquad \text{A.17}$$

or:

$$\frac{d\mathbf{u}}{d\mathbf{x}} = -\left(\frac{\partial \mathbf{h}}{\partial \mathbf{u}}\right)^{-1} \frac{\partial \mathbf{h}}{\partial \mathbf{x}} \qquad \text{A.18}$$

In the reduced space, the first-order necessary condition for optimality requires that an optimum is a stationary point or that the reduced gradient of the objective function vanishes at the optimum. An expression for the reduced gradient can be derived using the definition of an exact differential:

$$dP = \frac{\partial P}{\partial \mathbf{x}} d\mathbf{x} + \frac{\partial P}{\partial \mathbf{u}} d\mathbf{u} \qquad \text{A.19}$$

Thus, the reduced gradient is:

$$\nabla_r P = \frac{\partial P}{\partial \mathbf{x}} + \frac{\partial P}{\partial \mathbf{u}} \frac{d\mathbf{u}}{d\mathbf{x}} \qquad \text{A.20}$$

Incorporating Equation A.18 yields:

$$\nabla_r P = \frac{\partial P}{\partial \mathbf{x}} - \frac{\partial P}{\partial \mathbf{u}} \left(\frac{\partial \mathbf{h}}{\partial \mathbf{u}}\right)^{-1} \frac{\partial \mathbf{h}}{\partial \mathbf{x}} \qquad \text{A.21}$$

The second-order necessary condition for optimality in the reduced space, requires that conclusions be drawn regarding the reduced Hessian of the objective function. The reduced Hessian must be positive definite for an unique minimum or negative definite for an unique maximum. An expression for the reduced Hessian is obtained by differentiating the reduced gradient expression (Equation A.21) in the reduced space of the optimization problem, as follows:

$$\nabla_r^2 P = \frac{d}{d\mathbf{x}}\left(\frac{\partial P}{\partial \mathbf{x}}\right) + \frac{d}{d\mathbf{x}}\left(\frac{\partial P}{\partial \mathbf{u}}\frac{d\mathbf{u}}{d\mathbf{x}}\right) \qquad \text{A.22}$$

but:

$$\frac{d}{d\mathbf{x}}\left(\frac{\partial P}{\partial \mathbf{x}}\right) = \frac{\partial^2 P}{\partial \mathbf{x}^2} + \frac{d\mathbf{u}^T}{d\mathbf{x}}\frac{\partial^2 P}{\partial \mathbf{u}\,\partial \mathbf{x}} \qquad \text{A.23}$$

and:

$$\frac{d}{d\mathbf{x}}\left(\frac{\partial P}{\partial \mathbf{u}}\frac{d\mathbf{u}}{d\mathbf{x}}\right) = \left(\frac{\partial^2 P}{\partial \mathbf{x}\,\partial \mathbf{u}} + \frac{d\mathbf{u}^T}{d\mathbf{x}}\frac{\partial^2 P}{\partial \mathbf{u}^2}\right)\frac{d\mathbf{u}}{d\mathbf{x}} + \sum_{j=1}^{m}\frac{\partial P}{\partial u_j}\frac{d^2 u_j}{d\mathbf{x}^2} \qquad \text{A.24}$$

After performing the appropriate substitutions and simplifications the expression for the reduced Hessian of the profit function becomes:

$$\nabla_r^2 P = \sum_{j=1}^{m}\frac{\partial P}{\partial u_j}\frac{d^2 u_j}{d\mathbf{x}^2} + \frac{\partial^2 P}{\partial \mathbf{x}^2} - \frac{\partial \mathbf{h}^T}{\partial \mathbf{x}}\left(\frac{\partial \mathbf{h}^T}{\partial \mathbf{u}}\right)^{-1}\frac{\partial^2 P}{\partial \mathbf{u}\,\partial \mathbf{x}} - \frac{\partial^2 P}{\partial \mathbf{x}\,\partial \mathbf{u}}\left(\frac{\partial \mathbf{h}}{\partial \mathbf{u}}\right)^{-1}\frac{\partial \mathbf{h}}{\partial \mathbf{x}} + \frac{\partial \mathbf{h}^T}{\partial \mathbf{x}}\left(\frac{\partial \mathbf{h}^T}{\partial \mathbf{u}}\right)^{-1}\frac{\partial^2 P}{\partial \mathbf{u}^2}\left(\frac{\partial \mathbf{h}}{\partial \mathbf{u}}\right)^{-1}\frac{\partial \mathbf{h}}{\partial \mathbf{x}} \qquad \text{A.25}$$

These developments allow expression of the reduced properties of an optimization problem in terms of the partial derivatives of the active constraints and the objective function. Such expressions provide a basis for determining the adequacy of a process model.

Notice that all of the terms required for the evaluation of the reduced Hessian are either easily evaluated or have been previously determined, with the exception of:

$$\sum_{j=1}^{m} \frac{\partial p}{\partial u_j} \frac{d^2 u_j}{d\mathbf{x}^2} \qquad \text{A.26}$$

The Hessians of the dependent variables, with respect to the independent variables, can be determined by reapplication of the Implicit Function Theorem to each the row of Equation A.18. Considering the "i^{th}" row, corresponding to the "i^{th}" element of **h**:

$$\frac{\partial}{\partial \mathbf{x}}\left[\frac{\partial h_i}{\partial \mathbf{x}} + \frac{\partial h_i}{\partial \mathbf{u}} \frac{d\mathbf{u}}{d\mathbf{x}}\right] + \frac{d\mathbf{u}}{d\mathbf{x}}^T \frac{\partial}{\partial \mathbf{u}}\left[\frac{\partial h_i}{\partial \mathbf{x}} + \frac{\partial h_i}{\partial \mathbf{u}} \frac{d\mathbf{u}}{d\mathbf{x}}\right] = 0 \qquad \text{A.27}$$

Equation A.27 can be expanded to yield:

$$\frac{\partial^2 h_i}{\partial \mathbf{x}^2} + \frac{\partial^2 h_i}{\partial \mathbf{x} \partial \mathbf{u}} \frac{d\mathbf{u}}{d\mathbf{x}} + \sum_{j=1}^{m} \frac{\partial h_i}{\partial u_j} \frac{d^2 u_j}{d\mathbf{x}^2} + \frac{d\mathbf{u}}{d\mathbf{x}}^T \frac{\partial^2 h_i}{\partial \mathbf{u} \partial \mathbf{x}} + \frac{d\mathbf{u}}{d\mathbf{x}}^T \frac{\partial^2 h_i}{\partial \mathbf{u}^2} \frac{d\mathbf{u}}{d\mathbf{x}} = 0 \qquad \text{A.28}$$

which is a set of linear equations with the only unknown terms as the elements of the Hessians of the dependent variables. There are m dependent variables with each Hessian containing n^2 elements, for a total of mn^2 unknown quantities. Since Equation A.28 represents a set of m matrix equations (each containing n^2 elements) and the Jacobian of the active constraint set with respect to the dependent variables is nonsingular (Equation A.15), the Hessians of the dependent variables can be uniquely determined.

Finally it is worthwhile to note the equivalence of Equations A.25 and A.5 in representing the reduced Hessian of the profit function. To show this equivalence, comparison of Equations A.4 and A.21 gives a possible realization for **Z** of:

$$Z = \begin{bmatrix} I \\ \frac{du}{dx} \end{bmatrix} \quad \text{A.29}$$

Then expanding Equation A.5 yields:

$$\nabla_r^2 P = \frac{\partial^2 P}{\partial \mathbf{x}^2} + \frac{d\mathbf{u}}{d\mathbf{x}}^T \frac{\partial^2 P}{\partial \mathbf{u} \partial \mathbf{x}} + \frac{\partial^2 P}{\partial \mathbf{x} \partial \mathbf{u}} \frac{d\mathbf{u}}{d\mathbf{x}} + \frac{d\mathbf{u}}{d\mathbf{x}}^T \frac{\partial^2 P}{\partial \mathbf{u}^2} \frac{d\mathbf{u}}{d\mathbf{x}} - \sum_{i=1}^{m} \mu_i \left[\frac{\partial^2 h_i}{\partial \mathbf{x}^2} + \frac{\partial^2 h_i}{\partial \mathbf{x} \partial \mathbf{u}} \frac{d\mathbf{u}}{d\mathbf{x}} + \frac{d\mathbf{u}}{d\mathbf{x}}^T \frac{\partial^2 h_i}{\partial \mathbf{u} \partial \mathbf{x}} + \frac{d\mathbf{u}}{d\mathbf{x}}^T \frac{\partial^2 h_i}{\partial \mathbf{u}^2} \frac{d\mathbf{u}}{d\mathbf{x}} \right] \quad \text{A.30}$$

Using Equation A.28, Equation A.30 simplifies to:

$$\nabla_r^2 P = \frac{\partial^2 P}{\partial \mathbf{x}^2} + \frac{d\mathbf{u}}{d\mathbf{x}}^T \frac{\partial^2 P}{\partial \mathbf{u} \partial \mathbf{x}} + \frac{\partial^2 P}{\partial \mathbf{x} \partial \mathbf{u}} \frac{d\mathbf{u}}{d\mathbf{x}} + \frac{d\mathbf{u}}{d\mathbf{x}}^T \frac{\partial^2 P}{\partial \mathbf{u}^2} \frac{d\mathbf{u}}{d\mathbf{x}} + \sum_{i=1}^{m} \mu_i \left[\sum_{j=1}^{m} \frac{\partial h_i}{\partial u_j} \frac{d^2 u_j}{d\mathbf{x}^2} \right] \quad \text{A.31}$$

Equation A.31 can rewritten as:

$$\nabla_r^2 P = \frac{\partial^2 P}{\partial \mathbf{x}^2} + \frac{d\mathbf{u}}{d\mathbf{x}}^T \frac{\partial^2 P}{\partial \mathbf{u} \partial \mathbf{x}} + \frac{\partial^2 P}{\partial \mathbf{x} \partial \mathbf{u}} \frac{d\mathbf{u}}{d\mathbf{x}} + \frac{d\mathbf{u}}{d\mathbf{x}}^T \frac{\partial^2 P}{\partial \mathbf{u}^2} \frac{d\mathbf{u}}{d\mathbf{x}} + \sum_{j=1}^{m} \boldsymbol{\mu}^T \frac{\partial \mathbf{h}}{\partial u_j} \frac{d^2 u_j}{d\mathbf{x}^2} \quad \text{A.32}$$

Comparison of the first derivative of the Lagrangian with respect to the independent variable (x) and Equation A.21 gives:

$$\boldsymbol{\mu}^T = \frac{\partial P}{\partial \mathbf{u}} \left(\frac{\partial \mathbf{h}}{\partial \mathbf{u}} \right)^{-1} \quad \text{A.33}$$

Then, Equation A.32 becomes:

$$\nabla_r^2 P = \frac{\partial^2 P}{\partial \mathbf{x}^2} + \frac{d\mathbf{u}}{d\mathbf{x}}^T \frac{\partial^2 P}{\partial \mathbf{u} \partial \mathbf{x}} + \frac{\partial^2 P}{\partial \mathbf{x} \partial \mathbf{u}} \frac{d\mathbf{u}}{d\mathbf{x}} + \frac{d\mathbf{u}}{d\mathbf{x}}^T \frac{\partial^2 P}{\partial \mathbf{u}^2} \frac{d\mathbf{u}}{d\mathbf{x}} + \sum_{j=1}^{m} \frac{\partial P}{\partial \mathbf{u}} \left(\frac{\partial \mathbf{h}}{\partial \mathbf{u}} \right)^{-1} \frac{\partial \mathbf{h}}{\partial u_j} \frac{d^2 u_j}{d\mathbf{x}^2} \qquad \text{A.34}$$

which simplifies to:

$$\nabla_r^2 P = \frac{\partial^2 P}{\partial \mathbf{x}^2} + \frac{d\mathbf{u}}{d\mathbf{x}}^T \frac{\partial^2 P}{\partial \mathbf{u} \partial \mathbf{x}} + \frac{\partial^2 P}{\partial \mathbf{x} \partial \mathbf{u}} \frac{d\mathbf{u}}{d\mathbf{x}} + \frac{d\mathbf{u}}{d\mathbf{x}}^T \frac{\partial^2 P}{\partial \mathbf{u}^2} \frac{d\mathbf{u}}{d\mathbf{x}} + \sum_{j=1}^{m} \frac{\partial P}{\partial u_j} \frac{d^2 u_j}{d\mathbf{x}^2} \qquad \text{A.35}$$

Equations A.25 and A.35 are easily shown as equivalent by making use of Equation A.18. Then, the approaches of Section A.1 and A.3 yield the same results for the reduced Hessian of the profit function, with one possible representation for the null space of the active constraint set (**Z**) given in Equation A.29.

Appendix B: Derivation of Upper Error Bounds For Grid Adequacy Method

In Section 2.1 (Problem 2.8) a grid method was presented for numerically determining Point-Wise Model Adequacy. Inequalities 2.9 or 2.10 gave bounds for the possible errors using this method. In this appendix, the expressions for theses bounds are derived in detail.

The numerical method of Problem 2.8 for determining Point-Wise Model Adequacy does not guarantee an optimum of the model at the given plant optimum ($\mathbf{x}^*_p$). The grid method generates a value of the adjustable parameters ($\boldsymbol{\beta}$) for which:

$$P(\mathbf{x}_p^* + \delta\mathbf{x}_i, \boldsymbol{\beta}) > P(\mathbf{x}_p^*, \boldsymbol{\beta}) \qquad \text{B.1}$$

The dependent variables ($\mathbf{u}$) and the fixed parameters ($\boldsymbol{\alpha}$) have been eliminated from the notation in this section for clarity. Minimization has been assumed for these derivations; however, developments are applicable to maximization as well.

In order to determine the effects of grid spacing and problem geometry on uncertainty in the location of the model-based optimum, consider the model-based minimization which has been shown to be Point-Wise Adequate using the grid method of Equation 2.8, where the grid has been selected sufficiently small that:

$$P(\mathbf{x}) = P_0 + \mathbf{c}^T\mathbf{x} + \frac{1}{2}\mathbf{x}^T\mathbf{H}\mathbf{x} + o(\|\mathbf{x}-\mathbf{x}_p^*\|^3) \qquad \text{B.2}$$

and $\|\mathbf{x}-\mathbf{x}^*_p\|^3$ is negligible within the neighbourhood defined by the grid. Using

Equation B.2 to expand Inequality B.1 yields:

$$P_0 + c^T (x_p^* + \delta x_i) + \frac{1}{2} (x_p^* + \delta x_i)^T H (x_p^* + \delta x_i) > P_0 + c^T x_p^* + \frac{1}{2} (x_p^*)^T H x_p^* \qquad \text{B.3}$$

Simplifying:

$$[c^T + (x_p^*)^T H] \, \delta x_i + \frac{1}{2} \delta x_i^T H \, \delta x_i > 0 \qquad \text{B.4}$$

Although the adjustable parameters (β) have been set so as to satisfy Inequality B.1, consider the situation where the minimum of the model based optimization (x^0) is some distance from the true process optimum (x^*_p), then:

$$x^0 = x_p^* + \epsilon \qquad \text{B.5}$$

Substituting Equation B.5 into Inequality B.4 yields:

$$[c^T + (x^0 - \epsilon)^T H] \, \delta x_i + \frac{1}{2} \delta x_i^T H \, \delta x_i > 0 \qquad \text{B.6}$$

At the optimum of the model-based optimization problem:

$$\nabla_x P \Big|_{x^0} = c^T + (x^0)^T H = 0 \qquad \text{B.7}$$

Reduces Inequality B.6 to:

$$-\epsilon^T H \, \delta x_i + \frac{1}{2} \delta x_i^T H \, \delta x_i > 0 \qquad \text{B.8}$$

or:

$$\delta x_i^T H \, \delta x_i > 2 \epsilon^T H \, \delta x_i \qquad \text{B.9}$$

Since the reduced Hessian (H) of the model-based problem is real and symmetric and the model-based problem is strongly Point-Wise Adequate, the Hessian has a complete set of orthonormal eigenvectors (V) such that:

$$\mathbf{H}\,\mathbf{V} = \mathbf{V}\,\boldsymbol{\Lambda} \qquad \text{B.10}$$

Using these eigenvectors as a basis for the reduced space, the grid perturbations can be expressed as:

$$\boldsymbol{\delta}\mathbf{x}_i = \mathbf{V}\,\boldsymbol{\eta} \qquad \text{B.11}$$

and the difference between the true process and model-based optimum as:

$$\boldsymbol{\epsilon} = \mathbf{V}\,\mathbf{v} \qquad \text{B.12}$$

Substituting Equation B.11 and B.12 into Inequality B.9 yields:

$$\boldsymbol{\eta}^T \mathbf{V}^T \mathbf{H}\,\mathbf{V}\,\boldsymbol{\eta} > 2\,\mathbf{v}^T \mathbf{V}^T \mathbf{H}\,\mathbf{V}\,\boldsymbol{\eta} \qquad \text{B.13}$$

Using Equation B.10 to simplify Inequality B.13 gives:

$$\boldsymbol{\eta}^T \boldsymbol{\Lambda}\,\boldsymbol{\eta} > 2\,\mathbf{v}^T \boldsymbol{\Lambda}\,\boldsymbol{\eta} \qquad \text{B.14}$$

The left-hand side of Inequality B.14 can be rewritten as:

$$\boldsymbol{\eta}^T \boldsymbol{\Lambda}\,\boldsymbol{\eta} = \sum_{j=1}^{n} \lambda_j\, \eta_j^2 \qquad \text{B.15}$$

but:

$$\|\boldsymbol{\eta}\|^2 \bullet \max\{|\lambda_j|\} > \sum_{j=1}^{n} \lambda_j\, \eta_j^2 \qquad \text{B.16}$$

The right-hand side of Inequality B.14 can be rewritten as:

$$2\,\mathbf{v}^T \boldsymbol{\Lambda}\,\boldsymbol{\eta} = 2 \sum_{j=1}^{n} \lambda_j\, v_j\, \eta_j \qquad \text{B.17}$$

but:

$$2\sum_{j=1}^{n}\lambda_j v_j \eta_j \;>\; 2\,\|\mathbf{v}\|\,\|\boldsymbol{\eta}\|\cos\theta\bullet\min\{|\lambda_j|\} \qquad \text{B.18}$$

where θ is the angle between the vectors ν and η.

Using the relationships in B.14, B.16 and B.18 to get an upper bound estimate for the magnitude of ν:

$$\|\mathbf{v}\| \;<\; \frac{\|\boldsymbol{\eta}\|}{2\cos\theta}\,\frac{\max\{|\lambda_j|\}}{\min\{|\lambda_j|\}} \qquad \text{B.19}$$

An expression for the condition number (κ_2) of the matrix **H** is:

$$\kappa_2 \;=\; \rho(\mathbf{H})\bullet\rho(\mathbf{H}^{-1}) \;=\; \frac{\max\{|\lambda_j|\}}{\min\{|\lambda_j|\}} \qquad \text{B.20}$$

It can easily be shown that:

$$\begin{aligned} \|\boldsymbol{\delta}\mathbf{x}_i\| &= \|\boldsymbol{\eta}\| \\ \|\boldsymbol{\epsilon}\| &= \|\mathbf{v}\| \\ (\boldsymbol{\delta}\mathbf{x}_i)^T\boldsymbol{\epsilon} &= \boldsymbol{\eta}^T\mathbf{v} \end{aligned} \qquad \text{B.21}$$

Combining the expressions in Inequality B.19, Equations B.20 and B.21 produces:

$$\|\boldsymbol{\epsilon}\| \;<\; \frac{\|\boldsymbol{\delta}\mathbf{x}_i\|}{2\cos\theta}\,\kappa_2 \qquad \text{B.22}$$

This expression gives an upper bound for the distance between the given process optimum and the solution to the model-based optimization problem. From Inequality B.22 it is evident that this distance depends on the grid spacing, the angle between perturbations in the grid and the conditioning of the reduced Hessian for the model-based problem.

The grid design used in the case studies was set such that adjacent perturbations were orthogonal. Thus:

$$\theta_{max} = \frac{\pi}{4} \qquad \text{B.23}$$

Hence, Inequality B.22 becomes:

$$\| \boldsymbol{\epsilon} \| < \frac{\max\{\| \boldsymbol{\delta x}_i \|\}}{\sqrt{2}} \kappa_2 \qquad \text{B.24}$$

Then, using the grid method for determining Point-Wise Model Adequacy will yield a set of adjustable parameters ($\boldsymbol{\beta}$) for which the model-based optimum ($\mathbf{x}^o$) is contained within a hypersphere centred on the plant optimum ($\mathbf{x}^*_p$), with radius given in Inequality B.24.

Finally, it was recommended that when possible the grid should be aligned with the eigenvectors of the performance function's reduced Hessian. When this is done, the estimate of the maximum distance between the plant optimum and model-based optimum can be reduced to its smallest value. Consider that when:

$$\boldsymbol{\delta x}_i = \eta_i \mathbf{v}_i \qquad \text{B.25}$$

so that Inequality B.9 becomes:

$$\eta_i \mathbf{v}_i^T \mathbf{H} \mathbf{v}_i \eta_i > 2\boldsymbol{\epsilon}^T \mathbf{H} \mathbf{v}_i \eta_i \qquad \text{B.26}$$

but by definition:

$$\mathbf{H} \mathbf{v}_i = \lambda_i \mathbf{v}_i \qquad \text{B.27}$$

Thus, Inequality B.26 reduces to:

$$\| \mathbf{v}_i \| \lambda_i \eta_i^2 > 2\boldsymbol{\epsilon}^T \mathbf{v}_i \lambda_i \eta_i \qquad \text{B.28}$$

Simplifying:

$$\|\mathbf{v}_i\|^2 \eta_i \;>\; \|\boldsymbol{\epsilon}\| \, \|\mathbf{v}_i\| \cos\theta \qquad \text{B.29}$$

Recalling that the eigenvectors of the reduced Hessian are orthonormal and that the maximum angle is given by Equation B.23, Inequality B.29 becomes:

$$\|\boldsymbol{\epsilon}\| < \frac{\max\{\|\boldsymbol{\delta}\mathbf{x}_i\|\}}{\sqrt{2}} \qquad \text{B.30}$$

Thus, when the grid is chosen to align with the eigenvectors of the reduced Hessian, the resulting uncertainty in the location of the model-based optimum is independent of the conditioning of the optimization problem. In this case, using the grid method of determining Point-Wise Model Adequacy will produce a set of adjustable parameters such that the model-based optimum lies within a hypersphere centred on the plant optimum, where Inequality B.30 gives the maximum radius.

Appendix C: Bias Update Convergence

In Section 3.2 it was stated that in some cases a Real-Time Optimization system using bias update can be guaranteed to converge to the plant optimum. This appendix presents a Bias Update Convergence Theorem and its proof.

Bias Update Convergence Theorem:

A model-based Real-Time Optimization system, using bias model updating, will converge to the true plant optimum providing: i) all model equations and constraints are linear, ii) the active constraint set uniquely defines the solution of the model-based optimization problem (i.e. the model-based optimization problem is fully-constrained as defined in Section 2.2), and iii) the model-based optimization is Point-Wise Accurate according to Definition 3.1 in Section 3.2.

Proof:

Consider the Real-Time Optimization problem with Bias Update, as in Figure 3.1, with linear constraints operating an open-loop stable plant. The underlying model-based optimization problem is:

$$\min_{\mathbf{x}} \quad P(\mathbf{x})$$
$$\text{subject to:} \qquad \mathbf{A}_m \mathbf{x} \geq \mathbf{b}_L + \boldsymbol{\beta}_L \qquad \mathbf{Q}_m \mathbf{x} \geq \mathbf{b}_I + \boldsymbol{\beta}_I \tag{C.1}$$

with plant-model mismatch in the coefficient matrices of the inequality constraints (**A** and **Q**). If the process model is Point-Wise Accurate, with the constraints associated with $\mathbf{A}_m$ active at the plant optimum, the RTO system will converge to the plant optimum providing the bias term is appropriately filtered in the update phase, providing that the optimization problem is fully-constrained (i.e. rank($\mathbf{A}_m$) = dim(x)). This can be shown by considering the operations performed at the kth iteration:

1) bias update,

$$\boldsymbol{\beta}_{L,k} = \mathbf{F}(z)\ (\mathbf{A}_m - \mathbf{A}_p)\ \mathbf{x}_{k-1} \tag{C.2}$$

2) followed by an optimization, which is equivalent to solving the set of simultaneous linear equations given by the active constraint set,

$$\mathbf{A}_m \mathbf{x}_k = \mathbf{b}_L + \boldsymbol{\beta}_{L,k} \tag{C.3}$$

Substituting Equation C.2 into Equation C.3 and simplifying yields:

$$\mathbf{x}_k = \mathbf{A}_m^{-1} \mathbf{b}_L + \mathbf{A}_m^{-1} \mathbf{F}(z)\ (\mathbf{A}_m - \mathbf{A}_p)\ \mathbf{x}_{k-1} \tag{C.4}$$

but the optimum of the model-based problem with zero bias can be defined:

$$\mathbf{x}_m^* = \mathbf{A}_m^{-1} \mathbf{b}_L \tag{C.5}$$

and if we define a transformed filter:

$$\mathbf{F}(z) = \mathbf{A}_m \mathbf{G}(z)\ \mathbf{A}_m^{-1} \tag{C.6}$$

then Equation C.4 becomes:

$$\mathbf{x}_k = \mathbf{x}_m^* + G(z)\,(\mathbf{I} - \mathbf{A}_m^{-1}\mathbf{A}_p)\,\mathbf{x}_{k-1} \tag{C.7}$$

This difference equation will converge as $k \rightarrow \infty$ providing the filter is designed such that:

$$\left\| G(z)\,(\mathbf{I} - \mathbf{A}_m^{-1}\mathbf{A}_p) \right\|_2 < 1 \tag{C.8}$$

to give the final value of:

$$\mathbf{x}_\infty = \left[\mathbf{I} - G(1)\,(\mathbf{I} - \mathbf{A}_m^{-1}\mathbf{A}_p)\right]^{-1}\mathbf{x}_m^* \tag{C.9}$$

If the filter is designed such that it has unity steady-state gain, Equation C.9 simplifies to:

$$\mathbf{x}_\infty = \left[\mathbf{A}_m^{-1}\mathbf{A}_p\right]^{-1}\mathbf{x}_m^* \tag{C.10}$$

or:

$$\mathbf{x}_\infty = \mathbf{A}_p^{-1}\mathbf{A}_m\mathbf{x}_m^* \tag{C.11}$$

Since:

$$\mathbf{A}_m\mathbf{x}_m^* = \mathbf{b}_L \tag{C.12}$$

Equation C.11 can be rewritten:

$$\mathbf{x}_\infty = \mathbf{A}_p^{-1}\mathbf{b}_L \tag{C.13}$$

since $\mathbf{b}_L$ is the same for both the plant and model:

$$\mathbf{x}_p^* = \mathbf{A}_p^{-1}\mathbf{b}_L \tag{C.14}$$

and:

$$\mathbf{x}_{\infty} = \mathbf{x}_p^* \qquad \text{C.15}$$

More simply, for the linear constraint case, the Point-Wise Model Accurate system of Problem C.1 will converge to the plant optimum providing the filter is designed to ensure stability of the matrix product in Inequality C.8 and has unity steady-state gain. These results are not unexpected due to the similarity between the model-based optimization system of Figure 3.1 and a multivariable IMC controller [Garcia and Morari (1985)]; however, there are significant differences between these two technologies, since the system of Figure 3.1 contains a model-based optimization at its core, instead of the conventional set of controller equations found in the IMC design.

Appendix D: Numerical Derivative Data

This appendix contains the data used for finite difference approximation to the derivatives required for the Point-Wise Stability calculations and the approximation of the covariance matrix **Q** for the predicted optimimal manipulated variable values. Each section of this appendix presents, for a specific example, tables containing the parametric sensitivity of the model-based optimization problem ($dx^*_m/d\beta$), the sensitivity of the parameter estimation problem to the process measurements ($d\beta/dz$) and the process measurement derivatives (dz/dx). The tabular data of this appendix was used to perform the calculations for the examples in Chapters 4, 5 and 6.

The general approach to finite differencing used for producing the tabular data in this appendix included solving a given problem (optimization, parameter estimation or simulation) after perturbing a specific problem variable. The perturbations were selected to be small with respect to the magnitude of the problem variable which was perturbed, yet large with respect to the convergence tolerances of the specific problem which was to be solved. The linearity of the resulting finite difference approximations were tested by comparing the results of: both positive and negative perturbations, as well as a reduction of the perturbation size.

D.1 Williams-Otto Reactor (Chapter 4)

The following tables give the data used in the finite difference approximations to the sensitivities of the model-based optimization and parameter estimation problems, as well as plant derivatives, for the Williams-Otto reactor example of Section 4.3.2. The nomenclature used in the tables given in this section is:

F_B ≡ feed rate of Reactant B to the reactor (kg/s).

F_R ≡ effluent flow rate from the reactor (kg/s).

T_R ≡ reactor temperature (K).

X_i ≡ weight fraction of component "i" in the reactor effluent.

ϕ_i ≡ frequency factor in Arrhenius relationship for reaction "i" (s^{-1}).

ζ_i ≡ activation energy in Arrhenius relationship for reaction "i" (K).

The data in Table D.1 were produced by varying the adjustable parameters used in the model-based optimization problem by $\pm 0.1\%$ of their nominal values.

Table D.1: Williams-Otto Parametric Sensitivity of Optimization ($dx^*_m/d\beta$).

	ϕ_1	ϕ_2	ζ_1	ζ_2
F_B	4.026×10^{-6}	4.159×10^{-12}	-1.079×10^{-3}	-4.476×10^{-5}
T_R	1.329×10^{-6}	-6.695×10^{-10}	4.440×10^{-3}	4.056×10^{-3}

The data presented in Table D.2 were produced by perturbing the process measurements used in the parameter estimation problem by 0.3%, 0.15% and 0.5% of nominal values for flows, temperatures and compositions, respectively.

Table D.2: Williams-Otto Reactor Sensitivity of Parameter Estimation ($d\beta/dz$).

	ϕ_1	ϕ_2	ζ_1	ζ_2
F_B	7.3376×10^4	1.014×10^{10}	-273.9	-942.3
T_R	-1.5901×10^4	-2.416×10^9	59.34	224.3
X_a	-2.822×10^6	-3.596×10^{11}	1.053×10^4	3.340×10^4
X_b	-2.019×10^6	-1.968×10^{11}	7539	1.828×10^4
X_e	4.651×10^5	0	-1731	0
X_g	0	1.929×10^{10}	0	-1.792×10^4
X_p	1.233×10^5	-2.455×10^{10}	-460.3	2.280×10^4
F_R	-1.1059×10^4	-4.243×10^9	41.28	394.1

The data given in Table D.3 were developed by perturbing the independent manipulated variables of the plant simulation by 0.3% and 0.15% of the nominal values for the feed rate of Reactant B (F_B) and the reactor Temperature (T_R), respectively.

Table D.3: Williams-Otto Reactor Measurement Derivatives (dz/dx).

	F_B	T_R
F_B	1.000	0.000
T_R	0.000	1.000
X_a	-2.222×10^{-2}	-2.945×10^{-3}
X_b	8.222×10^{-2}	-5.051×10^{-3}
X_e	-2.684×10^{-2}	4.213×10^{-3}
X_g	-2.421×10^{-2}	4.005×10^{-3}
X_p	-5.348×10^{-3}	7.717×10^{-4}
F_R	1.000	0.000

D.2 Heat Exchanger Network (Chapter 4)

The following tables give the data used in the finite difference approximations to the sensitivities of the model-based optimization and parameter estimation problems, as well as plant derivatives, for the heat exchanger network example of Section 4.3.3.

The data in Table D.4 were produced by varying the adjustable parameters used in the model-based optimization problem by $\pm1.35\%$ and $\pm0.809\%$ of their nominal values for β_1 and β_2, respectively.

Table D.4: Heat Exchanger Parametric Sensitivity of Optimization ($dx^*_m/d\beta$).

	β_1	β_2
$r = F_2 / F_1$	1.5463×10^{-3}	-1.0825×10^{-3}

The data in Table D.5 were produced by varying the plant measurements used in the parameter estimation problem by ±0.333% of their nominal values.

Table D.5: Heat Exchanger Sensitivity of Parameter Estimation ($d\beta/dz$).

	$r = F_2 / F_1$	T_4	T_5	T_{11}	T_{21}
β_1	178.4408	3.3746	0	-1.7436	0
β_2	132.6660	0	3.6456	0	-2.1050

The data in Tale D.6 were produced by varying the fraction (r) of exchanger network total feed rate F_1 that is diverted to F_2 by ±0.333% of its nominal value, in the plant simulation.

Table D.6: Heat Exchanger Plant Measurement Derivatives (dz/dx).

	$r = F_2 / F_1$	T_4	T_5	T_{11}	T_{21}
$r = F_2 / F_1$	1.0000	-74.3830	42.7560	-67.3990	30.1430

D.3 Williams-Otto Reactor (Chapter 5)

The following tables give the data used in the finite difference approximations to the sensitivities of the model-based optimization and parameter estimation problems, as well as plant derivatives, for the Williams-Otto reactor example of Section 5.3.1. The nomenclature used in the tables given in this section is:

F_B ≡ feed rate of Reactant B to the reactor (kg/s).

F_R ≡ effluent flow rate from the reactor (kg/s).

T_R ≡ reactor temperature (K).

X_i ≡ weight fraction of component "i" in the reactor effluent.

ϕ_i ≡ frequency factor in Arrhenius relationship for reaction "i" (s^{-1}).

ζ_i ≡ activation energy in Arrhenius relationship for reaction "i" (K).

The data in Table D.7 were produced by varying the adjustable parameters used in the model-based optimization problem by ±0.1% of their nominal values. The data presented in Table D.8 were produced by perturbing the process measurements used in the parameter estimation problem by 0.3%, 0.15% and 0.5% of nominal values for flows, temperatures and compositions, respectively.

Table D.7: Williams-Otto Parametric Sensitivity of Optimization ($dx^*_m/d\beta$).

	Frequency Factors Adjustable		Activation Energies Adjustable	
	ϕ_1	ϕ_2	ζ_1	ζ_2
F_B	7.309×10^{-9}	2.940×10^{-16}	-9.867×10^{-4}	-3.953×10^{-5}
T_R	3.405×10^{-9}	-3.935×10^{-13}	4.112×10^{-3}	3.287×10^{-3}

Table D.8: Williams-Otto Reactor Sensitivity of Parameter Estimation ($d\beta/dz$).

	Frequency Factors Adjustable		Activation Energies Adjustable	
	ϕ_1	ϕ_2	ζ_1	ζ_2
F_B	3.641×10^{7}	1.218×10^{13}	-269.9	-897.6
T_R	-1.124×10^{7}	-4.060×10^{12}	69.50	249.5
X_a	-1.793×10^{9}	-5.567×10^{14}	1.329×10^{4}	4.102×10^{4}
X_b	-1.051×10^{9}	-2.513×10^{14}	7787	1.852×10^{4}
X_e	2.423×10^{8}	0	-1796	0
X_g	0	2.432×10^{14}	0	-1.792×10^{4}
X_p	5.900×10^{7}	-3.309×10^{14}	-437.0	2.438×10^{4}
F_R	-5.414×10^{6}	-4.785×10^{12}	40.13	352.6

The data given in Table D.9 were developed by perturbing the independent manipulated variables of the plant simulation by 0.3% and 0.15% of the nominal values for the feed rate of Reactant B (F_B) and the reactor Temperature (T_R), respectively.

Table D.9: Williams-Otto Reactor Measurement Derivatives (dz/dx).

	F_B	T_R
F_B	1.000	0.000
T_R	0.000	1.000
X_a	-1.784×10^{-2}	-2.697×10^{-3}
X_b	7.802×10^{-2}	-4.486×10^{-3}
X_e	-2.670×10^{-2}	3.578×10^{-3}
X_g	-2.609×10^{-2}	3.985×10^{-3}
X_p	-4.654×10^{-3}	4.607×10^{-4}
F_R	1.000	0.000

D.4 Williams-Otto Plant (Chapter 6)

The following tables give the data used in the finite difference approximations to the sensitivities of the model-based optimization and parameter estimation problems, as well as plant derivatives, for the Williams-Otto plant case study of Chapter 6. The nomenclature used in the tables given in this section is:

F_B ≡ feed rate of Reactant B to the reactor (kg/s).

F_{DW} ≡ flowrate of cooling water through the condenser (kg/s).

F_G ≡ flowrate of by-product stream G from the decanter (kg/s).

F_L ≡ flowrate of recycle stream L to the reactor (kg/s).

F_P ≡ flowrate of product stream P from the column (kg/s).

F_{RS} ≡ flowrate of steam through the reactor heating coils (kg/s).

F_{XW} ≡ flowrate of cooling water through the reaction cooler (kg/s).

N ≡ number of ideal trays in the distillation column.

$T_{IN,DS}$ ≡ inlet hot water temperature to reboiler (K).

$T_{OUT,DS}$ ≡ outlet hot water temperature from reboiler (K).

$T_{OUT,DW}$ ≡ outlet cooling water temperature from condenser (K).

$T_{OUT,XW}$ ≡ outlet cooling water temperature from reaction cooler (K).

T_R ≡ reactor temperature (K).

U_{cond} ≡ heat transfer coefficient of the condenser (J/m^2Ks).

U_{cool} ≡ heat transfer coefficient of the reaction cooler (J/m^2Ks).

U_{rbl} ≡ heat transfer coefficient of the reboiler (J/m^2Ks).

$X_{J,i}$ ≡ weight fraction of component "i" in Stream "J".

α ≡ relative volatility of the mixture in the distillation column..

ϕ_i ≡ frequency factor in Arrhenius relationship for reaction "i" (s^{-1}).

ζ_i ≡ activation energy in Arrhenius relationship for reaction "i" (K).

The data in Tables D.10 through D.18 were produced by varying the adjustable parameters used in the model-based optimization problem by ±0.1% of their nominal values. The data presented in Tables D.19 through D.27 were produced by perturbing the process measurements used in the parameter estimation problem by 0.3%, 0.15% and 0.5% of nominal values for flows, temperatures and compositions, respectively. The data given in Tables D.28 through D.36 were generated by perturbing the independent manipulated variables of the plant simulation by 0.3%, 0.3%, and 0.15 % of the nominal values for the feed rate of Reactant B (F_B), the flowrate of the recycle stream (FL) and the reacor temperature (T_R), respectively.

Table D.10: Williams-Otto Plant Optimization Parametric Sensitivity ($dx^*_m/d\beta$) for Model1 at F_A = 1.563 kg/s Disturbance Level.

	F_B	F_L	T_R
ϕ_1	-1.507×10^{-8}	-8.320×10^{-8}	-1.042×10^{-7}
ϕ_2	1.309×10^{-11}	8.213×10^{-11}	-5.293×10^{-11}
α	-0.3771	4.6624	-2.0206
U_{cond}	-4.483×10^{-5}	6.718×10^{-4}	-3.033×10^{-4}
U_{rbl}	-9.152×10^{-7}	-2.628×10^{-5}	-6.533×10^{-6}
U_{cool}	-1.522×10^{-2}	0.3433	5.371×10^{-2}

Table D.11: Williams-Otto Plant Optimization Parametric Sensitivity ($dx^*_m/d\beta$) for Model1 at F_A = 1.827 kg/s Disturbance Level.

	F_B	F_L	T_R
ϕ_1	-1.651×10^{-8}	2.624×10^{-8}	-8.370×10^{-8}
ϕ_2	1.264×10^{-11}	2.616×10^{-11}	-5.374×10^{-11}
α	-0.3127	$-9.671\times10\text{-}2$	-2.413
U_{cond}	-1.443×10^{-5}	-2.885×10^{-6}	-1.859×10^{-4}
U_{rbl}	-1.153×10^{-7}	2.057×10^{-8}	-3.461×10^{-6}
U_{cool}	-3.1057×10^{-4}	-1.744×10^{-3}	7.266×10^{-2}

Table D.12: Williams-Otto Plant Optimization Parametric Sensitivity ($dx^*_m/d\beta$) for Model1 at F_A = 2.092 kg/s Disturbance Level.

	F_B	F_L	T_R
ϕ_1	-1.391×10^{-8}	1.953×10^{-8}	-6.447×10^{-8}
ϕ_2	1.055×10^{-11}	3.263×10^{-11}	-5.725×10^{-11}
α	-0.2873	-0.2997	-1.977
U_{cond}	-1.443×10^{-5}	-1.376×10^{-5}	-1.761×10^{-4}
U_{rbl}	9.940×10^{-7}	1.102×10^{-6}	2.753×10^{-6}
U_{cool}	-3.106×10^{-4}	-1.672×10^{-3}	8.003×10^{-2}

Table D.13: Williams-Otto Plant Optimization Parametric Sensitivity ($dx^*_m/d\beta$) for Model2 at F_A = 1.563 kg/s Disturbance Level.

	F_B	F_L	T_R
ζ_1	1.165×10^{-2}	6.579×10^{-3}	1.229×10^{-3}
ζ_2	-5.586×10^{-4}	-3.379×10^{-3}	2.800×10^{-3}
α	-0.4181	4.8738	-2.222
U_{cond}	-4.883×10^{-5}	7.105×10^{-4}	-3.326×10^{-4}
U_{rbl}	-2.870×10^{-8}	-5.904×10^{-8}	1.710×10^{-6}
U_{cool}	-1.462×10^{-2}	0.3246	5.687×10^{-2}

Table D.14: Williams-Otto Plant Optimization Parametric Sensitivity ($dx^*_m/d\beta$) for Model2 at F_A = 1.827 kg/s Disturbance Level.

	F_B	F_L	T_R
ζ_1	1.574×10^{-3}	-2.783×10^{-3}	1.081×10^{-2}
ζ_2	-6.199×10^{-4}	-1.332×10^{-3}	1.074×10^{-3}
α	-0.3447	5.682×10^{-2}	-2.809
U_{cond}	-1.798×10^{-5}	1.332×10^{-6}	-2.544×10^{-4}
U_{rbl}	2.389×10^{-6}	2.389×10^{-6}	-4.879×10^{-5}
U_{cool}	-1.672×10^{-4}	-2.962×10^{-3}	7.372×10^{-2}

Table D.15: Williams-Otto Plant Optimization Parametric Sensitivity ($dx^*_m/d\beta$) for Model2 at F_A = 2.092 kg/s Disturbance Level.

	F_B	F_L	T_R
ζ_1	1.452×10^{-3}	-2.368×10^{-3}	9.321×10^{-3}
ζ_2	-5.828×10^{-4}	-1.882×10^{-3}	1.789×10^{-3}
α	-0.3641	-0.3086	-2.6583
U_{cond}	-1.820×10^{-5}	-1.176×10^{-5}	-2.250×10^{-4}
U_{rbl}	2.389×10^{-6}	4.778×10^{-6}	-1.121×10^{-5}
U_{cool}	-7.167×10^{-5}	-3.297×10^{-3}	7.898×10^{-2}

Table D.16: Williams-Otto Plant Optimization Parametric Sensitivity ($dx^*_m/d\beta$) for Model3 at F_A = 1.563 kg/s Disturbance Level.

	F_B	F_L	T_R
ϕ_1	-1.833×10^{-8}	-1.024×10^{-7}	-1.282×10^{-7}
ϕ_2	1.406×10^{-11}	9.074×10^{-11}	-6.009×10^{-11}
ζ_1	1.215×10^{-3}	6.624×10^{-3}	1.155×10^{-2}
ζ_2	-5.513×10^{-4}	-3.458×10^{-3}	3.840×10^{-4}
α	-0.3051	4.035	-1.644
N	-1.332×10^{-2}	0.1240	-7.761×10^{-2}

Table D.17: Williams-Otto Plant Optimization Parametric Sensitivity ($dx^*_m/d\beta$) for Model3 at F_A = 1.827 kg/s Disturbance Level.

	F_B	F_L	T_R
ϕ_1	-2.254×10^{-8}	3.746×10^{-8}	-1.175×10^{-7}
ϕ_2	1.399×10^{-11}	6.083×10^{-11}	-6.857×10^{-11}
ζ_1	1.260×10^{-3}	4.029×10^{-3}	1.073×10^{-2}
ζ_2	-6.268×10^{-4}	-1.336×10^{-3}	1.059×10^{-3}
α	-0.2000	3.239×10^{-2}	-1.806
N	-1.497×10^{-2}	4.092×10^{-2}	-9.850×10^{-2}

Table D.18: Williams-Otto Plant Optimization Parametric Sensitivity ($dx^*_m/d\beta$) for Model3 at F_A = 2.092 kg/s Disturbance Level.

	F_B	F_L	T_R
ϕ_1	-2.027×10^{-8}	3.088×10^{-8}	-9.690×10^{-8}
ϕ_2	1.371×10^{-11}	4.524×10^{-11}	-7.980×10^{-11}
ζ_1	1.423×10^{-3}	-2.336×10^{-3}	9.314×10^{-3}
ζ_2	-5.855×10^{-4}	-1.905×10^{-4}	1.794×10^{-4}
α	-0.2363	1.2017	-1.833
N	-1.468×10^{-2}	-1.324×10^{-2}	-9.750×10^{-2}

Table D.19: Williams-Otto Plant Parameter Estimation Sensitivity (dβ/dz) for Model1 at F_A = 1.563 kg/s Disturbance Level.

	ϕ_1	ϕ_2	α	U_{cond}	U_{rbl}	U_{cool}
F_B	1.912×10^{7}	4.153×10^{9}	-1.784×10^{-2}	0	0	6.072×10^{-2}
F_G	5.393×10^{6}	2.459×10^{11}	4.491×10^{-2}	0	0	3.110×10^{-2}
F_L	-1.104×10^{6}	3.078×10^{9}	2.213×10^{-2}	0	0	5.954×10^{-2}
F_P	-2.058×10^{7}	5.458×10^{10}	-0.2283	0	0	-5.776×10^{-3}
F_{DW}	-2.057×10^{5}	5.457×10^{8}	-4.708×10^{-3}	0.1658	1.552×10^{-2}	-5.776×10^{-5}
F_{RS}	-8.959×10^{6}	-2.424×10^{10}	-1.505×10^{-2}	0	0	2.093×10^{-4}
F_{XW}	-2.053×10^{5}	5.392×10^{8}	-2.291×10^{-2}	0	0	-1.456×10^{-2}
T_R	-6.010×10^{6}	-6.254×10^{9}	-6.108×10^{-4}	0	0	2.320×10-3
$T_{IN,DS}$	-4.667×10^{4}	1.238×10^{8}	-9.453×10^{-3}	3.9761	0.1528	-1.310×10^{-5}
$T_{OUT,DS}$	-4.669×10^{4}	1.238×10^{8}	8.625×10^{-3}	-3.9761	-0.4176	-1.310×10^{-5}
$T_{OUT,DW}$	4.667×10^{4}	1.238×10^{8}	-1.364×10^{-2}	89.09	8.532×10^{-2}	-1.310×10^{-5}
$T_{OUT,XW}$	-4.561×10^{4}	1.075×10^{8}	-5.382×10^{-4}	0	0	0.1120
$X_{D,a}$	7.747×10^{7}	3.673×10^{11}	-3.211	124.96	-1.507	2.084×10^{-2}
$X_{D,b}$	1.215×10^{8}	4.424×10^{11}	-1.312	124.96	-1.507	8.668×10^{-2}
$X_{D,c}$	-4.048×10^{8}	5.799×10^{11}	18.79	62.50	-0.7533	8.072×10^{-2}
$X_{D,p}$	2.072×10^{8}	-4.124×10^{11}	-95.65	124.96	-1.507	9.981×10^{-2}
$X_{P,a}$	-1.526×10^{10}	-1.809×10^{13}	56.46	-99.67	-1.200	-1.200
$X_{P,b}$	-1.264×10^{10}	-1.190×10^{13}	17.73	-99.67	-1.200	-2.975
$X_{P,c}$	9.786×10^{9}	-1.133×10^{13}	-18.38	-49.82	0.6002	-2.759

Table D.20: Williams-Otto Plant Parameter Estimation Sensitivity (dβ/dz) for Modell at F_A = 1.827 kg/s Disturbance Level.

	ϕ_1	ϕ_2	α	U_{cond}	U_{rbl}	U_{cool}
F_B	2.301×10^{7}	-2.007×10^{9}	2.989×10^{-3}	-1.028×10^{-5}	0	6.316×10^{-2}
F_G	9.564×10^{6}	2.631×10^{11}	6.432×10^{-2}	-1.079×10^{-5}	0	3.252×10^{-3}
F_L	-1.138×10^{6}	2.793×10^{9}	2.425×10^{2}	-4.505×10^{-6}	0	6.151×10^{-2}
F_P	2.304×10^{7}	-6.233×10^{10}	2.220×10^{-1}	-1.351×10^{-3}	-1.723×10^{-5}	5.734×10^{-3}
F_{DW}	-3.666×10^{1}	9.732×10^{4}	-2.223×10^{-3}	1.658×10^{-1}	1.504×10^{-2}	0
F_{RS}	-7.043×10^{6}	-3.202×10^{10}	7.417×10^{-3}	-1.351×10^{-4}	-1.835×10^{-6}	9.250×10^{-4}
F_{XW}	3.432×10^{2}	-6.826×10^{6}	-6.268×10^{-6}	-9.011×10^{-6}	0	-1.612×10^{-2}
T_R	-6.747×10^{6}	-7.279×10^{9}	-8.535×10^{-5}	0	0	3.183×10^{-3}
$T_{IN,DS}$	-6.093×10^{-2}	2.143×10^{2}	-8.215×10^{-3}	3.858	1.481×10^{-1}	0
$T_{OUT,DS}$	-2.041	5.359×10^{3}	8.401×10^{-3}	-3.858	-4.052×10^{-1}	0
$T_{OUT,DW}$	-6.093×10^{-2}	2.143×10^{2}	-1.251×10^{-2}	8.864×10^{1}	8.602×10^{-2}	0
$T_{OUT,XW}$	7.799×10^{2}	-1.541×10^{7}	-1.434×10^{-5}	1.226×10^{-5}	1.899×10^{-7}	1.130×10^{-1}
$X_{D,a}$	8.497×10^{7}	3.580×10^{11}	-2.290	1.251×10^{2}	-1.501	3.750×10^{-2}
$X_{D,b}$	1.489×10^{8}	3.854×10^{11}	-1.087	1.251×10^{2}	-1.501	8.571×10^{-2}
$X_{D,e}$	-3.894×10^{8}	5.468×10^{11}	2.158×10^{1}	6.256×10^{1}	-7.502×10^{-1}	8.678×10^{-2}
$X_{D,p}$	2.651×10^{8}	-5.613×10^{11}	-1.009×10^{2}	1.853×10^{4}	-1.501	1.026×10^{-1}
$X_{P,a}$	-1.305×10^{10}	-1.829×10^{13}	4.346×10^{1}	-1.005×10^{2}	1.203	-1.507
$X_{P,b}$	-1.457×10^{10}	-1.332×10^{13}	1.944×10^{1}	-1.004×10^{2}	1.203	-2.897
$X_{P,e}$	1.049×10^{10}	-1.260×10^{13}	-1.678×10^{1}	-5.023×10^{1}	6.019×10^{-1}	-2.842

Table D.21: Williams-Otto Plant Parameter Estimtaion Sensitivity (dβ/dz) for Model1 at F_A = 2.092 kg/s Disturbance Level.

	ϕ_1	ϕ_2	α	U_{cond}	U_{rbl}	U_{cool}
F_B	-2.532×10^{7}	2.831×10^{9}	-8.965×10^{-4}	-9.011×10^{-5}	-1.416×10^{-6}	5.921×10^{-2}
F_G	9.722×10^{6}	2.944×10^{11}	6.373×10^{-2}	-9.011×10^{-5}	-1.442×10^{-6}	2.431×10^{-3}
F_L	-1.047×10^{6}	2.839×10^{9}	2.367×10^{-2}	6.307×10^{-5}	0	5.813×10^{-2}
F_P	-2.505×10^{7}	6.995×10^{10}	2.248×10^{-1}	-2.703×10^{-3}	-3.712×10^{-5}	4.897×10^{-3}
F_{DW}	-5.505	9.449×10^{3}	-2.308×10^{-3}	1.690×10^{-1}	1.500×10^{-2}	0
F_{RS}	-8.257×10^{6}	3.611×10^{10}	8.722×10^{-3}	-9.011×10^{-5}	-1.005×10^{-6}	9.041×10^{-4}
F_{XW}	-2.332×10^{2}	6.697×10^{6}	-5.554×10^{-6}	0	0	-1.582×10^{-2}
T_R	-7.520×10^{6}	8.134×10^{9}	-1.076×10^{-4}	3.066×10^{-6}	0	4.028×10^{-3}
$T_{IN,DS}$	-9.048	4.758×10^{4}	-8.543×10^{-3}	3.819	1.479×10^{-1}	0
$T_{OUT,DS}$	-3.655×10^{1}	3.001×10^{3}	8.734×10^{-3}	-3.819	-4.051×10^{-1}	0
$T_{OUT,DW}$	-1.888	5.359×10^{3}	-1.312×10^{-2}	8.744×10^{1}	8.670×10^{-2}	0
$T_{OUT,XW}$	-5.540×10^{2}	1.585×10^{7}	-1.326×10^{-5}	-9.199×10^{-6}	0	1.168×10^{-1}
$X_{D,a}$	8.132×10^{7}	4.627×10^{11}	-2.151	1.241×10^{2}	-1.494	4.695×10^{-2}
$X_{D,b}$	1.891×10^{8}	4.257×10^{11}	-1.394	1.242×10^{2}	-1.494	7.670×10^{-2}
$X_{D,e}$	-4.488×10^{8}	6.321×10^{11}	2.007×10^{1}	6.211×10^{1}	-7.469×10^{-1}	8.388×10^{-2}
$X_{D,p}$	-3.040×10^{8}	6.903×10^{11}	-9.850×10^{1}	1.242×10^{2}	-1.494	9.395×10^{-2}
$X_{P,a}$	-1.191×10^{10}	1.967×10^{13}	3.938×10^{1}	-1.004×10^{2}	1.206	-1.778
$X_{P,b}$	-1.760×10^{10}	1.520×10^{13}	2.531×10^{1}	-1.004×10^{2}	1.206	-2.604
$X_{P,e}$	-1.207×10^{10}	1.450×10^{13}	-1.713×10^{1}	-5.020×10^{1}	6.035×10^{-1}	-2.735

Table D.22: Williams-Otto Plant Parameter Estimation Sensitivity (dβ/dz) for Model2 at F_A = 1.563 kg/s Disturbance Level.

	ζ_1	ζ_2	α	U_{cond}	U_{rbl}	U_{cool}
F_B	-2.308×10^{2}	9.600×10^{1}	-1.745×10^{-2}	6.307×10^{-4}	8.371×10^{-6}	6.129×10^{-2}
F_G	-6.858×10^{1}	5.558×10^{3}	4.486×10^{-2}	7.208×10^{-4}	8.371×10^{-6}	3.177×10^{-3}
F_L	-1.368×10^{1}	7.079×10^{1}	2.218×10^{-2}	-4.505×10^{-6}	0	6.006×10^{-2}
F_P	-2.522×10^{2}	1.253×10^{3}	-2.276×10^{-1}	7.659×10^{-3}	1.255×10^{-4}	-5.818×10^{-3}
F_{DW}	-2.522	1.253×10^{1}	-4.669×10^{-3}	1.660×10^{-1}	1.549×10^{-2}	-5.818×10^{-5}
F_{RS}	1.083×10^{2}	5.590×10^{2}	-1.498×10^{-2}	7.659×10^{-4}	1.255×10^{-5}	2.427×10^{-4}
F_{XW}	-2.518	1.238×101	-2.283×10^{-3}	9.011×10^{-5}	1.255×10^{-6}	-1.479×10^{-2}
T_R	7.259×10^{1}	1.437×10^{2}	-6.080×10^{-4}	4.088×10^{-6}	0	2.369×10^{-3}
$T_{IN,DS}$	-5.724×10^{-1}	2.844	-9.340×10^{-3}	3.967	1.522×10^{-1}	-1.319×10^{-5}
$T_{OUT,DS}$	-5.723×10^{-1}	2.843	8.512×10^{-3}	-3.967	-4.162×10^{-1}	-1.319×10^{-5}
$T_{OUT,DW}$	-5.723×10^{-1}	2.843	-1.352×10^{-2}	8.911×10^{1}	8.561×10^{-2}	-1.319×10^{-5}
$T_{OUT,XW}$	-5.605×10^{-1}	2.472	-5.360×10^{-4}	1.226×10^{-5}	0	1.117×10^{-1}
$X_{D,a}$	-9.180×10^{2}	8.416×10^{3}	-3.149	1.247×10^{2}	-1.509	2.046×10^{-2}
$X_{D,b}$	-1.423×10^{3}	1.013×10^{4}	-1.270	1.247×10^{2}	-1.509	8.683×10^{-2}
$X_{D,e}$	-4.890×10^{3}	1.314×10^{4}	1.916×10^{1}	6.240×10^{1}	-7.541×10^{-1}	8.082×10^{-2}
$X_{D,p}$	-2.534×10^{3}	9.317×10^{3}	-9.651×10^{1}	1.247×10^{2}	-1.509	1.003×10^{-1}
$X_{P,a}$	2.009×10^{5}	4.658×10^{5}	5.533×10^{1}	-9.970×10^{1}	1.203	-1.196
$X_{P,b}$	1.627×10^{5}	2.941×10^{5}	1.697×10^{1}	-9.969×10^{1}	1.203	-3.002
$X_{P,e}$	-1.130×10^{5}	2.783×10^{5}	-1.795×10^{1}	-4.983×10^{1}	6.022×10^{-1}	-2.783

Table D.23: Williams-Otto Plant Parameter Estimation Sensitivity (dβ/dz) for Model2 at F_A = 1.827 kg/s Disturbance Level.

	ζ_1	ζ_2	α	U_{cond}	U_{rbl}	U_{cool}
F_B	-2.439×10^{2}	3.874×10^{1}	3.099×10^{-3}	-3.153×10^{-4}	-4.185×10^{-6}	6.291×10^{-2}
F_G	-1.012×10^{2}	5.082×10^{3}	6.440×10^{-2}	-3.153×10^{-3}	-4.604×10^{-5}	3.218×10^{-3}
F_L	-1.183×10^{1}	5.401×10^{1}	2.422×10^{-2}	-1.351×10^{-5}	0	6.126×10^{-2}
F_P	-2.455×10^{2}	1.215×10^{3}	2.224×10^{-1}	-1.802×10^{-3}	-2.651×10^{-5}	5.650×10^{-3}
F_{DW}	-4.408×10^{-5}	8.816×10^{-5}	-2.231×10^{-3}	1.662×10^{-1}	1.506×10^{-2}	0
F_{RS}	7.560×10^{1}	6.328×10^{2}	7.600×10^{-3}	-1.802×10^{-4}	-2.754×10^{-6}	9.334×10^{-4}
F_{XW}	-2.027×10^{-3}	1.132×10^{-1}	-6.982×10^{-6}	1.072×10^{-3}	1.548×10^{-5}	-1.613×10^{-2}
T_R	7.007×10^{1}	1.396×10^{2}	-8.796×10^{-5}	-4.088×10^{-6}	0	3.273×10^{-3}
$T_{IN,DS}$	-3.407×10^{-6}	3.000×10^{-5}	-8.247×10^{-3}	3.857	1.481×10^{-1}	0
$T_{OUT,DS}$	-1.000×10^{-5}	3.000×10^{-5}	8.433×10^{-3}	-3.857	-4.054×10^{-1}	0
$T_{OUT,DW}$	0	5.900×10^{-4}	-1.256×10^{-2}	1.064×10^{2}	8.622×10^{-2}	0
$T_{OUT,XW}$	-7.790×10^{-3}	2.998×10^{-1}	-1.465×10^{-5}	0	0	1.134×10^{-1}
$X_{D,a}$	-9.086×10^{2}	7.062×10^{3}	-2.304	1.248×10^{2}	-1.502	3.745×10^{-2}
$X_{D,b}$	-1.593×10^{3}	7.583×10^{3}	-1.083	1.248×10^{2}	-1.501	8.636×10^{-2}
$X_{D,c}$	-4.175×10^{3}	1.066×10^{4}	2.144×10^{1}	6.243×10^{1}	-7.506×10^{-1}	8.678×10^{-2}
$X_{D,p}$	-2.829×10^{3}	1.092×10^{4}	-1.007×10^{2}	1.248×10^{2}	-1.501	1.022×10^{-1}
$X_{P,a}$	1.472×10^{5}	3.970×10^{5}	4.370×10^{1}	-1.004×10^{2}	1.205	-1.505
$X_{P,b}$	1.660×10^{5}	2.812×10^{5}	1.936×10^{1}	-1.004×10^{2}	1.205	-2.888
$X_{P,c}$	-1.071×10^{5}	2.653×10^{5}	-1.675×10^{1}	-5.020×10^{1}	6.031×10^{-1}	-2.838

Table D.24: Williams-Otto Plant Parameter Estimation Sensitivity (dβ/dz) for Model2 at F_A = 2.092 kg/s Disturbance Level.

	ζ_1	ζ_2	α	U_{cond}	U_{rbl}	U_{cool}
F_B	-2.379×10^{2}	4.724×10^{1}	-6.363×10^{-4}	-1.351×10^{-4}	-1.744×10^{-6}	5.889×10^{-2}
F_G	-9.129×10^{1}	4.945×10^{3}	6.363×10^{-2}	-2.252×10^{-4}	-3.184×10^{-6}	2.411×10^{-3}
F_L	-9.673	4.786×10^{1}	2.363×10^{-2}	-9.011×10^{-6}	0	5.781×10^{-2}
F_P	-2.366×10^{2}	1.187×10^{3}	2.248×10^{-1}	-1.802×10^{-3}	-2.870×10^{-5}	4.813×10^{-3}
F_{DW}	-1.763×10^{-4}	8.375×10^{-4}	-2.323×10^{-3}	1.698×10^{-1}	1.504×10^{-2}	0
F_{RS}	7.867×10^{1}	6.204×10^{2}	8.908×10^{-3}	-1.802×10^{-4}	-2.592×10^{-6}	9.083×10^{-4}
F_{XW}	-1.763×10^{-3}	1.119×10^{-1}	-4.919×10^{-6}	-9.011×10^{-6}	0	-1.575×10^{-2}
T_R	6.845×10^{1}	1.340×10^{2}	-1.105×10^{-4}	-3.066×10^{-6}	0	4.084×10^{-3}
$T_{IN,DS}$	0	9.693×10^{-6}	-8.595×10^{-3}	3.830	1.480×10^{-1}	0
$T_{OUT,DS}$	-2.000×10^{-5}	1.100×10^{-4}	8.788×10^{-3}	-3.830	-4.055×10^{-1}	0
$T_{OUT,DW}$	-1.000×10^{-4}	5.000×10^{-4}	-1.318×10^{-2}	1.131×10^{2}	8.678×10^{-2}	0
$T_{OUT,XW}$	-4.670×10^{-3}	2.699×10^{-1}	-1.305×10^{-5}	-4.088×10^{-6}	0	1.171×10^{-1}
$X_{D,a}$	-7.773×10^{2}	7.905×10^{3}	-2.175	1.243×10^{2}	-1.495	4.653×10^{-2}
$X_{D,b}$	-1.793×10^{3}	7.305×10^{3}	-1.389	1.243×10^{2}	-1.495	7.665×10^{-2}
$X_{D,e}$	-4.273×10^{3}	1.074×10^{4}	1.980×10^{1}	6.216×10^{1}	-7.474×10^{-1}	8.377×10^{-2}
$X_{D,p}$	-2.881×10^{3}	1.173×10^{4}	-9.794×10^{1}	1.243×10^{2}	-1.495	9.358×10^{-2}
$X_{P,a}$	1.189×10^{5}	3.721×10^{5}	3.983×10^{1}	-1.006×10^{2}	1.208	-1.766
$X_{P,b}$	1.792×10^{5}	2.803×10^{5}	2.519×10^{1}	-1.006×10^{2}	1.208	-2.599
$X_{P,e}$	-1.092×10^{5}	2.667×10^{5}	-1.709×10^{1}	-5.030×10^{1}	6.045×10^{-1}	-2.728

Table D.25: Williams-Otto Plant Parameter Estimation Sensitivity (dβ/dz) for Model3 at F_A = 1.563 kg/s Disturbance Level.

	ϕ_1	ϕ_2	ζ_1	ζ_2	α	N
F_B	-3.048×10^4	6.761×10^{11}	-2.322×10^2	-1.928×10^4	7.916×10^1	-4.191
F_G	-1.477×10^5	8.588×10^{11}	-6.000×10^1	-3.042×10^4	-2.880×10^1	1.704
F_L	-2.712×10^5	4.253×10^{10}	1.976×10^3	2.559×10^3	2.745×10^1	5.452
F_P	-1.779×10^5	2.049×10^{13}	2.471×10^2	-6.804×10^5	3.953×10^2	-2.173×10^1
F_{DW}	-4.294×10^3	6.691×10^{10}	2.561	-1.910×10^3	1.203	-7.217×10^{-2}
F_{RS}	-3.857×10^5	1.234×10^{12}	1.056×10^2	-3.654×10^4	3.144	-1.952×10^{-1}
F_{XW}	1.237×10^3	5.563×10^{10}	2.511	1.400×10^3	7.641	-4.061×10^{-1}
T_R	-1.077×10^4	2.696×10^{10}	7.217×10^1	-6.733×10^2	4.991×10^{-1}	-2.823×10^{-2}
$T_{IN,DS}$	-1.497×10^3	4.635×10^{10}	5.889×10^{-1}	-1.538×10^3	-2.089×10^{-1}	7.913×10^{-3}
$T_{OUT,DS}$	-6.145×10^3	1.199×10^{10}	4.754×10^{-1}	-3.383×10^2	-1.113×10^{-1}	-1.608×10^{-3}
$T_{OUT,DW}$	-5.638×10^2	4.686×10^{10}	5.751×10^{-1}	-1.559×10^3	1.657	-3.984×10^{-2}
$T_{OUT,XW}$	-7.335×10^2	2.668×10^{10}	5.795×10^{-1}	-8.005×10^2	1.883	-9.957×10^{-2}
$X_{D,a}$	-1.895×10^3	3.000×10^{12}	-9.727×10^2	-9.025×10^4	2.360×10^2	-1.728×10^1
$X_{D,b}$	-8.764×10^5	1.279×10^{13}	-1.533×10^3	-3.860×10^5	4.261×10^2	-2.493×10^1
$X_{D,c}$	-3.436×10^5	3.336×10^{12}	5.026×10^3	-1.044×10^5	3.881×10^2	2.471
$X_{D,p}$	-1.831×10^6	2.829×10^{12}	-2.510×10^3	-6.748×10^4	-4.985×10^3	2.117×10^2
$X_{P,a}$	-2.590×10^7	7.051×10^{12}	1.984×10^5	2.650×10^5	8.719×10^2	2.842×10^1
$X_{P,b}$	-2.186×10^7	3.094×10^{12}	1.654×10^5	3.765×10^5	1.015×10^3	-2.964×10^1
$X_{P,c}$	1.593×10^7	6.483×10^{12}	-1.148×10^5	4.470×10^5	7.916×10^2	-6.589×10^1

Table D.26: Williams-Otto Plant Parameter Estimation Sensitivity $(d\beta/dz)$ for Model3 at F_A = 1.827 kg/s Disturbance Level.

	ϕ_1	ϕ_2	ζ_1	ζ_2	α	N
F_B	-3.759×10^{5}	7.902×10^{11}	-2.146×10^{2}	-1.623×10^{4}	5.830×10^{1}	-3.051
F_G	-2.912×10^{5}	1.547×10^{12}	-7.275×10^{1}	-3.879×10^{4}	4.163	-1.703×10^{-1}
F_L	-4.076×10^{4}	2.698×10^{11}	1.488×10^{1}	-6.563×10^{3}	-1.309	1.004×10^{-1}
F_P	-2.285×10^{6}	1.306×10^{13}	2.789×10^{2}	-2.790×10^{5}	2.380×10^{2}	-1.296×10^{1}
F_{DW}	-3.917×10^{4}	2.681×10^{11}	3.023	-6.457×10^{3}	-1.171	5.875×10^{-2}
F_{RS}	-2.171×10^{5}	1.296×10^{12}	1.033×10^{2}	-2.704×10^{4}	1.756×10^{1}	-9.588×10^{-1}
F_{XW}	-1.947×10^{4}	1.047×10^{11}	2.737	-2.194×10^{3}	4.374	-2.323×10^{-1}
T_R	-2.733×10^{3}	4.614×10^{10}	7.051×10^{1}	-9.109×10^{2}	-2.401×10^{-1}	1.232×10^{-2}
$T_{IN,DS}$	-7.434×10^{2}	3.899×10^{10}	5.689×10^{-1}	-8.610×10^{2}	1.239×10^{-1}	-1.021×10^{-2}
$T_{OUT,DS}$	-6.001×10^{3}	3.303×10^{10}	4.719×10^{-1}	5.795×10^{2}	9.872×10^{-1}	-5.881×10^{-2}
$T_{OUT,DW}$	-4.745×10^{3}	2.674×10^{10}	6.264×10^{-1}	-5.660×10^{2}	4.995×10^{-1}	1.828×10^{-2}
$T_{OUT,XW}$	-2.764×10^{3}	5.122×10^{10}	5.992×10^{-1}	-1.185×10^{3}	2.776×10^{-1}	-1.557×10^{-2}
$X_{D,a}$	-2.875×10^{6}	1.499×10^{13}	-5.488×10^{2}	-3.246×10^{5}	1.464×10^{2}	-1.121×10^{1}
$X_{D,b}$	-1.518×10^{6}	1.276×10^{13}	-1.261×10^{3}	-2.744×10^{5}	1.546×10^{2}	-1.008×10^{1}
$X_{D,e}$	-4.040×10^{6}	3.318×10^{13}	4.537×10^{3}	-8.061×10^{5}	5.131×10^{2}	-1.023×10^{-1}
$X_{D,p}$	-2.878×10^{6}	1.419×10^{13}	-2.474×10^{3}	-2.882×10^{5}	6.698×10^{2}	-1.606×10^{2}
$X_{P,a}$	-1.841×10^{7}	4.191×10^{13}	1.458×10^{5}	-6.836×10^{5}	1.809×10^{2}	4.668×101
$X_{P,b}$	-1.969×10^{7}	1.382×10^{13}	1.661×10^{5}	-9.438×10^{3}	7.956×10^{1}	2.107×10^{1}
$X_{P,e}$	-1.760×10^{7}	1.782×10^{13}	-1.065×10^{5}	-1.185×10^{5}	2.221×10^{2}	-3.376×10^{1}

Table D.27: Williams-Otto Plant Parameter Estimation Sensitivity (dβ/dz) for Model3 at F_A = 2.092 kg/s Disturbance Level.

	ϕ_1	ϕ_2	ζ_1	ζ_2	α	N
F_B	-1.474×10^{6}	2.371×10^{12}	-2.357×10^{2}	5.954×10^{4}	2.332×10^{1}	-1.298
F_G	3.595×10^{5}	9.537×10^{10}	-6.229×10^{1}	-2.143×10^{3}	-4.050	2.781×10^{-1}
F_L	-1.252×10^{5}	1.345×10^{11}	1.014×10^{1}	-5.127×10^{3}	-2.202	1.519×10^{-1}
F_P	-6.517×10^{6}	6.544×10^{11}	1.458×10^{2}	1.926×10^{4}	-2.265×10^{2}	1.244×10^{1}
F_{DW}	-3.363×10^{4}	9.836×10^{9}	1.901	-3.252×10^{2}	-1.466	7.660×10^{-2}
F_{RS}	-2.234×10^{5}	2.466×10^{11}	1.059×10^{2}	-7.487×10^{3}	-2.251×10^{1}	1.248
F_{XW}	1.445×10^{5}	4.624×10^{10}	4.401	1.372×10^{3}	-7.364×10^{-1}	3.792×10^{-2}
T_R	-2.909×10^{4}	5.251×10^{9}	6.848×10^{1}	-4.872×10^{1}	-7.887×10^{-1}	4.397×10^{-2}
$T_{IN,DS}$	1.691×10^{4}	2.847×10^{10}	7.760×10^{-1}	7.851×10^{2}	-3.053×10^{-1}	1.338×10^{-2}
$T_{OUT,DS}$	-3.272×10^{3}	4.688×10^{9}	5.843×10^{-1}	-1.539×10^{2}	-3.165×10^{-1}	1.024×10^{-2}
$T_{OUT,DW}$	7.084×10^{2}	1.158×10^{10}	5.483×10^{-1}	3.422×10^{2}	8.504×10^{-1}	9.542×10^{-4}
$T_{OUT,XW}$	-3.335×10^{3}	1.826×10^{9}	5.860×10^{-1}	-6.079×10^{1}	-3.991×10^{-1}	2.168×10^{-2}
$X_{D,a}$	-8.744×10^{6}	3.146×10^{12}	-5.957×10^{2}	-1.115×10^{5}	-5.504×10^{1}	-1.480×10^{-1}
$X_{D,b}$	4.706×10^{7}	2.399×10^{13}	-8.465×10^{2}	6.180×10^{5}	-4.367×10^{2}	2.259×10^{1}
$X_{D,c}$	-1.482×10^{7}	1.206×10^{13}	4.793×10^{3}	-4.412×10^{5}	-3.705×10^{1}	2.801×10^{1}
$X_{D,p}$	-5.399×10^{6}	1.487×10^{13}	-2.659×10^{3}	-5.358×10^{5}	-5.544×10^{2}	-1.023×10^{2}
$X_{P,a}$	-4.406×10^{7}	1.327×10^{12}	1.172×10^{5}	3.294×10^{5}	1.692×10^{3}	-3.490×10^{1}
$X_{P,b}$	-3.616×10^{7}	2.643×10^{13}	1.793×10^{5}	9.596×10^{5}	9.521×10^{2}	-1.717×10^{1}
$X_{P,c}$	3.544×10^{7}	6.360×10^{13}	-1.086×10^{5}	1.597×10^{6}	-2.645×10^{2}	-7.762

Table D.28: Williams-Otto Plant Measurement Derivatives (dz/dx) for Modell at F_A = 1.563 kg/s Disturbance Level.

	F_B	F_L	T_R
F_B	1	0	0
F_G	-9.932×10^{-2}	6.248×10^{-3}	2.087×10^{-2}
F_L	0	1	0
F_P	7.990×10^{-2}	4.876×10^{-3}	2.354×10^{-3}
F_{DW}	-2.332	1.008	-8.907×10^{-1}
F_{RS}	4.743×10^{-2}	3.368×10^{-2}	3.008×10^{-3}
F_{XW}	1.997	1.998	4.433×10^{-1}
T_R	0	0	1
$T_{IN,DS}$	-8.353×10^{-1}	5.932×10^{-1}	-5.299×10^{-2}
$T_{OUT,DS}$	-3.574×10^{-1}	2.539×10^{-1}	-2.268×10^{-2}
$T_{OUT,DW}$	-4.760×10^{-2}	2.688×10^{-2}	8.879×10^{-2}
$T_{OUT,XW}$	-1.437×10^{-1}	1.431×10^{-1}	6.658×10^{-2}
$X_{D,a}$	-3.546×10^{-2}	3.968×10^{-4}	-3.052×10^{-3}
$X_{D,b}$	-1.188×10^{-1}	1.342×10^{-3}	-4.230×10^{-3}
$X_{D,c}$	-7.009×10^{-2}	1.522×10^{-3}	7.578×10^{-3}
$X_{D,p}$	-6.856×10^{-3}	2.274×10^{-4}	7.605×10^{-4}
$X_{P,a}$	-1.895×10^{-3}	1.912×10-5	-1.539×10-4
$X_{P,b}$	-6.039×10^{-3}	6.498×10^{-5}	-2.037×10^{-4}
$X_{P,c}$	-3.802×10^{-3}	8.426×10^{-5}	4.116×10^{-4}

Table D.29: Williams-Otto Plant Measurement Derivatives (dz/dx) for Modell at F_A = 1.827 kg/s Disturbance Level.

	F_B	F_L	T_R
F_B	1	0	0
F_G	-8.761×10^{-2}	6.681×10^{-3}	2.448×10^{-2}
F_L	0	1	0
F_P	8.924×10^{-2}	5.538×10^{-3}	3.437×10^{-3}
F_{DW}	-1.948	1.521	-4.076×10^{-1}
F_{RS}	3.499×10^{-2}	3.073×10^{-2}	5.496×10^{-4}
F_{XW}	1.854	1.855	4.397×10^{-1}
T_R	0	0	1
$T_{IN,DS}$	-6.607×10^{-1}	5.416×10^{-1}	-9.690×10^{-3}
$T_{OUT,DS}$	-2.640×10^{-1}	2.319×10^{-1}	-4.150×10^{-3}
$T_{OUT,DW}$	-1.807×10^{-2}	7.749×10^{-2}	5.260×10^{-3}
$T_{OUT,XW}$	-1.472×10^{-1}	1.467×10^{-1}	6.732×10^{-2}
$X_{D,a}$	-4.734×10^{-2}	4.874×10^{-4}	-3.193×10^{-3}
$X_{D,b}$	-1.141×10^{-1}	1.470×10^{-3}	-5.119×10^{-3}
$X_{D,e}$	-5.297×10^{-2}	1.715×10^{-3}	8.689×10^{-3}
$X_{D,p}$	-5.163×10^{-3}	2.361×10^{-4}	8.708×10^{-4}
$X_{P,a}$	-2.509×10^{-3}	2.308×10^{-5}	-1.580×10^{-4}
$X_{P,b}$	-5.830×10^{-3}	7.172×10^{-5}	-2.487×10^{-4}
$X_{P,e}$	-2.860×10^{-3}	9.402×10^{-5}	4.698×10^{-4}

Table D.30: Williams-Otto Plant Measurement Derivatives (dz/dx) for Model1 at F_A = 2.092 kg/s Disturbance Level.

	F_B	F_L	T_R
F_B	1	0	0
F_G	-7.315×10^{-2}	6.054×10^{-3}	2.665×10^{-2}
F_L	0	1	0
F_P	9.832×10^{-2}	4.951×10^{-3}	4.385×10^{-3}
F_{DW}	-1.746	1.094	-3.510×10^{-1}
F_{RS}	2.220×10^{-2}	2.877×10^{-2}	0
F_{XW}	1.787	1.788	4.884×10^{-1}
T_R	0	0	1
$T_{IN,DS}$	-3.909×10^{-1}	5.070×10^{-1}	0
$T_{OUT,DS}$	-1.675×10^{-1}	2.171×10^{-1}	0
$T_{OUT,DW}$	-2.644×10^{-2}	1.415×10^{-2}	-5.700×10^{-3}
$T_{OUT,XW}$	-1.348×10^{-1}	1.344×10^{-1}	6.618×10^{-2}
$X_{D,a}$	-5.808×10^{-2}	4.492×10^{-4}	-3.100×10^{-3}
$X_{D,b}$	-1.095×10^{-1}	1.277×10^{-3}	-5.756×10^{-3}
$X_{D,e}$	-3.727×10^{-2}	1.480×10^{-3}	9.283×10^{-3}
$X_{D,p}$	-3.581×10^{-3}	2.151×10^{-4}	9.309×10^{-4}
$X_{P,a}$	-3.055×10^{-3}	2.078×10^{-5}	-1.500×10^{-4}
$X_{P,b}$	-5.616×10^{-3}	6.236×10^{-5}	-2.817×10^{-4}
$X_{P,e}$	-2.002×10^{-3}	8.101×10^{-5}	4.999×10^{-4}

Table D.31: Williams-Otto Plant Measurement Derivatives (dz/dx) for Model2 at F_A = 1.563 kg/s Disturbance Level.

	F_B	F_L	T_R
F_B	1	0	0
F_G	-9.726×10^{-2}	6.303×10^{-3}	2.069×10^{-2}
F_L	0	1	0
F_P	7.780×10^{-2}	4.935×10^{-3}	2.557×10^{-3}
F_{DW}	-5.606	9.669×10^{-1}	-1.195×10^{-1}
F_{RS}	4.742×10^{-2}	3.345×10^{-2}	2.855×10^{-3}
F_{XW}	1.983	1.984	4.390×10^{-1}
T_R	0	0	1
$T_{IN,DS}$	-8.335×10^{-1}	5.893×10^{-1}	-5.030×10^{-2}
$T_{OUT,DS}$	-3.574×10^{-1}	2.522×10^{-1}	-2.153×10^{-2}
$T_{OUT,DW}$	-6.431×10^{-1}	3.328×10^{-2}	-5.068×10^{-2}
$T_{OUT,XW}$	-1.450×10^{-1}	1.446×10^{-1}	6.677×10^{-2}
$X_{D,a}$	-3.513×10^{-2}	4.043×10^{-4}	-3.053×10^{-3}
$X_{D,b}$	-1.180×10^{-1}	1.359×10^{-3}	-4.246×10^{-3}
$X_{D,e}$	-6.969×10^{-2}	1.546×10^{-3}	7.597×10^{-3}
$X_{D,p}$	-6.822×10^{-3}	2.282×10^{-4}	7.626×10^{-4}
$X_{P,a}$	-1.877×10^{-3}	1.951×10^{-5}	-1.539×10^{-4}
$X_{P,b}$	-5.996×10^{-3}	6.577×10^{-5}	-2.043×10^{-4}
$X_{P,e}$	-3.776×10^{-3}	8.553×10^{-5}	4.123×10^{-4}

Table D.32: Williams-Otto Plant Measurement Derivatives (dz/dx) for Model2 at F_A = 1.827 kg/s Disturbance Level.

	F_B	F_L	T_R
F_B	1	0	0
F_G	-8.573×10^{-2}	6.560×10^{-3}	2.420×10^{-2}
F_L	0	1	0
F_P	8.727×10^{-2}	5.438×10^{-3}	3.682×10^{-3}
F_{DW}	-1.934	1.155	-4.140×10^{-1}
F_{RS}	3.495×10^{-2}	3.049×10^{-2}	5.957×10^{-4}
F_{XW}	1.845	1.846	4.436×10^{-1}
T_R	0	0	1
$T_{IN,DS}$	-6.158×10^{-1}	5.373×10^{-1}	-1.049×10^{-2}
$T_{OUT,DS}$	-2.636×10^{-1}	2.301×10^{-1}	-4.500×10^{-3}
$T_{OUT,DW}$	-1.675×10^{-2}	1.467×10^{-2}	5.860×10^{-3}
$T_{OUT,XW}$	-1.467×10^{-1}	1.458×10^{-1}	6.724×10^{-2}
$X_{D,a}$	-4.712×10^{-2}	4.802×10^{-4}	-3.196×10^{-3}
$X_{D,b}$	-1.138×10^{-1}	1.445×10^{-3}	-5.156×10^{-3}
$X_{D,e}$	-5.284×10^{-2}	1.685×10^{-3}	8.731×10^{-3}
$X_{D,p}$	-5.151×10^{-3}	2.332×10^{-4}	8.753×10^{-4}
$X_{P,a}$	-2.497×10^{-3}	2.277×10^{-5}	-1.580×10^{-4}
$X_{P,b}$	-5.810×10^{-3}	7.045×10^{-5}	-2.504×10^{-4}
$X_{P,e}$	-2.851×10^{-3}	9.235×10^{-5}	4.719×10^{-4}

Table D.33: Williams-Otto Plant Measurement Derivatives (dz/dx) for Model2 at F_A = 2.092 kg/s Disturbance Level.

	F_B	F_L	T_R
F_B	1	0	0
F_G	-7.228×10^{-2}	5.962×10^{-3}	2.639×10^{-2}
F_L	0	1	0
F_P	9.667×10^{-2}	4.871×10^{-3}	4.607×10^{-3}
F_{DW}	-1.738	1.145	-4.051×10^{-1}
F_{RS}	2.255×10^{-2}	2.866×10^{-2}	7.758×10^{-5}
F_{XW}	1.784	1.786	4.930×10^{-1}
T_R	0	0	1
$T_{IN,DS}$	-3.971×10^{-1}	5.050×10^{-1}	-1.360×10^{-3}
$T_{OUT,DS}$	-1.701×10^{-1}	2.163×10^{-1}	-5.900×10^{-4}
$T_{OUT,DW}$	-2.600×10^{-2}	2.380×10^{-2}	3.190×10^{-3}
$T_{OUT,XW}$	-1.340×10^{-1}	1.333×10^{-1}	6.606×10^{-2}
$X_{D,a}$	-5.755×10^{-2}	4.421×10^{-4}	-3.106×10^{-3}
$X_{D,b}$	-1.091×10^{-1}	1.256×10^{-3}	-5.445×10^{-3}
$X_{D,c}$	-3.750×10^{-2}	1.455×10^{-3}	9.300×10^{-3}
$X_{D,p}$	-3.604×10^{-3}	2.132×10^{-4}	9.329×10^{-4}
$X_{P,a}$	-3.027×10^{-3}	2.047×10^{-5}	-1.503×10^{-4}
$X_{P,b}$	-5.597×10^{-3}	6.133×10^{-5}	-2.822×10^{-4}
$X_{P,c}$	-2.014×10^{-3}	7.958×10^{-5}	5.006×10^{-4}

Table D.34: Williams-Otto Plant Measurement Derivatives (dz/dx) for Model3 at F_A = 1.563 kg/s Disturbance Level.

	F_B	F_L	T_R
F_B	1	0	0
F_G	-9.684×10^{-2}	5.957×10^{-3}	2.062×10^{-2}
F_L	0	1	0
F_P	7.865×10^{-2}	4.626×10^{-3}	2.534×10^{-3}
F_{DW}	-2.128	1.448	-5.323×10^{-1}
F_{RS}	4.654×10^{-2}	3.322×10^{-2}	3.172×10^{-3}
F_{XW}	1.984	1.985	4.554×10^{-1}
T_R	0	0	1
$T_{IN,DS}$	-8.194×10^{-1}	5.851×10^{-1}	-5.588×10^{-2}
$T_{OUT,DS}$	-3.508×10^{-1}	2.504×10^{-1}	-2.392×10^{-2}
$T_{OUT,DW}$	-1.057×10^{-2}	5.668×10^{-2}	2.200×10^{-2}
$T_{OUT,XW}$	-1.406×10^{-1}	1.398×10^{-1}	6.632×10^{-2}
$X_{D,a}$	-3.615×10^{-2}	3.811×10^{-4}	-3.074×10^{-3}
$X_{D,b}$	-1.192×10^{-1}	1.284×10^{-3}	-4.326×10^{-3}
$X_{D,e}$	-6.967×10^{-2}	1.452×10^{-3}	7.701×10^{-3}
$X_{D,p}$	-6.811×10^{-3}	2.219×10^{-4}	7.734×10^{-4}
$X_{P,a}$	-1.930×10^{-3}	1.832×10^{-5}	-1.548×10^{-4}
$X_{P,b}$	-6.061×10^{-3}	6.204×10^{-5}	-2.084×10^{-4}
$X_{P,e}$	-3.776×10^{-3}	8.045×10^{-5}	4.181×10^{-4}

Table D.35: Williams-Otto Plant Measurement Derivatives (dz/dx) for Model3 at F_A = 1.827 kg/s Disturbance Level.

	F_B	F_L	T_R
F_B	1	0	0
F_G	-8.503×10^{-2}	6.542×10^{-3}	2.414×10^{-2}
F_L	0	1	0
F_P	8.738×10^{-2}	5.432×10^{-3}	3.741×10^{-3}
F_{DW}	-2.206	1.073	-4.888×10^{-1}
F_{RS}	3.444×10^{-2}	3.032×10^{-2}	5.483×10^{-4}
F_{XW}	1.836	1.837	4.426×10^{-1}
T_R	0	0	1
$T_{IN,DS}$	-6.069×10^{-1}	5.344×10^{-1}	-9.660×10^{-3}
$T_{OUT,DS}$	-2.600×10^{-1}	2.288×10^{-1}	-4.140×10^{-3}
$T_{OUT,DW}$	-6.259×10^{-2}	1.057×10^{-3}	1.891×10^{-2}
$T_{OUT,XW}$	-1.467×10^{-1}	1.462×10^{-1}	6.731×10^{-2}
$X_{D,a}$	-4.771×10^{-2}	4.822×10^{-4}	-3.197×10^{-3}
$X_{D,b}$	-1.141×10^{-1}	1.447×10^{-3}	-5.189×10^{-3}
$X_{D,e}$	-5.254×10^{-2}	1.689×10^{-3}	8.768×10^{-3}
$X_{D,p}$	-5.122×10^{-3}	2.328×10^{-4}	8.789×10^{-4}
$X_{P,a}$	-2.527×10^{-3}	2.285×10^{-5}	-1.580×10^{-4}
$X_{P,b}$	-5.830×10^{-3}	7.053×10^{-5}	-2.520×10^{-4}
$X_{P,e}$	-2.834×10^{-3}	9.251×10^{-5}	4.738×10^{-4}

Table D.36: Williams-Otto Plant Measurement Derivatives (dz/dx) for Model3 at F_A = 2.092 kg/s Disturbance Level.

	F_B	F_L	T_R
F_B	1	0	0
F_G	-7.094×10^{-2}	5.889×10^{-3}	2.615×10^{-2}
F_L	0	1	0
F_P	9.646×10^{-2}	4.811×10^{-3}	4.748×10^{-3}
F_{DW}	-1.883	$9.837\times10\text{-}1$	$-3.823\times10\text{-}1$
F_{RS}	2.185×10^{-2}	2.842×10^{-2}	9.029×10^{-5}
F_{XW}	1.772	1.773	4.942×10^{-1}
T_R	0	0	1
$T_{IN,DS}$	-3.848×10^{-1}	5.008×10^{-1}	-1.590×10^{-3}
$T_{OUT,DS}$	-1.648×10^{-1}	2.144×10^{-1}	-6.800×10^{-4}
$T_{OUT,DW}$	-4.981×10^{-2}	2.997×10^{-3}	-1.100×10^{-3}
$T_{OUT,XW}$	-1.340×10^{-1}	1.332×10^{-1}	6.606×10^{-2}
$X_{D,a}$	-5.831×10^{-2}	4.394×10^{-4}	-3.100×10^{-3}
$X_{D,b}$	-1.095×10^{-1}	$1.245\times10\text{-}3$	$-5.810\times10\text{-}3$
$X_{D,e}$	-3.700×10^{-2}	1.441×10^{-3}	9.336×10^{-3}
$X_{D,p}$	-3.556×10^{-3}	2.111×10^{-4}	9.366×10^{-4}
$X_{P,a}$	-3.065×10^{-3}	2.031×10^{-5}	-1.498×10^{-4}
$X_{P,b}$	-5.617×10^{-3}	6.069×10^{-5}	-2.842×10^{-4}
$X_{P,e}$	-1.987×10^{-3}	7.878×10^{-5}	5.024×10^{-4}