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The enhancement of a block-oriented modeling method to improve inference and prediction

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The enhancement of a block-oriented modeling method to improve inference and prediction

by

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in partial fulfillment of the requirements for the degree of

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To my incredible, encouraging, and loving support system. Thanks!
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CHAPTER I. INTRODUCTION

1. General Introduction

Processes in industry have become more complicated and there is an increased demand to maintain tighter control, and meet tighter specifications. This increase in complexity is leading to linear modeling becoming less useful than non-linear modeling at obtaining accurate models. Process identification requires identification of the model structure and estimating unknown model parameters. The control literature is filled with methods to identify model forms and estimate unknown parameters. However there has not been any significant focus on improving statistical inference by minimizing the number of dynamic model parameters. In addition, process noise can also make it difficult to detect changes between the true process and signal noise. Previous work, presented by Rietz [1], used an on-line change point algorithm, which requires accurate change point detection. However, it can be difficult to determine a suitable change point algorithm. Therefore, this work seeks to enhance predictive modeling by minimizing the number of estimated parameters to improve statistical inference and by proposing an algorithm that treats each sampling time as an input change and therefore eliminates the need for change point detection.

2. Motivation

Rollins et al [2] introduced a closed-form continuous-time exact solution to the single input, single output (SISO) Hammerstein system which was later known as H-BEST [3]; and similarly, W-BEST for Wiener systems [4]. It is very common for processes to have multiple
inputs and multiple outputs (MIMO). In MIMO processes the number of dynamic model parameters can be quite large. MIMO processes can be decomposed into multiple input, single output (MISO) equations such that each output depends on a unique set of parameters. This condition will restrict reduction of the number of estimated parameters by not allowing different outputs to depend on the same parameters. In Chapter 3 we propose a methodology to reduce the number of estimated parameters which increases the number of degrees of freedom for error and thus improves statistical inference.

Rietz [1] presented a prediction algorithm that uses on-line change point detection. Not only can it be difficult to determine a suitable change point algorithm but our work has suggested that it may not be sufficient due to the dynamic nature of process equipment controlling inputs. To overcome the requirement of accurate change point detection, we developed a prediction algorithm to treat each sampling instant as an input change point. This algorithm is derived and presented in Chapter 4. Our proposed “classical algorithm” or “C-algorithm,” is unrestricted to the type of input sequence or dynamic order of the process. In this chapter we also compare it to the approach in [1] using data from a real tank level process.

3. Problems and Objectives

Bhandari and Rollins [3] modeled a simulated Continuous Stirred Tank Reactor (CSTR) using their W-BEST approach. Reactants A and B enter the CSTR as two different streams, they react to form product C. The reaction taking place in the CSTR is second-order and exothermic which gives the process strong non-linear and interactive behavior [3]. The process model consists of the overall mass balance, component A and B mole balances and
energy balances on the tank and jacket contents. This is a MIMO system with 7 inputs and 5 outputs. However, since there is linear dependency between the concentration outputs the study consists of only 4 outputs and 7 inputs. This work presents a methodology to apply multiresponse estimation (ME) to transfer function modeling. ME is applied to the process in [3] with the goal of maximizing statistical inference without adversely affecting fit. This will be accomplished by setting parameters equal that are not significantly different.

The real process used in Chapter 4 is a SISO tank level system. The input variable for the experiment is the inlet flow rate which is controlled to achieve or maintain the desired tank level. The response variable is the tank height. The outlet flow rate from the tank is not measured or controlled; it is a function of the tank height since the manual valve was left fully open. This work proposes a BEST Classical algorithm which uses each sampling time as an input change thus eliminating the need for input change point detection.

4. Organization of Thesis

Chapter 2 begins with a review of previous work in theoretical and semi-theoretical modeling. Chapter 2 also discusses current approaches to non-linear modeling. The application of a new method for reducing the number of estimated dynamic model parameters in transfer function modeling is presented in Chapter 3. A research and development note introducing the proposed prediction algorithm which uses each sampling time as an input change is presented in Chapter 4. Finally, Chapter 5 includes general conclusions as well as potential future research avenues.
LITERATURE CITED


CHAPTER II. LITERATURE REVIEW

1. Background

There has been a lot of work done in the field of theoretical modeling and some work in semi-theoretical modeling of chemical processes. Currently, in transfer function modeling, for multiple-input, single-output (MISO) or multiple-input, multiple-output (MIMO) processes, each output depends on a unique set of parameters. This condition restricts parameter reduction and does not allow different outputs to depend on the same parameters. Multiresponse estimation (ME) was developed by Box and Draper [1] to overcome the least squares estimation (LSE) limitation that outputs on the same run cannot be correlated. ME has been applied in first principle modeling in the chemical engineering literature where theoretical knowledge produces a minimum set of parameters as different outputs theoretically depend on the same model parameters (see [2]-[5]). However, no previous work has been found applying ME in transfer function modeling. There also has been no work identified that uses ME in process system identification to minimize the number of estimated parameters.

As mentioned above, in some situations it is possible to measure multiple outputs. It is useful in these situations to combine information from all the measured responses to provide more precise parameter estimation and to determine more realistic models [6]. Box and Draper [1] derived a determinant parameter estimation criterion for multiresponse data. Using this criterion, [6] presents a generalization of the Gauss-Newton optimization method. They also describe a convergence criterion for this optimization method, and discuss how to modify the method if there are singularities in the data [6].
2. Approaches

A popular approach to nonlinear transfer function modeling is block-oriented modeling. Block-oriented modeling uses mathematical blocks to represent physical systems. The inputs are transformed in blocks using nonlinear static gain equations or linear dynamic equations and outputs from blocks are either intermediate variables that input to other blocks or are final output responses. The arrangement of blocks defines the type of system. The two most common structures are Hammerstein and Wiener. For the Hammerstein system, the inputs enter the first block, which is a static nonlinear function of the inputs and passes its output to a linear dynamic block which gives the outputs. A limitation of the Hammerstein system is its inability to directly treat systems with nonlinear dynamics [7]. Many methods have been applied to nonlinear systems. These include, but are not limited to: Nonlinear Auto-Regressive Moving Average with eXogenous inputs (NARMAX) modeling, artificial neural networks (ANN), wavelets, and Volterra series (page 2 of [7]).

Most of the block-oriented modeling articles in the literature only address independently distributed noise or the so called “white” noise (e.g., see [8]-[15].) However, this is an insufficient representation of a “real” system which will inevitably have serially correlated noise due to these error sources [16]. A few studies have been found involving serially correlated noise in block-oriented modeling. These included the works of: Cao and Gertler [35]; Zhu [36]; David and Bastin [37]; Chen and Fassois [38]; as discussed by Haist et.al. [16]. These studies did not employ methods that separate identification of these structures. Only a few of these studies specifically addressed Wiener or Hammerstein systems and none of them involved the modeling of physical systems.
3. Review of Modeling Approaches

There are several different modeling approaches that can be implemented within model predictive control (MPC). The two fundamental approaches to modeling a process are a theoretical and an empirical approach, with the semi-theoretical approach and semi-empirical approach falling between. A brief discussion of these four approaches is given below.

*Theoretical*

This approach, also referred to as the “first principles” model, utilizes the principles of physics and chemistry to describe the complete details of the system. It relies on a fundamental understanding of all phenomena involved, and the lack of such understanding is the biggest limitation of this method.

*Empirical*

The other extreme of theoretical modeling is the empirical approach which relies exclusively on process data to arrive at the model and requires no understanding of the underlying physical phenomena. Since the choice of the model structure is more a matter of convenience and familiarity than of process knowledge, this method is sometimes referred to as the “black-box” approach. Given that all information for the model is obtained from data, the experimental requirements can be quite large. This need for huge amounts of data becomes the biggest limitation in cases of dynamic modeling. However, in situations where dynamic prediction is not the ultimate goal, empirical models can be obtained from a limited amount of data, making their use more practical.
**Semi-theoretical**

The semi-theoretical approach is similar to the theoretical approach. However, it is more practical because it uses the understanding of the process to arrive at the model, and also uses a limited amount of data to get estimates of model parameters. The applicability of this method is severely limited when fundamental knowledge of the process is lacking.

**Semi-empirical**

The semi-empirical approach uses process behavior to provide the appropriate model structure and obtains parameter estimates from a relatively small amount of data. The data requirements can be reduced (compared to empirical models) by intelligent choice of model form. An advantage of this approach is that the data has some fundamental significance in the context of the process and the model parameters typically have physical meaning. Thus this approach retains the benefits of the empirical and theoretical approaches while at the same time attempting to overcome their limitations.

This section examined the different modeling approaches. Some of the empirical approaches that are commonly used are described more specifically below.

4. **Empirical Modeling Methods**

This section presents the various empirical modeling methods that have been used in an MPC framework. The general model equation is of the form given by Eq. 1 below:

\[
\hat{Y}_{i+1} = f(Y_i, Y_{i-1}, Y_{i-2}, \ldots, X_i, X_{i-1}, X_{i-2}, \ldots; \theta) + \varepsilon_{i+1}
\]  

(1)

where
\( \hat{Y}_{i+1} \) = predicted value of the output at the \((i+1)^{th}\) time instant

\( X_i \) = input at \(i^{th}\) time instant

\( \theta \) = vector of parameters (typically will not have physical meaning)

\( \varepsilon_{i+1} \) = error term at \((i+1)^{th}\) time instant.

Every empirical model requires sampling of the outputs and the inputs at constant and equal rates. However, they differ primarily in the choice of the function \( f \). The various empirical model representations are:

i. \textit{Convolution model:} This is a non-parametric model that is also referred to as the \textit{step response model}. The model coefficient \( a(i) \) is simply the process output response, \( y \), sampled at time interval \( i \) to a step change in the input made at time \( 0 \). The number of sampling times it takes the process to reach 95\% of its ultimate value is the approximate number of coefficients required \((N)\). The advantage of this method is that it is easy to obtain, however the number of terms required can be quite large (as high as 50-60 or more). The form of the convolution model is given in Eq. 2.

\[
\hat{y}(k) = y_0 + \sum_{i=1}^{N} a(i)x(k-i) \tag{2}
\]

where \( \hat{y}(k) \) is the predicted value at time instant \( k \), \( y_0 \) is the initial value of the output \( y \), and \( x(k-i) \) is the input at time instant \((k-i)\). As can be seen from Eq. 2, the output depends on all the previous input changes over the model horizon, \( N \). A different version of the same model, known as an \textit{impulse response model}, uses the change in \( y \) from its previous value as the model coefficient. Limitations of this method are that it cannot be used for integrating processes and it can be difficult to apply to more complex processes. The original
implementations of MPC used the convolution models (impulse response [17] and step response [18]).

**ii. State space models:** The state-space model is parametric and can be described by Eqs. 3 and 4 below.

\[ X(k) = A(\theta)X(k - 1) + B(\theta)u(k - 1) + v(k - 1) \]  
\[ \hat{Y}(k) = C(\theta)X(k) + w(k) \]  

where \( X(k) \) is the input state vector at time \( k \), \( u(k) \) is the vector of manipulated variables, and \( \hat{Y}(k) \) is the predicted output vector. The matrices \( A, B, \) and \( C \) are of appropriate dimensions and may be functions of the parameter vector \( \theta \). The vectors \( v(k) \) and \( w(k) \) are the process disturbance and measurement noise vectors, respectively. The state space model may use a transfer function or step responses to obtain terms in the matrices \( A, B \) and \( C \).

Advantages of using the state-space model above are that it is linear and can be easily modified to handle constraints. However, the method requires uniform process sampling.

**iii. Time Series or Input/Output Models:** These models may be moving average or auto-regressive models or a combination of both. The most general form of such a model is the ARMAX (auto regressive moving average with exogenous inputs) form given by Eq. 5 below.

\[ \hat{Y}(k) + a_1 Y(k - 1) + \ldots + a_n Y(k - n) = b_1 u(k - 1) + \ldots + b_m u(k - m) + c_1 e(k - 1) + \ldots + c_r (k - r) \]  

where \( y(k), u(k) \) and \( e(k) \) are the output, the input, and the error at time \( k \). Since these models are discrete in time they also require real and constant rate sampling.
iv. **Artificial Neural Network (ANN):** The ANN models, first developed and used for biological nervous systems, consist of input and output layers with one or more hidden layers between them. The input layer and the hidden layers consist of a series of nodes, which are interconnected and give a single output. The nodes for the hidden and the output layer are determined by summing the results of the previous layers with their interconnecting weights and then transferring their sum through an activation function. The model parameters are obtained by minimization of deviation between actual and predicted values in the training data set. Validation of the fitted model is done by using a test data set. If there is good agreement between the fit and the test, then the entire procedure is repeated. A disadvantage or limitation of this approach is that it may result in a model that fits only two particular input sequences, the training and the test sequences.

v. **Multi-scale Models:** These models use wavelet transformations and represent signals in such a way that time and scale (frequency) localization can be obtained. This framework makes it possible to retain scale-based characteristics of the process, i.e., the model captures the dynamics involving different time rates. By retaining the scale-based characteristics it is possible for the model to include different inputs at different sampling rates. However, it is still necessary to have an equal and constant sampling rate for a particular input.

The extensive use of empirical models in MPC has been due to the fact that no knowledge about the process is required. Their use seems more attractive with the availability of large process databases. An empirical approach would probably be the easiest, if the purpose of a model were curve fitting. However, there are a number of issues that need to be addressed when empirical models are used in a predictive setting, as shown by Chen.
and Rollins [20]. One important consideration is the information content of the data set used for model development. Knowledge about the process is gained from the data, and therefore the data requirements for empirical model building can be quite large. Another requirement for using empirical methods is that the sampling rates must remain equal and constant, which is not always the case. Another consideration is that extrapolation with empirical models is extremely risky, and in a multivariate situation it might not be easy to ascertain the input region.

Semi-empirical models offer an attractive alternative for overcoming some of the limitations mentioned above. As previously discussed, their strengths include the fact that data sets required for model building are not huge, they do not require online sampling, mild extrapolation is acceptable, and the model parameters typically have physical meaning. For these reasons, the semi-empirical modeling approach was selected to be used in development of the predictive control framework that was proposed by Rollins et al. [17] and referred to as H-BEST. More details are presented in the following sections.

5. H-BEST

The H-BEST approach was first introduced by Rollins et al. [17] and falls under the category of semi-empirical modeling. This approach used semi-empirical models to represent process behavior and used a novel algorithm for prediction. The semi-empirical model (SEM) form used for this purpose was a first order plus dead time (FOPDT) model and a limited amount of dynamic data were used to obtain parameter estimates. The predictive performance of H-BEST was shown to be vastly superior to the performance of empirical techniques such as artificial neural networks (ANN) and linear regression (LR).
The basic steps for H-BEST model development in [17] for the SISO case are: (1) the model identification is performed through step tests, (2) the ultimate change in the response is modeled as a function of the input using linear regression, and (3) the dynamic parameters are estimated using nonlinear regression.

The model is then incorporated in the H-BEST algorithm, for prediction purposes. The H-BEST algorithm was written so that the output variable depended only on the most recent input change. This property eliminated propagation of modeling errors in order to make the model accurate and easy to implement.

For an input change occurring at time $t_1$ a generic representation of the H-BEST algorithm in [17] is given below:

For $t > t_1$,

$$\hat{Y}(t) = \hat{Y}(t_1) + \left( f(X(t);\hat{\theta}) - \hat{Y}(t_1) + Y(0) \right) g((t - t_1);\hat{\theta})S(t - t_1)$$

(7)

where $\hat{Y}(t)$ is the estimated output response at time $t$; $Y(0)$ is the measured value of the output at the initial time ($t = 0$); $X(t)$ is a vector that contains the values of the process variables at time $t$; $\hat{\theta}$ is a vector that contains the estimates of the steady state response parameters determined from the current input conditions; $f(X(t);\hat{\theta})$ is the function that computes the change in the ultimate response for input $X(t)$; $\hat{\theta}$ is a vector that contains the estimates of the dynamic parameters determined from the current input conditions; $g(t - t_1;\hat{\theta})$ is the semi-empirical non-linear function that computes the dynamic portion of the response such that as $t \to \infty$, the function, $g \to 1$; and $S(t - t_1)$ is the shifted unit step function. Note that at $t_1$, $\hat{Y}(t) = \hat{Y}(t_1)$, and as $t \to \infty$, $\hat{Y}(t) \to Y(0) + f(X(t);\hat{\theta})$. Thus, the algorithm provides proper initial and limiting behavior.
6. Related Work

More recently, H-BEST has been applied to processes with more complex dynamics [21], to a real process in open-loop [22] and closed-loop situations [23], and to human thermoregulation [24]. While all the previous applications are single-input, single-output (SISO), its application to continuous time MIMO processes is presented in [7] and [25] and a discrete-time application for a MIMO process in presented in [26].

In order to evaluate competing designs in the context of nonlinear dynamic system identification for Hammerstein systems, [27] studied the information efficiency of the Statistical Design of Experiments (SDOE) and Pseudo Random Sequences Design (PRSD) approaches. This work was continued in [28] which evaluated SDOE against PRS under D-optimal efficiency for Wiener Systems. For Hammerstein and Wiener continuous-time modeling, [29] proposes compact algorithms under sinusoidal input sequences that depend only on the most previous input changes and provides exact solutions that are applicable to MIMO systems. More continuous-time modeling is presented in [30] with an analytical solution to Hammerstein and Wiener systems with second-order plus-lead (SOPL) dynamic behavior for sinusoidal input changes.

Further work has been done in the field of human thermoregulation with [31] demonstrating that a semi-empirical continuous-time, block oriented modeling approach is capable of accurately predicting human thermoregulatory response. Also, [32] discusses a mechanism to obtain a human thermoregulatory system model without subjecting the individual to an environmental chamber experiment by creating a library of model structures with the assistance of theoretical knowledge and extensive test subject data from environmental chambers over the domain of human attributes and experimental conditions.
Other work using BEST consists of [33] which demonstrates the greater accuracy H-BEST has over discrete-time modeling in modeling a high purity distillation column. Also, [34] presents a continuous time “unrestricted” algorithm which is not restricted by steady-state conditions between input changes. Finally, [16] proposes a model building methodology that is able to separately determine the steady state, dynamic and noise model structures.

LITERATURE CITED

CHAPTER III. MINIMIZING THE NUMBER OF DYNAMIC PARAMETERS TO IMPROVE STATISTICAL INFERENCE IN BLOCK-ORIENTED MODELING

A paper submitted to Computers & Chemical Engineering

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Abstract

In process identification (i.e., dynamic model development) information on the precision and reliability of a parameter estimate is conveyed by a confidence interval. The best confidence interval is the one with the shortest width for a given level of confidence. Confidence interval widths widen as the standard error increases or as the number of estimated parameters increases. This article focuses on minimizing the width of confidence intervals by reducing the number of estimated dynamic parameters in the context of block-oriented modeling. This objective is accomplished by the development of a procedure that finds parameter equivalencies within (intra) and between (inter) the functional forms for the responses (i.e., outputs). It is important to recognize that the least squares estimation criterion is not valid under inter-parameter equivalency. However, the multiresponse criterion does not have this limitation and is used in this work. For the seven (7) input, five (5) output, simulated CSTR from Bhandari and Rollins (2003), the number of estimated dynamic parameters was reduced from 84 to 23. This reduction resulted in a 50% decrease in confidence interval width for a given level of confidence or, equivalently, an increase in confidence level from 50% to 99.9% for a fixed interval width.

Key words: Block-oriented modeling, Multiresponse estimation, System identification, Nonlinear regression.
1. Introduction

Block-oriented modeling (BOM), a sub-class of Volterra modeling (Henson and Seborg, 1997; Doyle et al., 2002), is an active area of research in the system identification literature (Zhu, 2002; Bai, 2003; Gomez and Baeyens, 2004; Park et al., 2006; Rollins et al., 2006). Processes that can be described by series and/or parallel arrangement of nonlinear static blocks and linear dynamic blocks are said to have block-oriented structures. One of the simplest and most popular systems is the Hammerstein structure, which consists of a nonlinear (N) static gain block followed by a linear (L) dynamic block and is said to have “NL structure.” Another popular system is the Wiener structure which reverses this order and has “LN structure.” The popularity of BOM comes from its ability to effectively describe nonlinear static and dynamic behavior for physical and biological systems from intelligent model structures (i.e., linear transfer function structures) under relatively low parametrization. Nonetheless, as the dynamic model order rises to explain complex behavior and as the number of measured outputs grows, the total number of parameters can become quite large which adversely affects statistical inference. (By statistical inference we mean a formal statistical method that seeks to infer truth about model parameters at a specified level of significance which includes confidences intervals and hypothesis testing.) For example, in a seven input, five output process where each output depends on a second-order plus lead (SOPL) dynamic function for each input, there are 105 dynamic parameters. This model is said to be a decomposed multiple-input, single-output (MISO) system of equations where each of the five outputs has its own set of parameters and is written independently of other outputs (Nells, 2001). A block diagram of a decomposed MISO Wiener block-oriented system of $q$ outputs is shown in Figure 1.
While the systems identification literature is filled with methods to identify model forms and estimate unknown parameters, we have not found any significant focus on improving statistical inference by minimizing the number of estimated dynamic model parameters.

The general form for a $100(1 - \alpha)\%$ confidence interval (CI) for some parameter $\theta$ is

$$\hat{\theta} \pm F\left(\nu_1, \nu_2; \alpha\right)s_{\hat{\theta}}$$

where $\hat{\theta}$ is the estimate (or estimator) of $\theta$, $F\left(\nu_1, \nu_2; \alpha\right)$ is the critical value, $\nu_1$ is the number of degrees of freedom associated with the number of estimated parameters ($P$), $\nu_2$ is the number of degrees of freedom associated with the number of samples minus $P$, and $s_{\hat{\theta}}$ is the estimated standard error of $\hat{\theta}$. Note that for $\alpha = 0.05$, Eq. 1 is a 95% CI for $\theta$. In the context of BOM, this work focuses on minimizing the width of Eq. 1 by minimizing the critical value which, for a fixed sample size, decreases as $P$ decreases. Thus, our goal is to develop a procedure for BOM that effectively obtains a minimum set of estimated parameters (i.e., the smallest $P$) without adversely affecting prediction accuracy. We will accomplish this goal by finding sets of parameters that are not statistically significantly different from one another, setting them equal to each other, and estimating only one parameter for each set. In the common way that BOM is applied, each response has its own set of parameters and reducing the number of estimated parameters based on determining sets of equivalent parameters is not widely practiced, especially in discrete-time modeling.

While it is acceptable to use the least squares criterion under intra-parameter equivalency (PE), this criterion is not valid for inter-PE. That is, least squares is not valid when outputs depend on the same parameters that are candidates for estimation (Bates and
Watts, 1988). To address this limitation, our proposed procedure uses the multiresponse criterion (Box and Draper, 1965) which does not suffer from this limitation. Multiresponse estimation (ME) has been applied in first principle modeling in the chemical engineering literature where theoretical knowledge produces outputs that depend on the same model parameters (see Mezaki and Butt, 1969; Ziegel and Gorman, 1980; Stewart, et al., 1992; Rollins and Davis, 1994; Stewart, et al., 1998; Singh, 1999; Asprey and Macchietto, 2000; Chen and Asprey, 2003). However, this appears to be the first application of ME in BOM. Moreover, we have not found the use of ME in process identification to minimize the number of estimated parameters using PE. Using this determinant criterion, we present a methodology for systematically reducing the number of estimated dynamic parameters to a minimum number using intra- and inter-PE. Although we present this approach in the context of continuous-time (CT) modeling, our proposed approach is also applicable to discrete-time (DT) modeling.

**Figure 1.** A description of the general MIMO Wiener model structure (decomposed to \( q \) MISO blocks) with \( i = 1, \ldots, q \) outputs and \( j = 1, \ldots, p \) inputs. There is one set of blocks for each of the \( q \) outputs. For each set of blocks, each of the \( p \) inputs \((u_j)\) passes through a separate linear dynamic block \((G_{ij})\) and produces an intermediate variable, \( v_{ij} \), that is an
element of the vector $v_i$. Each $v_i$ passes through a non-linear static function $f_i(v_i)$ and generates the output $y_i$.

This article presents the proposed approach using the following outline. In Section 2, we discuss ME and present the model, the objective criterion, parameter inference regions, and discuss practical issues. Section 3 presents the problem from literature that we will use to demonstrate the effectiveness of this approach. The process is the simulated continuous-stirred tank reactor (CSTR) introduced by Bhandari and Rollins (2003). It has seven inputs and five outputs. They modeled this process using a CT Wiener approach called “W-BEST.” Section 4 will introduce and apply the proposed approach to this problem and demonstrate a substantial improvement in statistical inference while maintaining the test model performance obtained by Bhandari and Rollins. Concluding remarks are given in Section 5.

2. Multiresponse Estimation

Multiresponse estimation (ME) was developed by Box and Draper (1965) to overcome the least squares estimation (LSE) limitation that outputs on the same run cannot be correlated. When outputs depend on the same model parameters, ME exploits the combined information provided by outputs to improve estimation of the model parameters (Bates and Watts, 1988). LSE is not able to combine this information to improve parameter inference and thus, loses to ME in this context. Following Bates and Watts (1988), in the notation of Fig. 1, the multiresponse model is given as:

$$ y_i(t_i) = y_{ki} = f_i(v_{i1}, \ldots, v_{ik}; \theta) + Z_i(t_i) = f_i(v_{ki}; \theta) + Z_{ki} $$

where $i = 1, \ldots, q$, $k = 1, \ldots, N$, $v_{ki} = [v_{ki1}, v_{ki2}, \ldots, v_{kip}]$, $Z_{ki}$ is the noise term and $\theta$ is a $P$ by 1 vector of all the dynamic parameters to be estimated. Note that $N$ is now being used as the sample size and will retain this definition from here out. All other model parameters (e.g.,
the static model parameters) are assumed to be known for convenience. Note that in the W-BEST approach the static model is independently determined before the dynamic model. The noise term is normally distributed with

\[ E[Z_i] = 0 \quad \text{and} \quad H[Z_i, Z_{im}] = \begin{cases} \{\Sigma\}_{im} & k = r \\ 0 & k \neq r \end{cases} \]

where \( \Sigma \) is a fixed \( q \) by \( q \) covariance matrix. That is, measurements from different times are independent but observations at the same time may be correlated. In contrast, LSE requires all observations to be uncorrelated. Let \( Y \) be the \( N \) by \( q \) matrix of observed values of outputs and \( H(\theta) \) be the \( N \) by \( q \) matrix of the expected outputs, then the \( N \) by \( q \) residual matrix is defined as

\[ Z(\theta) = Z = Y - H(\theta) \]

Now we may write the multiresponse objective criterion as the set of parameter estimates of \( \theta \) that minimizes

\[ |Z^TZ| \]

ME was derived from a statistical Bayesian approach and following Box and Tiao (1973), Bates and Watts (1988) recommend the following approximate 100(1 - \( \alpha \))% highest posterior density (HPD) region for \( \theta \)

\[ |Z^TZ| - |\tilde{Z}^T\tilde{Z}| < s^2 F_{\alpha, P, N-P} \]

where

\[ s^2 = \frac{|\tilde{Z}^T\tilde{Z}|}{N - P} \]
\( \hat{Z} \) is the estimate of \( Z \), and \( F_{\alpha, P, N-P} \) is the 100(1 - \( \alpha \))th percentile of the F-distribution with \( P \) numerator and \( N - P \) denominator degrees of freedom, respectively. As Eq. 7 shows, the size of this region is minimized when the right side is minimized, that is, as \( P \), for a fixed \( s \), is minimized, because the reduction of \( P \) also reduces \( F_{\alpha, P, N-P} \), for a fixed \( N \). Therefore, the goal of the proposed method is to minimize the number of estimated parameters, \( P \). To use Eq. 7, Bates and Watts (1988) indicate that such regions would have to be determined numerically and displayed in contour plots. For an equation for individual approximate 100(1 - \( \alpha \))% HPD intervals (i.e., for single parameters) see Bates and Watts (1988).

3. The CSTR

This section presents the physical process that we will use to demonstrate our proposed method. The process is a simulated CSTR that Bhandari and Rollins (2003) (BR) modeled using their W-BEST approach. A simplified diagram of the CSTR is given in Fig. 2. Reactants A and B enter the CSTR as two different flow streams and form product C. The second-order, exothermic reaction taking place in the CSTR gives the process strong nonlinear and interactive behavior. The process model consists of the overall mass balance, component (A and B) mole balances, and energy balances on tank and jacket contents. The input variables are the feed flowrate of A (\( q_{AF} \)), the feed temperature of A (\( T_{AF} \)), the feed concentration of A (\( C_{AF} \)), the feed flowrate of B (\( q_{BF} \)), the feed temperature of B (\( T_{BF} \)), the feed concentration of B (\( C_{BF} \)) and the coolant flowrate to the jacket (\( q_c \)). The output variables are the concentrations of species A, B and C in the reactor (i.e., \( C_A \), \( C_B \), and \( C_C \), respectively), the temperature in the tank (\( T \)), and the coolant temperature (\( T_C \)) in the jacket. Thus, in all, this process has seven (7) inputs and five (5) outputs. However, due to linear
dependencies for the three concentration outputs (i.e., you only need two to determine all three) we eliminated $C_c$ from our evaluation (see Bates and Watts for a discussion on dependencies among outputs and their impact on ME which uses research from Box, et al., 1973; and McLean et al. 1979). Therefore, our study consists of four (4) outputs and seven (7) inputs.

![Figure 2. Schematic of the CSTR from Bhandari and Rollins (2003).](image)

BR effectively modeled this process as a decomposed MISO Wiener system. For the training data, the $R^2$ values were 99% and higher for all the outputs. As Figure 1 shows, for this Wiener system, each output has two types of blocks associated with it. As shown, each input enters its own linear dynamic block. The unobservable outputs from these blocks (i.e., the $v_{ij}$'s) are collected in a vector and passed to a single nonlinear static block which gives the fitted output response. The focus of this study is on reducing the number of estimated dynamic parameters for the terms represented in the linear dynamic blocks which BR
determined to be a second-order-plus-lead (SOPL) transfer function for each block. This model form is given below:

$$g_y(t) = 1 + \frac{\gamma_y - \alpha_y}{\alpha_y - \beta_y} e^{-\frac{t}{\alpha_y}} + \frac{\gamma_y - \beta_y}{\beta_y - \alpha_y} e^{-\frac{t}{\beta_y}}$$

(9)

In Eq. 9, $\alpha_{ij}$ is the dominant time constant, $\beta_{ij}$ is also a time constant and $\gamma_{ij}$ is a lead parameter. We are not using the common Greek letter $\tau$ for these parameters to better distinguish them. The BR estimates for these parameters are given in Table 1. Equivalent parameter sets in the tables are represented by the same color within parameter types. From the colors in Table 1 one can see that for this case, one value of $\alpha_{ij}$ and one value of $\beta_{ij}$ was used for each output but all $\gamma_{ij}$ estimates were different (indicated by no coloring). Thus, the number of estimated dynamic parameters for the BR case is 36 ($4 + 4 + 28$). Note that since the equivalent parameters are contained in the same output (i.e., intra-PE), LSE is appropriate to use for this case. In the next section we will present our proposed multiresponse parameter minimization strategy that will significantly reduce the number of estimated parameters and thereby, make a substantial reduction to the right side of Eq. 7 (i.e., a substantial improvement in inference), while maintaining test set prediction accuracy (i.e., relative SSPE’s close to one).

4. Application of the Proposed Approach to the CSTR

In this section we present a methodology to apply ME to BOM to minimize $P$. More specifically, we will apply ME to block-oriented Wiener modeling with the goal of maximizing statistical inference without adversely affecting prediction accuracy. This goal will be accomplished using a systematic procedure for finding sets of parameters that are not significantly different from one another and estimating only one parameter for each set. For
their CSTR, BR assumed, based on intuition, that the time constants for each output were the same and estimated only one for each type per output. However, in this section we present a procedure for systematically reducing the number of estimated parameters using evidence provided by the values of the estimates. The complete PE procedure is given by the following steps:

1. Using an appropriate method, determine the static and dynamic model structures and parameter estimates under a full set of dynamic model parameters using LSE from the training data.
2. Determine SSPE’s for all the outputs for the testing data.
3. Using the estimates from Step 1 as the starting values, determine estimates for the full set of dynamic parameters using the multiresponse determinant criterion, i.e., Eq. 6, and the model determined in Step 1. This is the base case.
4. Determine SSPE’s for the current case using the testing data.
5. Determine the right-hand side of Eq. 7, i.e., \( P_s^2 F_{a_p,N-p} \) for the current case.
6. Reduce the number of estimated dynamic parameters by grouping them into equivalent sets.
7. Using the training data with the equivalent sets determined in Step 6, determine the estimate for each set using ME.
8. Repeat Step 4
9. Repeat Step 5
10. If \( P_s^2 F_{a_p,N-p} \) decreases and the SSPE’s do not increase too much repeat Steps 6 to 9; otherwise stop.

Because of the complexity of the objective function, good starting values are critical in ME as well as the choice of the estimation algorithm. We had success using the Solver tool in the Microsoft Office Excel 2003 software package when using the starting values from the full set of parameters determined from LSE and recommend this as a procedure for obtaining starting values. While is it beyond the scope of this article to explain the use of Solver, we provide the following assistance for using it for ME. For a fixed set of starting values for the parameters, determine \( Z \) from Eq. 5. Next, using the product of \( Z^T Z \), determine its determinant using Eq. 6. Then run the Solver routine by selecting the cell where the
determinant value is stored as the target cell to be minimized and select the parameters to be changed. **Solver** will change the values of the selected parameters to meet the convergence tolerances set by the user and indicate if the run converged to a solution. If the run is not successful, the user can enter different starting values and rerun **Solver**.

For the CSTR, the model structures as indicated by Step 1 were obtained by BR. The structure for the dynamic model is given by Eq. 9 and the static nonlinear model is given in BR. This procedure is carried out with the static nonlinear model fixed, i.e., ME is used only for the dynamic parameters.

The SSPE’s in Step 2 are determined from LSE for the full set of parameters to compare with the ME SSPE’s to confirm that ME is providing a comparable fit to LSE. Step 3 establishes the performance for the base case which is the full set of ME parameters. When the number of parameters for this case is large, the fit will likely be extremely good and it is not likely that the final reduced set case will fit as well. However, when the final reduced set of parameters is much less than the full set of the base case and has excellent fit, the principle of parsimony and improvement in statistical inference justifies selection of the final case over the base case. As the procedure indicates, Steps 6-9 are repeated until a lower limit in the number of estimated parameters is found based on the criterion of excellent SSPE performance.
Table 1. Dynamic parameters estimates – DR case. P = 36.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$C_A$</th>
<th>$C_B$</th>
<th>$T$</th>
<th>$T_C$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_{1j}$</td>
<td>0.70</td>
<td>0.64</td>
<td>0.52</td>
<td>0.52</td>
</tr>
<tr>
<td>$\alpha_{2j}$</td>
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<td>0.64</td>
<td>0.52</td>
<td>0.52</td>
</tr>
<tr>
<td>$\alpha_{3j}$</td>
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<td>0.64</td>
<td>0.52</td>
<td>0.52</td>
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<td>$\alpha_{4j}$</td>
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<td>0.64</td>
<td>0.52</td>
<td>0.52</td>
</tr>
<tr>
<td>$\alpha_{5j}$</td>
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<td>0.64</td>
<td>0.52</td>
<td>0.52</td>
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<tr>
<td>$\alpha_{6j}$</td>
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<td>0.64</td>
<td>0.52</td>
<td>0.52</td>
</tr>
<tr>
<td>$\alpha_{7j}$</td>
<td>0.70</td>
<td>0.64</td>
<td>0.52</td>
<td>0.52</td>
</tr>
<tr>
<td>$\beta_{1j}$</td>
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<td>0.62</td>
<td>0.52</td>
<td>0.53</td>
</tr>
<tr>
<td>$\beta_{2j}$</td>
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<td>0.62</td>
<td>0.52</td>
<td>0.53</td>
</tr>
<tr>
<td>$\beta_{3j}$</td>
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<td>0.62</td>
<td>0.52</td>
<td>0.53</td>
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<tr>
<td>$\beta_{4j}$</td>
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<td>0.62</td>
<td>0.52</td>
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<td>$\beta_{5j}$</td>
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<td>$\beta_{6j}$</td>
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<td>0.62</td>
<td>0.52</td>
<td>0.53</td>
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<tr>
<td>$\beta_{7j}$</td>
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<td>0.62</td>
<td>0.52</td>
<td>0.53</td>
</tr>
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<td>1.70</td>
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<td>-0.06</td>
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<tr>
<td>$\gamma_{6j}$</td>
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<td>0.60</td>
<td>0.40</td>
<td>0.29</td>
<td>0.30</td>
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</tbody>
</table>

We will now apply the above procedure to the CSTR where $N = 580$. Step 1 was discussed above. In Step 2, the SSPE’s for the full set ($P = 84$) using LSE were similar to the SSPE’s for the full set using ME in Step 3. The SSPE’s for all the cases are in Table 2. The ME full set of parameters is given in Table 3 as Case 1 since it represents the first iteration in reducing the number of estimated dynamic parameters using ME.
Table 2. SSPE results for all the cases in the CSTR simulation study.

<table>
<thead>
<tr>
<th>Case</th>
<th>Absolute SSPE</th>
<th>Relative SSPE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$C_A \times 10^3$</td>
<td>$C_B \times 10^3$</td>
</tr>
<tr>
<td>BR</td>
<td>7.59</td>
<td>7.27</td>
</tr>
<tr>
<td>1</td>
<td>5.75</td>
<td>6.03</td>
</tr>
<tr>
<td>2</td>
<td>6.56</td>
<td>6.05</td>
</tr>
<tr>
<td>3</td>
<td>7.40</td>
<td>6.15</td>
</tr>
<tr>
<td>4</td>
<td>8.06</td>
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<td>8.06</td>
<td>6.18</td>
</tr>
<tr>
<td>6</td>
<td>6.50</td>
<td>6.17</td>
</tr>
</tbody>
</table>

Table 3. The full set of ME parameters – Case 1. $P = 84$.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$C_A$</th>
<th>$C_B$</th>
<th>$T$</th>
<th>$T_C$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_{1j}$</td>
<td>1.23</td>
<td>1.20</td>
<td>2.34</td>
<td>1.19</td>
</tr>
<tr>
<td>$\alpha_{2j}$</td>
<td>1.24</td>
<td>0.49</td>
<td>0.55</td>
<td>0.57</td>
</tr>
<tr>
<td>$\alpha_{3j}$</td>
<td>0.75</td>
<td>0.72</td>
<td>0.64</td>
<td>0.63</td>
</tr>
<tr>
<td>$\alpha_{4j}$</td>
<td>0.59</td>
<td>0.55</td>
<td>0.53</td>
<td>0.64</td>
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<tr>
<td>$\alpha_{5j}$</td>
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<td>0.92</td>
<td>0.77</td>
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<tr>
<td>$\alpha_{6j}$</td>
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<td>0.47</td>
<td>0.34</td>
<td>0.52</td>
</tr>
<tr>
<td>$\alpha_{7j}$</td>
<td>0.56</td>
<td>0.62</td>
<td>0.49</td>
<td>0.21</td>
</tr>
<tr>
<td>$\beta_{1j}$</td>
<td>1.11</td>
<td>1.20</td>
<td>0.48</td>
<td>1.19</td>
</tr>
<tr>
<td>$\beta_{2j}$</td>
<td>0.37</td>
<td>0.72</td>
<td>0.55</td>
<td>0.57</td>
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<td>$\beta_{3j}$</td>
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<td>0.19</td>
<td>0.28</td>
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<td>0.55</td>
<td>0.53</td>
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<tr>
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<td>0.70</td>
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<td>0.54</td>
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<tr>
<td>$\beta_{6j}$</td>
<td>0.61</td>
<td>0.47</td>
<td>0.65</td>
<td>0.52</td>
</tr>
<tr>
<td>$\beta_{7j}$</td>
<td>0.55</td>
<td>0.62</td>
<td>0.49</td>
<td>0.64</td>
</tr>
<tr>
<td>$\gamma_{1j}$</td>
<td>1.93</td>
<td>0.25</td>
<td>4.39</td>
<td>3.72</td>
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<tr>
<td>$\gamma_{6j}$</td>
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<td>-0.93</td>
<td>0.01</td>
<td>-0.10</td>
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<tr>
<td>$\gamma_{7j}$</td>
<td>0.20</td>
<td>0.33</td>
<td>0.25</td>
<td>0.01</td>
</tr>
</tbody>
</table>

From comparing Tables 1 and 3, it appears that the BR decision to make the time constants (i.e., the $\alpha$’s and $\beta$’s) for each output an equivalent set was not a good one. As one
can see from Table 3, $\alpha_{1j}, j = 1$ to $4$, $\alpha_{21}$, $\beta_{11}$, $\beta_{12}$ and $\beta_{14}$ appear to be significantly larger than the other time constants. Nonetheless, there appears to be several possible equivalent sets.

Table 4 gives the results for the right-hand side of Eq. 7, i.e., $P s^2 F_{a,P,N-P}$, as required by Step 5. Comparing the results for Cases BR and 1, $P s^2 F_{a,P,N-P}$ for Case 1 is much lower indicating a substantial improvement in statistical inference over Case BR even though the BR value of $P$ is much lower (36 vs. 84). As Table 4 shows, the difference is in the considerably smaller value of $|Z^T Z|$, which translate to a much smaller value for $s^2$ for Case 1. Consequently, since our goal was to find the smallest value of $P s^2 F_{a,P,N-P}$, we used Table 3 to develop equivalent parameter sets for the next case.

The variations in the colors in Table 5 indicate the equivalent parameter sets we chose for Case 2. These selections were obtained by setting parameters equal based on the results contained in Table 3. For example, in Table 3, $\alpha_{11} = 1.23$, $\alpha_{12} = 1.20$, $\alpha_{14} = 1.19$ and $\alpha_{21} = 1.24$; hence, in Table 5 we set $\alpha_{11} = \alpha_{12} = \alpha_{14} = \alpha_{21}$. The result that you see in Table 5 is the value we obtained for $\alpha_{11}$, $\alpha_{12}$, $\alpha_{14}$, and $\alpha_{21}$ after estimation under the constraint that $\alpha_{11} = \alpha_{12} = \alpha_{14} = \alpha_{21}$. To facilitate convergence, the initial values that we used for this case were taken from Table 3. In particular, Table 5 shows the values for all the parameter estimates after applying ME. Note that, in addition to the color variations, the equivalent sets in Table 5 can be distinguished by the parameters that are the same. This completes Steps 6 and 7 in the proposed procedure.
Table 4. Determination of the term $\text{Ps}^2 F_{a,P,N-P}$ for all cases with $\alpha = 0.05$.

| Case | P   | (N-P) | $|Z'|^2 | s^2 | F_{a,P,N-P} | \text{Ps}^2 F_{a,P,N-P} | \text{Ratio to Case 6} | % Change to Case 6 |
|------|-----|-------|-------|-----|-------------|-------------------------|------------------------|---------------------|
| BR   | 36  | 544   | 3.14  | 5.77| 1.44        | 229.1                   | 4.98                   | 79.9                |
| 1    | 84  | 496   | 0.52  | 1.05| 1.30        | 114.5                   | 1.90                   | 47.5                |
| 2    | 35  | 545   | 0.89  | 1.64| 1.44        | 82.9                    | 1.38                   | 27.5                |
| 3    | 32  | 548   | 0.90  | 1.65| 1.46        | 77.3                    | 1.29                   | 22.2                |
| 4    | 26  | 554   | 0.92  | 1.66| 1.52        | 65.4                    | 1.09                   | 8.1                 |
| 5    | 25  | 555   | 0.93  | 1.67| 1.53        | 63.7                    | 1.06                   | 5.6                 |
| 6    | 23  | 557   | 0.94  | 1.69| 1.55        | 60.1                    | 1.00                   | 0.0                 |

Table 5. The ME parameters for Case 2. $P = 35$.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$C_A$</th>
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<th>$T$</th>
<th>$T_C$</th>
</tr>
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<td>0.65</td>
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</tr>
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<td>0.35</td>
<td>0.03</td>
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</table>
33

As one compares the relative SSPE values from Table 2 for Cases 1 and 2 (i.e., Step 8) there are slight increases for all but one of the outputs. However, with a reduction in parameters from 84 (Case 1) to 35 (Case 2), the benefit in the reduction of \( P S^2 F_{a,P,N-P} \), as shown in Table 4, appears to justify Case 2 over Case 1 (Step 9). Therefore, as indicated in Step 10, we repeated Steps 6-9 for Case 3.

As before, the most reliable estimates, i.e., the ones in Table 5, were used to determine the equivalent sets and initial values for Case 3. The final parameter values for this case are shown in Appendix A, as well as Cases 4 and 5. The SSPE and \( P S^2 F_{a,P,N-P} \) results are contained in Tables 2 and 4, respectively. As these tables show, we repeated Steps 6-9 until Case 6, the final case. As Table 2 shows, the relative SSPE’s for Case 6 are very close to Case 2. Moreover, Table 4 shows an improvement in \( P S^2 F_{a,P,N-P} \) with each case. (Note the stability of \( s^2 \).) For the term \( P S^2 F_{a,P,N-P} \), Cases BR and 1 are about five times and two times larger than Case 6, respectively. \( P \) for Case 6 is 23 which is much lower than Case BR (\( P = 35 \)) and Case 1 (\( P = 84 \)). Case 6 was our final case because we could not reduce \( P \) more without significantly increasing SSPE in Step 10. Therefore, our recommended dynamic parameters and the equivalent sets (Case 6) for this process are given in Table 6.

5. Concluding Remarks

The method that we proposed in this article is a model refinement procedure. We recommend it as a final step in model development to comply with the principle of parsimony which seeks simplicity with high significance. We are suggesting that the proposed method be applied after all model forms and parameters are obtained for the full model. This includes the static model, the dynamic model and even the noise model.
Although all model forms and the static model parameters should be held fixed when applying this procedure, the dynamic and noise parameters should be allowed to change. However, only the dynamic parameters should be formed into equivalent sets during this procedure.

Although we have demonstrated the proposed approach using a continuous-time (CT) model, this procedure is also applicable to discrete-time (DT) models. For example, Rollins and Bhandari (2004) also modeled the CSTR using their DT W-BEST method. The number of dynamic parameters in their final model is the same as the number in the CT model in Bhandari and Rollins (2003), i.e., there are three parameters for each dynamic term. Hence, these parameters could be placed in a table, equivalent sets could be formed, and the proposed procedure applied as it was in this article. Therefore, we recommend the proposed procedure as a model refinement tool for DT methods also.

The procedure that we proposed is an informal parameter equivalency (PE) method for reducing the number of estimated dynamic parameters. It is informal because PE decisions are made intuitively and not by formal statistical testing. More research will be needed to formalize this procedure. Completion of this research will pave the way for the development of algorithms similar to step-wise regression parameter elimination procedures, and perhaps provide a more efficient and automated procedure. One should note the following key differences between automated PE procedure needed for block-oriented modeling and the step-wise parameter elimination procedures found in statistical software packages. In addition to parameter estimates with vastly different distributions, which alone disqualifies step-wise regression as a possible procedure for this application, this type of procedure is vastly different from the one needed. In step-wise regression, parameters are
tested for *existence* but here we are testing parameters for *equivalency*. Furthermore, the step-wise models are linear in parameters and nested, and the goal is model reduction (i.e., model discrimination). In contrast, block-oriented models are non-nested and nonlinear in the dynamic parameters, and model reduction is not the goal, but reduction in the number of *estimated* parameters. Hence, the step-wise regression algorithms are not useful in this application.

Table 6. The ME parameters for Case 6. P = 23.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$\alpha_1$</th>
<th>$\alpha_2$</th>
<th>$\alpha_3$</th>
<th>$\alpha_4$</th>
<th>$\alpha_5$</th>
<th>$\alpha_6$</th>
<th>$\alpha_7$</th>
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<td></td>
<td></td>
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<td>0.64</td>
<td>0.64</td>
<td>0.64</td>
<td>0.64</td>
<td>0.64</td>
<td>0.64</td>
</tr>
<tr>
<td>$T$</td>
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<td>0.64</td>
<td>0.64</td>
<td>0.64</td>
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<td>$T_C$</td>
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<td>0.64</td>
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</tr>
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<td></td>
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</tr>
</tbody>
</table>
LITERATURE CITED

NOMENCLATURE

$C_{Af}$ Feed stream A inlet concentration
$C_{Bf}$ Feed stream B inlet concentration
$C_A$ Concentration of A in the reactor
$C_B$ Concentration of B in the reactor
$f$ Nonlinear static gain function
$F_{P,N-P}$ The $100(1-\alpha)$th percentile of the $F$-distribution with $P$ numerator and $N-P$ denominator degrees of freedom
$g$ Linear dynamic function
$N$ Number of samples or “Nonlinear” on page 2.
$P$ Number of estimated parameters
$q_c$ Coolant flowrate
$q$ Outlet flowrate
$q_{Af}$ Feed A flowrate
$q_{Bf}$ Feed B flowrate
$R^2$ The percent of explained variation
$s^2$ Estimated standard error
$t_k$ Time for $k^{th}$ sample
$T_{Af}$ Stream A inlet temperature
$T_{Bf}$ Stream B inlet temperature
$T_{ci}$ Coolant inlet temperature
$T_C$ Coolant Temperature in the jacket
$T$ Tank Temperature in the reactor
$v(t)$ Vector of intermediate variables for Wiener system
$u$ Input variable
$y$ Observed output
$Y$ Vector of measured outputs
$Z$ Residual matrix

Greek Letters

$\alpha$ Dominant time constant
$\beta$ Smaller time constant
$\gamma$ Lead parameter
$\Sigma$ Variance-covariance matrix

Subscripts

$j$ Input
$i$ Output
$k$ The $k^{th}$ sample

Abbreviations

BOM Block-oriented Modeling
BR Bhandari and Rollins (2003)
CSTR Continuous Stirred Tank Reactor
CT Continuous-time
DT Discrete-time
HPD Highest Posterior Density
LSE Least Squares Estimation
ME Multiresponse Estimation
MIMO Multiple Input, Multiple Output
MISO Multiple Input, Single Output
PE Parameter Equivalency
SISO Single Input, Single Output
SOPL Second-order Plus Lead
SSPE Sum of Squared Prediction Error
W-BEST Wiener Block-oriented Exact Solution Technique

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Table 1. Dynamic parameters estimates – DR case. P = 36.
Table 2. SSPE results for all the cases in the CSTR simulation study.
Table 3. The full set of ME parameters – Case 1. P = 84.
Table 4. Determination of the term $P^2 \text{F}_{\alpha,p,N-p}$ for all cases with $\alpha = 0.05$.
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LIST OF FIGURE CAPTIONS

Figure 1. A description of the general MIMO Wiener model structure (decomposed to q MISO blocks) with $i = 1, ..., q$ outputs and $j = 1, ..., p$ inputs. There is one set of blocks for each of the q outputs. For each set of blocks, each of the p inputs $(u_j)$ passes through a separate linear dynamic block $(G_{ij})$ and produces an intermediate variable, $v_{ij}$, that is an element of the vector $V_i$. Each $v_i$ passes through a non-linear static function $f_i(v_i)$ and generates the output $y_i$.

Figure 2. Schematic of the CSTR from Bhandari and Rollins (2003).
CHAPTER IV. A GENERAL BLOCK ORIENTED MODELLING ALGORITHM FOR STEP INPUT CHANGES

A research note to be submitted to ISA Transactions

Gabrielle L. Larson and Derrick K. Rollins, Sr.

1. Introduction

As processes in industry have become more complicated, linear modeling has become less useful than nonlinear modeling at obtaining accurate models. Block oriented modeling (BOM) is one type of nonlinear modeling approach currently used and receiving much attention [1-5]. In block-oriented modeling, static and dynamic behavior are represented in separate blocks and arranged in a network. The network consists of nonlinear (N) static gain blocks and linear (L) dynamic blocks. The two most popular systems, by simplicity, are the Hammerstein and Wiener systems. As shown in Fig. 1, the first block in the Hammerstein system is the static gain function which is typically nonlinear in the inputs. This function enters the second block consisting of a linear dynamic transfer function. Thus, the Hammerstein system is said to be “NL.” The Wiener system is similar to the Hammerstein system, but reverses the order of the blocks and is thus, “L.N.” The Wiener system allows each input to have separate dynamics. Other systems, generally called Sandwich systems, are combinations of Hammerstein and Wiener (e.g., LNL or NLN, etc.) [6].
Rollins et al. [7] first introduced a closed-form continuous-time exact solution to the single input, single output (SISO) Hammerstein system using a model building technique called the "Block-oriented Exact Solution Technique" or BEST [8]. For Hammerstein modeling it is called "H-BEST", similarly "W-BEST" for modeling Wiener systems. There are several different modeling approaches that can be implemented within model predictive control (MPC); theoretical, empirical, semi-theoretical and semi-empirical modeling. Block oriented modeling uses a semi-empirical approach. Semi-empirical modeling uses a model form with phenomenological interpretation and uses data to estimate unknown parameters [9]. A process model structure is assumed based upon knowledge of the process dynamics which allows the process to be identified as a type of block-oriented system, commonly either Hammerstein or Wiener. Experimental data are then used to estimate model parameters and coefficients.

There are three main benefits of the semi-empirical (i.e. block-oriented) approach. The first one is that the model structure has a physical basis. Another advantage is that there is weak reliance on experimental data compared to empirical modeling. The third benefit is that the model parameters have physical meaning that can be adjusted with changing process
conditions. The goal of the BEST approach is to effectively model a variety of systems under different conditions of specific input changes.

The successful implementation of BEST is dependent on its ability to predict output behavior accurately. One of the stated attributes of BEST is exact solutions to Hammerstein and Wiener systems. However, the two prediction algorithms developed to date are exact under specific conditions only. The first BEST prediction algorithm was developed by [7] and gives an exact solution to a true Hammerstein system under first order dynamic models or sequential step test input sequences (i.e. step input changes where after each input change the process is allowed to come to steady state). For a mathematical proof see [8]. This solution is called the “restricted algorithm” or the “R-algorithm.” The second prediction algorithm was developed by [9] and gives an exact solution to a true Hammerstein system for sequential step input changes. This solution is called the “unrestricted algorithm” or the “U-algorithm” and its proof can be found in [9]. The advantage of the R-algorithm is that it is simple to implement and “compact.” By “compact” we mean that it depends on a small number of previous input changes and for this algorithm it is only one. Therefore this algorithm is commonly used in model building when step tests are used as in the procedures developed for H-BEST in [8] and W-BEST in [10]. However, the disadvantage is that processes are not usually operated with only step test type input changes and using this algorithm to predict under normal operating conditions can lead to significant model mismatch. For this reason [9] developed the U-algorithm which is also compact depending only on two previous input changes. The disadvantage of this algorithm is its complexity to implement.
Due to the limitations of current BEST algorithms in predicting output behavior this work develops new algorithms that give exact solutions to Wiener and Hammerstein systems under no restrictions. The name given to this set of algorithms is the “classical algorithm” or the “C-algorithm.” In Section 2 we derive the exact solutions for Hammerstein and Wiener C-algorithms. In Section 3 we apply the H-BEST C-algorithm to a level process study by Rietz [11]. This section demonstrates the accuracy of the C-algorithm using real process data for model prediction under fast input sampling (i.e. input changes). Concluding remarks are given in Section 4.

2. Derivation of Classical Algorithm

This section derives the C-algorithms for Hammerstein and Wiener systems. For convenience we will assume input changes at each sampling time. Thus we are assuming that we can approximate input behavior by piecewise step input sequences based on the sampling time. However, this is not a restriction to the C-algorithm. The C-algorithm will be derived using the input sequence description given in Fig. 2.

Figure 2. Step input sequence for the C-algorithm derivation
2.1 Hammerstein C-algorithm

The C-algorithm for the Hammerstein system is derived using the input sequence shown in Fig. 2. The block diagram for the Hammerstein system is shown in Fig. 1a. From this figure we see that

\[ v(t) = f(u(t)) \]  

where \( f(u(t)) \) is an unrestricted function of all the inputs. From Fig. 2 \( u(t) \) can be written as

\[ u(t) = u_0 s(t) + (u_1 - u_0) s(t - t_1) + (u_2 - u_1) s(t - t_2) + \cdots + (u_k - u_{k-1}) s(t - t_k) \]  

and in the Laplace domain as

\[ U(s) = \frac{u_0}{s} + \frac{(u_1 - u_0)}{s} e^{-t_1 s} + \frac{(u_2 - u_1)}{s} e^{-t_2 s} + \cdots + \frac{(u_k - u_{k-1})}{s} e^{-t_k s} \]  

From Eqs. 1 and 2 \( v(t) \) is represented by Eq. 4 below:

\[ v(t) = v_0 s(t) + (v_1 - v_0) s(t - t_1) + (v_2 - v_1) s(t - t_2) + \cdots + (v_k - v_{k-1}) s(t - t_k) \]  

and in the Laplace domain as

\[ V(s) = \frac{v_0}{s} + \frac{(v_1 - v_0)}{s} e^{-t_1 s} + \frac{(v_2 - v_1)}{s} e^{-t_2 s} + \cdots + \frac{(v_k - v_{k-1})}{s} e^{-t_k s} \]  

From Fig. 1 the output in the Laplace domain can be represented as

\[ Y(s) = V(s) \cdot G(s) \]  

Therefore by substituting Eq. 5 into Eq. 6 we get
Now solving for the output in the time domain by inverting Eq. 7 we get

\[ y(t) = L^{-1} \left\{ v(s)G(s) \right\} \]

\[ = v_o L^{-1} \left\{ \frac{G(s)}{s} \right\} + (v_1 - v_0) L^{-1} \left\{ \frac{G(s)}{s} e^{-t_1 s} \right\} + (v_2 - v_1) L^{-1} \left\{ \frac{G(s)}{s} e^{-t_2 s} \right\} + \cdots + (v_k - v_{k-1}) L^{-1} \left\{ \frac{G(s)}{s} e^{-t_k s} \right\} \]

\[ = v_o g(t) s(t) + (v_1 - v_0) g(t - t_1) s(t - t_1) + (v_2 - v_1) g(t - t_2) s(t - t_2) + \cdots + (v_k - v_{k-1}) g(t - t_k) s(t - t_k) \]  

where

\[ g(t) = L^{-1} \left\{ \frac{G(s)}{s} \right\} \]  

As shown by this derivation Eq. 8 is an exact solution for a Hammerstein system under step input changes. By treating each sampling instant as an input change, when sampling is fast enough to accurately represent the input variability, Eq. 8 can accurately model Hammerstein type processes. When taken together, Eqs. 1, 8, and 9 represent the C-algorithm.
2.2 Wiener C-algorithm

The C-algorithm for the Wiener system is also derived using the input sequence shown in Fig. 2. The block diagram for the Wiener system is shown in Fig. 1b. From this figure we see that

\[ y(t) = f(v(t)) \]  

(13)

In addition the unobservable output variable of the linear block can be represented in the s-domain as

\[ V(s) = U(s) \cdot G(s) \]  

(14)

Transforming Eq. 14 to the t-domain gives

\[ v(t) = u_0 \cdot g(t) \cdot s(t) + (u_1 - u_0) \cdot g(t - t_1) \cdot s(t - t_1) + (u_2 - u_1) \cdot g(t - t_2) \cdot s(t - t_2) + \cdots + (u_k - u_{k-1}) \cdot g(t - t_k) \cdot s(t - t_k) \]  

(15)

Therefore Eq. 15 is an exact solution for a Wiener system under step input changes. When taken together, Eqs. 13-15 represent the C-algorithm for a Wiener system. Note that the C-algorithms depend on all past input changes which grows with sampling. Therefore, one drawback of this algorithm is this growth in terms. To address this problem we have modified the C-algorithm to carry only the number of terms representing the time interval of settling time. The fading memory C-algorithm is developed on the premise that \( g(t - t_k) \) will be one when \( t \) is much greater than \( t_k \). With this premise Eq. 8 is modified for use in the fading memory algorithm as given by Eq. 16 below.

\[ y(t) \approx v_{k-N} g(t - t_{k-N}) + \cdots + \left(v_{k-1} - v_{k-2}\right) g(t - t_1) \]  

(16)

Similarly, Eq. 15 is modified for use in the fading memory algorithm for a Wiener system as

\[ v(t) \approx u_{k-N} g(t - t_{k-N}) + \cdots + \left(u_{k-1} - u_{k-2}\right) g(t - t_1) \]  

(17)
where \( N \cdot \Delta t \) is approximately equal to the settling time with \( \Delta t \) as the sampling time.

In the next section we demonstrate the superiority of the C-algorithm over the U-algorithm for predicting output response under relatively fast sampling rates.

3. Algorithm Application

To evaluate the proposed method using real data, we applied our method to the SISO self-regulating tank level process shown in Figure 3. The input variable for the experiment is the inlet flow rate, \( q(t) \), which is controlled via a standard PI loop where the control valve in the inlet line is manipulated to achieve or maintain the desired set point. The outlet flow rate from the tank is neither measured nor controlled, rather is a function of the tank height and the position of the manual valve. For this study, the manual valve was left fully open. Since the outlet flow rate is not controlled, the process is self-regulating. The outlet (response variable) is the tank height, \( h(t) \). The data for this study is taken from [11].

![Figure 3. Tank Level System](image)
The model for this process was determined by [11] and was modeled as a Hammerstein process. The static function was determined to be

\[ v(t) = a + b(q - q_0) \]  

(18)

where \( a = 0.3468 \) and \( b = 85.2 \). The linear dynamic function was determined to be a first-order process with \( \tau = 499.51 \) seconds. Thus

\[ g(t) = 1 - e^{-\frac{t}{\tau}} \]  

(19)

Since this is a first order process the C-algorithm and the U-algorithm are equivalent. The U-algorithm is given by Eq. 20.

\[ \hat{h}(t) = \hat{h}(t - \Delta t) + \left( a + b \Delta q \right) + \left( h_0 - \hat{h}(t - \Delta t) \right) \left( 1 - e^{-\frac{\Delta t}{\tau}} \right) \]  

(20)

This algorithm differs from the one in [11] because in [11] the input set point changes were used and not the measured inputs at each sampling time. The fit of the model in [11] was not very good under input set point changes because of significant discrepancies between the values of set points and measured inputs. Rietz tried to correct this problem by developing a change point detection algorithm that better approximated the time of input changes but still did not see much improvement in the fit of the model. Figure 4 shows the fit of the U-algorithm and the C-algorithm based on treating each sampling time as an input change to the test input sequence given in [11]. As this figure shows, the algorithms agree exactly and fit the process very well. Rollins et al. [5] determined that the residuals from this model were serially correlated (an autoregressive process of order two) and applied a pre-whitening method to improve the fit. Therefore, the C-algorithm appears to provide an accurate way to predict BEST model response when inputs changes are rapid enough to not allow the process
to reach steady state between input changes, such as typically found under normal operating conditions.

![Figure 4](image.png)

**Figure 4.** Test sequence performance of $\hat{h}(t)$ for the real process based on treating each sampling time as an input change to the test input sequence given in [11]. Performance is excellent for both the U-algorithm and C-algorithm shown as “fit.”

4. Concluding Remarks

This note proposes a BEST prediction algorithm for predicting output behavior when input changes are too often to allow the process to reach steady state. This algorithm is called the classical algorithm or the C-algorithm and is unrestricted to the type of input sequence or a step test requirement for input changes. The C-algorithm would typically be the algorithm of choice under normal operating conditions or in situations where models are built from plant data as shown in [14] since under these conditions processes rarely reach steady state.
between input changes. One important drawback of the C-algorithm is that one term is added
each time the process is sampled. This can result in a prohibitively large number of terms.
We have addressed this problem by providing a modified algorithm that we call the fading
memory version and it will have a finite number of terms based on the settling time.

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CHAPTER V. CONCLUSIONS AND FUTURE WORK

1. Conclusions

As industry continues to advance, the need for better process control has increased. Model predictive control is one promising solution that creates better control by predicting future behavior of the process. For this strategy to be successful, the model of the process must be accurate. In order to have an accurate model, the model parameters need to be estimated correctly. However, in many cases there are a large number of parameters and estimation can be difficult and time consuming. Ideally, to have an accurate and useable model, it is necessary to reduce the number or estimated parameters by only using the parameters that are most influential for prediction without adversely affecting the model accuracy.

In Chapter 3, this work proposed a methodology to obtain an efficient set of dynamic model parameters in MIMO process modeling. The proposed method is a model refinement procedure and would be a final step in model development. This approach was demonstrated using a continuous-time (CT) model, however this procedure is also applicable to discrete-time models.

The objective of this work has been to present a new method for reducing the number of dynamic model parameters in transfer function modeling. By exploiting multiresponse estimation, which allows outputs to depend on the same parameters, a method was created that determines sets of parameters within and across responses (i.e., outputs) that can be made equivalent without significantly affecting accuracy. Reducing the number of model parameters without adversely affecting model accuracy narrows the width of confidence
intervals for model parameters. That is, for a specific interval width, it raises the level of confidence.

For the seven (7) input, five (5) output simulated CSTR from [1], the number of dynamic parameters was reduced from 84 to 23. This reduction resulted in a 50% decrease in confidence interval width, which increases the confidence level from 50% to 99.9% for a fixed interval width.

Previous methods for predicting output response under relatively fast sampling use an on-line change point algorithm, which requires accurate change point detection. However, it can be difficult to determine a suitable change point algorithm. Since it is of interest to use as much information as possible in order to obtain better prediction, it is desirable to use each available input value.

The proposed BEST prediction algorithm, from Chapter 4, for predicting output behavior when input changes are too often to allow the process to reach steady state treats each sampling time as an input change. Treating each sampling time as an input change, eliminates the requirement of input change point detection. This approach allows the algorithm to be updated at every input change. This algorithm, which is unrestricted to the type of input sequence, is called the classical algorithm or the C-algorithm. Under conditions where processes rarely reach steady state between input changes, such as normal operating conditions, the C-algorithm would typically be preferred. However, one difficulty with using the C-algorithm is that one term is added each time the process is sampled, which can result in a prohibitively large number of terms. A modified algorithm, called the fading memory version, has been provided to address this problem. The fading memory version of the C-
algorithm has a finite number of terms based on the settling time and therefore is less cumbersome to use while at the same time providing excellent prediction.

2. Future Work

In Chapter 3 we proposed a procedure for an informal parameter reduction method for dynamic parameters. The next step would be to develop an algorithm that follows the procedure to automatically reduce the number of parameters. Ideally this new algorithm would know when the improved fit is acceptable or worth the reduction in parameters, and know when to stop trying to improve the fit. In order to know when to stop trying to improve fit a formal test would be necessary. Nonetheless, one could still develop a step-wise parameter equivalency algorithm similar to the step-wise regression procedures, and perhaps provide a more efficient and automated procedure than the one proposed in this work.

Chapter 4 proposed a BEST prediction algorithm for predicting output behavior when input changes are too often to allow the process to reach steady state. Frequently, under normal operating conditions, processes do not reach steady state and are more complex than a simple Hammerstein or Wiener process. Future work should begin to look at predicting output behavior for Sandwich processes when the input needs to pass through a “block” to become a useful input for a Hammerstein or Wiener block process. For example, if the pressure drop is being measured, but flowrate is needed as the input to a Wiener system, the pressure drop would need to pass through a non-linear block to be transformed before going into the LN Wiener system, resulting in a NLN Sandwich system. Similarly, when modeling a Hammerstein system with temperature as the input, the temperature will not immediately reach the target set point. Therefore, the temperature set point needs to pass through the linear dynamic block to be transformed for use in the NL Hammerstein system, therefore
becoming a LNL Sandwich system. Future work with predictive modeling includes extending the presented algorithms to develop useful procedures for modeling plant data. Ultimately creating a user-friendly modeling software that automates all of the methodologies for practical use.

LITERATURE CITED

## APPENDIX

### CASES 3, 4 AND 5

**Table A1.** The ME parameters for Case 3, P = 32.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$C_A$</th>
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<th>T</th>
<th>$T_C$</th>
</tr>
</thead>
<tbody>
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<td>$\alpha_{1j}$</td>
<td>1.20</td>
<td>1.20</td>
<td>2.28</td>
<td>1.20</td>
</tr>
<tr>
<td>$\alpha_{2j}$</td>
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<td>0.54</td>
<td>0.66</td>
<td>0.66</td>
</tr>
<tr>
<td>$\alpha_{3j}$</td>
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<td>0.66</td>
<td>0.66</td>
<td>0.66</td>
</tr>
<tr>
<td>$\alpha_{4j}$</td>
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<td>0.66</td>
<td>0.66</td>
<td>0.66</td>
</tr>
<tr>
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<td>0.66</td>
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<td>0.54</td>
<td>0.66</td>
</tr>
<tr>
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<td>0.66</td>
<td>0.54</td>
<td>0.54</td>
</tr>
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<td>1.16</td>
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<td>1.16</td>
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</tr>
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<td>0.47</td>
<td>0.47</td>
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<tr>
<td>$\beta_{6j}$</td>
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<td>0.49</td>
<td>0.47</td>
</tr>
<tr>
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</tr>
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<td>0.26</td>
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</tr>
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<td>$\gamma_{3j}$</td>
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<td>-0.09</td>
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<td>$\gamma_{4j}$</td>
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<td>0.11</td>
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Table A2. The ME parameters for Case 4, P = 26.

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<tr>
<th>Parameter</th>
<th>C_A j=1</th>
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<th>T j=3</th>
<th>T_C j=4</th>
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<tr>
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<td>0.66</td>
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<td>α_{5j}</td>
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<tr>
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</tr>
<tr>
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<tr>
<td>β_{1j}</td>
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<td>1.16</td>
<td>0.48</td>
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</tr>
<tr>
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</tr>
<tr>
<td>β_{3j}</td>
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<td>0.32</td>
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<td>0.48</td>
<td>0.48</td>
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<tr>
<td>β_{6j}</td>
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<td>0.48</td>
<td>0.48</td>
<td>0.48</td>
</tr>
<tr>
<td>β_{7j}</td>
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<td>0.48</td>
<td>0.48</td>
<td>0.26</td>
</tr>
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<td>γ_{1j}</td>
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<td>γ_{3j}</td>
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</tr>
<tr>
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<td>-0.88</td>
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</tr>
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<td>0.28</td>
<td>0.36</td>
<td>0.04</td>
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</tbody>
</table>
Table A3. The ME parameters for Case 5, $P = 25$.

<table>
<thead>
<tr>
<th>Parameter</th>
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</tr>
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<td>$\alpha_{j1}$</td>
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<td>1.44</td>
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<td>1.44</td>
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<tr>
<td>$\alpha_{j2}$</td>
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<tr>
<td>$\alpha_{j3}$</td>
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<td>0.65</td>
<td>0.65</td>
<td>0.65</td>
</tr>
<tr>
<td>$\alpha_{j4}$</td>
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<td>0.65</td>
<td>0.65</td>
<td>0.65</td>
</tr>
<tr>
<td>$\alpha_{j5}$</td>
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<td>0.92</td>
<td>0.65</td>
<td>0.65</td>
</tr>
<tr>
<td>$\alpha_{j6}$</td>
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<td>0.55</td>
<td>0.65</td>
</tr>
<tr>
<td>$\alpha_{j7}$</td>
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<td>0.65</td>
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<td>0.55</td>
</tr>
<tr>
<td>$\beta_{j1}$</td>
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<td>0.88</td>
<td>0.49</td>
<td>0.88</td>
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<tr>
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<td>0.49</td>
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<td>$\beta_{j3}$</td>
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<td>0.33</td>
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<tr>
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</tr>
<tr>
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<tr>
<td>$\gamma_{j4}$</td>
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<td>0.05</td>
</tr>
<tr>
<td>$\gamma_{j5}$</td>
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<td>0.13</td>
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<tr>
<td>$\gamma_{j6}$</td>
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<td>-0.88</td>
<td>0.05</td>
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<tr>
<td>$\gamma_{j7}$</td>
<td>0.20</td>
<td>0.28</td>
<td>0.37</td>
<td>0.05</td>
</tr>
</tbody>
</table>
ACKNOWLEDGMENTS

By finishing my coursework and then leaving campus to work full-time while finishing my research and thesis I took an unusual (and somewhat long and difficult) route pursuing and finishing this degree. Therefore, there are many people who deserve thanks and acknowledgement. I’m sure I’ll forget some, but these are the major players in my “support system.” I could not have done this without them.

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