ADAPTIVE DYNAMIC PROGRAMMING FOR HIGH-DIMENSIONAL, MULTICOLLINEAR STATE SPACES

by

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ABSTRACT

ADAPTIVE DYNAMIC PROGRAMMING FOR HIGH-DIMENSIONAL, MULTICOLLINEAR STATE SPACES

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Dynamic programming (DP) is a mathematical programming method for optimizing a system changing over time and has been used to solve multi-stage optimization problems in manufacturing systems, environmental engineering, and many other fields. Exact solutions are only possible for small problems or under very limiting restrictions, but computationally practical approximate DP methods now exist. Most continuous-state problems require discretization of the state space. A design and analysis of computer experiments (DACE) approach for approximate DP uses experimental design and statistical modeling to approximate the value function in continuous-state problems. However, ideal experimental designs are orthogonal, and when the state variables are correlated, ideal experimental designs will not appropriately represent the state space. In this dissertation, the Atlanta ozone pollution problem, which is known for having a multicollinear state space, is selected as our case study. For complex applications like air quality, the state transitions are not given as closed form equations. Rather, an advanced photochemical air quality, such as the Atlanta Urban Airshed Model (UAM), can

represent state transitions. However, the UAM is computationally impractical to be used directly in DP. Therefore, in adaptive DP (ADP), statistical metamodels are developed to provide computationally practical surrogates for state transitions. In the dissertation, three types of state transition metamodels for the Atlanta UAM are developed and implemented in ADP. The first type ignores the inherent collinearity between ozone concentrations at different times and monitoring sites and constructs metamodels that have deliberately high variance inflation factors (VIFs). The second type addresses the multicollinearity using classical regression analysis techniques to yield low VIFs. Finally, the third type develops metamodels that orthogonalize the state space. Results are compared under the base case of the Atlanta case study and 50 random hypothetical scenarios.

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CHAPTER 1

INTRODUCTION

1.1 Background

Dynamic Programming (DP) is a mathematical programming method used to solve a multi-stage optimization problem by breaking it down into a recursive sequence of decision steps over time. Developed by Bellman (1957), DP has been widely used in engineering, economic, social science and many other fields (Bertsekas, 2005, Adda & Cooper, 2003, Burkhauser, Butler, & Gumus, 2004). In this study, we focus on Stochastic DP (SDP), which involves uncertainty. The objective of an SDP problem is to minimize the expected cost (or maximize expected benefit) sequentially over several time stages subject to certain constraints. For a given stage, decisions are made based on current states of the system to minimize cost (or maximize benefit), and states then evolve to next stage based on the chosen decisions, the current states, and the realization of some uncertain components. The system's dynamics are represented by a state transition function. The SDP optimal solutions at a given time stage provide the minimum expected cost (maximum expected benefit) from the given time stage forward through the end of the time horizon. The basic elements of SDP used above can be described as follows:

1. Stage usually represents a particular point in time of the problem's planning horizon. The sequential nature of making decisions in DP evolves through a series of consecutive stages. The DP optimization problem is decomposed by these stages. The time horizon can be an infinite, but this dissertation focuses on the finite and discrete time horizon SDP problem.

2. A state variable holds information required to fully understand the system in order to making an appropriate decision at a particular stage. It also includes information that we need to

describe how the system evolves over time. Defining the state of the system is the most important part of DP problem (Powell, 2011). From a practical point of view, Powell (2011) defines the set of state variables as “the minimally dimensioned function of history that is necessary and sufficient to compute the decision function, the transition function, and the contribution function.” In order words, the set of state variables should be kept as small as possible to reduce the computational effort and mitigate the curse of dimensionality issue. If some state variables are never needed for making decisions, representing system dynamics, or contributing to the objective function, then those state variables should be dropped from the problem. State variables can be discrete, but the focus here is on the continuous state variable case.

3. A decision variable is a control or action that is chosen when the system is in a given state to minimize cost (or maximize benefit) for a particular time stage. Decision variables also represent how we control the system, and the resulting decision impacts how the system evolves to the next stage. In DP, a set of decision rules across the range of states is referred to as a policy for choosing an action.

4. The state transition represents the dynamics of the system. This function describes how the system evolves from one state to another as a result of the decisions and some uncertainties.

5. The objective function specifies the return/contribution (cost or benefit) being optimized over a time horizon. Since in an SDP problem, the objective function is sequentially optimized by stage, the return generated from one stage of the system is called the stage return. The total return accounts all previous stage returns by accumulating them in some manner. The purpose of an SDP problem is to determine the optimal expected total return achieved for each possible state of the system and store them as the future value function or cost-to-go function. This function provides the optimal return to operate the system as a function of the state variables from a given stage to the end of the time horizon.

To solve continuous-state problems, the state space is discretized and the future value function is approximated. For example, one could use a finite grid to discretize the state space, and then interpolate the optimal value function between grid points. However, in high-dimensional problems, a straightforward grid of points, corresponding to a full factorial experimental design, will grow exponentially as the number of state variables increases. This is one form of the “curse of dimensionality” that makes DP computationally intractable. Chen, Ruppert, and Shoemaker (1999) recognized that more efficient state space discretization can be achieved by using methods from design of experiments (DoE), where Chen et al. proposed the use of orthogonal array experimental designs in place of the full factorial design. This approach is based on design and analysis of computer experiments (DACE) from Chen, Tsui, Barton, and Meckesheimer (2006), where for DP the computer experiment is the optimization that occurs in each stage of the DP. To approximate the continuous future value function, Chen et al. employed a regression splines method.

Ideal experimental designs typically assume orthogonality (Chen et al., 2006), therefore, DoE will not appropriately represent the state space when the state variables are highly-correlated, as shown in Figure 1.1 (left figure). It is difficult to design an appropriate experimental design for the correlated case, since DoE provides ideal designs that are “square” (or circular), as shown in the right figure. To handle this multicollinearity issue, the state space can be orthogonalized by using an appropriate data mining technique before conducting DACE.

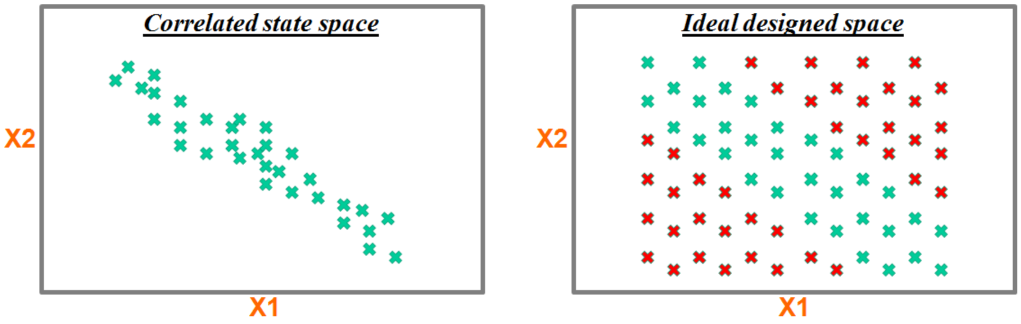

Figure 1.1 Correlated state space vs. Ideal designed space.

Additionally, in extremely high-dimensional SDP problems with more than 100 state variables, directly conducting DACE-based DP would require an extremely large experimental design under the assumption that all 100 or so state variables are important. However, often in practice, not all of these state variables are important, and it is not known in advance which ones should be maintained. Hence, data mining feature selection techniques with small exploratory experimental designs would provide important dimension reduction to reduce state space representation and DP computation.

Therefore, the research objectives in this dissertation are to apply data mining techniques: (1) to address multicollinearity in a DP state space, so as to enable the use of ideal experimental designs, and (2) to reduce the dimensionality of a high-dimensional DP problem. The case study of very high-dimensional SDP problem with highly correlated state variables is represented by an Atlanta ground-level ozone pollution problem (Yang , Chen, Chang, Murphy, & Tsai, 2007, Yang, Chen, Chang, Sattler, & Wen, 2009). In this case study, there are initially more than 500 variables over four time stages and ozone concentration variables at different locations and times are very highly correlated. It should be noted here that this case study uses the old ozone pollution standard that limits maximum hourly ozone to 0.12 parts per million. In order to compare against prior published results, this standard is maintained. For more recent work on identifying control strategies for ozone pollution, see Sule, Chen, and Sattler (2011).

1.2 Research Methodology Overview

These are two main issues, high dimension and multicollinearity, in SDP that this research seeks to address. Because the state transition function is a model representing the dynamics of the system, it is a function that can be used to determine the required variables that should be maintained to keep the SDP problem as small as possible. In this dissertation, data mining techniques are applied for modeling the state transition function. Data mining techniques are employed in this study for two purposes: (1) to orthogonalize a DP state space and enable the use of ideal experimental designs, and (2) to reduce the dimensionality of a DP problem.

In the next chapter (Chapter 2), the previous work related to this research is reviewed and a brief background of the data mining techniques used in this study is described. In Chapter 3, the Atlanta ozone pollution problem case study is introduced, including setting up the SDP problem and determining an metamodel of the complex air quality computer model, which is computationally impractical to use directly as the state transition function. Also in Chapter 3, various types of data mining techniques are explored in a preliminary study on the Atlanta ozone problem. In Chapter 4, general procedures for developing the state transition function are described for two different situations (low and high multicollinearity) in the first section, and then test cases for state transition modeling for the Atlanta ozone pollution problem are shown in another section. In Chapter 5, the proposed state transition functions are implemented in an adaptive DP (ADP) process, and tested under the base air quality case and 50 random hypothetical scenarios. Finally, in Chapter 6, conclusions and future work are discussed.

CHAPTER 2

LITERATURE REVIEW

2.1 Previous Study

This dissertation focuses on continuous-state SDP with a discrete and finite time horizon. The SDP formulation can been seen in (2.1), The objective is to minimize expected cost ($\mathrm{E}[c_t(.)]$) over T discrete stages, subject to certain constraints (Γ_t), where the expected value is taken over a random vector ($\boldsymbol{\varepsilon}_t$) with known probability distribution that models the stochasticity in the system. For a given current stage (t), the state variables ($\boldsymbol{x}_t$) specify the state of the system at the beginning of stage t, and the initial state of the system is represented by $\boldsymbol{x}_1$. The state transition function ($f_t(.)$) defines the transition of the state variables from the current stage ($\boldsymbol{x}_t$) to the next stage ($\boldsymbol{x}_{t+1}$).

$$\begin{aligned} &\min_{u_1,\ldots,u_T} E\left\{\sum_{t=1}^{T} c_t(\mathbf{x}_t, u_t, \boldsymbol{\varepsilon}_t)\right\} \\ &\text{s.t.} \quad \mathbf{x}_{t+1} = f_t(\mathbf{x}_t, u_t, \boldsymbol{\varepsilon}_t), \text{for } t = 1,\ldots,T-1 \\ &\qquad\; u_t \in \Gamma_t, \text{for } t = 1,\ldots,\; T \end{aligned} \tag{2.1}$$

Given the state $\boldsymbol{x}_t$ of the system at any stage t, we can solve for the future value function ($\boldsymbol{V}_t(\boldsymbol{x}_t)$) using the Bellman (1957) recursive equation (2.2), and the optimal policy $\boldsymbol{u}_t$ obtained from solving (2.2) is used to control the system at time stage t.

$$\begin{aligned} &V_t(x_t) = \min_{u_t} E\{c_t(\mathbf{x}_t, u_t, \boldsymbol{\varepsilon}_t) + V_{t+1}(x_{t+1})\} \\ &\text{s.t.} \quad \mathbf{x}_{t+1} = f_t(\mathbf{x}_t, u_t, \boldsymbol{\varepsilon}_t), \text{for } t = 1,\ldots,\; T-1 \\ &\qquad\; u_t \in \Gamma_t, \text{for } t = 1,\ldots,\; T \\ &\text{where } V_T(x_T) = c_T(x_T) \end{aligned} \tag{2.2}$$

The previous studies that are closely related to this dissertation include the work of Chen et. al. (1999), Tsai, Chen, Beck, and Chen (2004), Yang et al. (2007) and Yang et al. (2009).

Chen et. al. (1999) introduced a solution method using a statistical perspective on the high-dimensional, continuous-state SDP problem, and applied their method to inventory forecasting problems. This solution method use statistical experimental design for discretization of the state space and uses statistical modeling for future value function approximation. This DACE-based SDP solution method from Chen et al. (1999) is shown in Figure 2.1. In each DP stage *t*, an experimental design is used to specify values of the state variables, which are the predictor variables. The optimization computer experiment is solved for these designed state values to obtain the optimized objective value (future value), which is the response variable. Then a statistical model is constructed to estimate the future value function based on this dataset, with input (predictors) variables values taken from DoE and output (response) variables taken from optimization. More specifically, orthogonal arrays (OA) of strength 3 were used to discretize state spaces and multivariate adaptive regression splines (MARS) models were used to approximate future value functions.

```
1. For each stage $t$: Use DoE to sample $N$ points from the state space $\{\boldsymbol{x}_{jt}\}_{t=1}^{N}$.
2. In each stage $t = T - 1, \ldots, 1$:
    (a) For each sampled state point $\boldsymbol{x}_{jt}$, $j = 1, \ldots, N$, solve the minimization problem (1), where $t < T - 1$,
        the future value function $\mathbf{V}_{t+1}(\cdot)$ is estimated by $\hat{\mathbf{V}}_{t+1}(\cdot)$.
    (b) Construct the estimated $\hat{\mathbf{V}}_{t}(\cdot)$ via a statistical model using the data from step 2(a).
```

Figure 2.1 A general algorithm for solving continuous-state SDP problem (Chen et al., 1999).

Tsai et al (2004) utilized the continuous-state SDP solution approach based on the OA/MARS method (Chen et al., 1999) on a wastewater treatment system with up to 20 dimensions. Tsai et al. extends the OA/MARS method by focusing on improving MARS to be more flexible and more robust. The improved version of MARS used automatic stopping rules to reduce computational time and enabled a flexible implementation of MARS. In addition, a robust MARS algorithm was developed to give priority to lower-order terms to reduce the complexity and improve the robustness of the approximation model.

Yang et al. (2007) and Yang et al. (2009) developed a decision making framework (DMF) to solve a continuous-state SDP problem using similar structure to the approach developed by Chen et al. (1999). However, the dimension of the problem in Yang et al., which is the Atlanta ground-level ozone pollution studied in this dissertation, initially is more than 500. In this problem, the complex air quality model used to simulate ozone concentration over time is computational impractical to directly use as the state transition function in the DACE based SDP solution method. Hence, DACE methods, specifically Latin hypercube experimental designs and stepwise regression statistical models, were employed to construct state transition function metamodels as surrogates for the complex air quality model in the DP problem. To obtain the metamodels, Yang et al. (2007) proposed two phases: an exploratory mining phase and a metamodeling phase. After these two phases, dimension of the SDP problem was reduced to 25.

2.2 Data Mining for Computer Experiment

Data mining methods are employed in this study for two purposes: (1) to orthogonalize a DP state space and enable the use of ideal experimental designs, and (2) to reduce the dimensionality of a DP problem. In this research, feature selection and feature extraction data mining techniques are utilized and described as follows.

2.2.1. Feature Selection

Feature (variable) selection data mining techniques are used to reduce the size of a DP problem by identifying the important subset of the original features. The feature selection techniques used in this study include stepwise regression, regression trees (Breiman et al., 1984), and a multiple testing procedure based on the false discovery rate (FDR, Benjamini &

Hochberg, 1995). These techniques have been studied by Shih, Pilla, Kim, Rosenberger, and Chen (2006), who found that FDR worked well for the Atlanta ozone pollution problem from Yang (2004).

2.2.1.1 Stepwise Regression

Stepwise regression is an automatic variable selection procedure that uses forward selection and backward elimination processes. As in the forward-selection process, variables are added one by one to the model if they are statistically significant. Then all of the variables already included in the model are evaluated and insignificant variables are deleted. These forward selection with backward elimination processes are repeated until none of the variables outside of the model are significant. In this study, the significance level threshold for a variable to enter or to stay in the model was specified at 0.05.

2.2.1.2 Classification and Regression Trees

Classification and regression trees (CART) developed by Breiman , Friedman, Olshen, and Stone (1984) have become a very popular data mining tool for supervised learning. The CART forward algorithm uses binary recursive partitioning to separate the variable space into rectangular regions based on the similarity of the response values. In this research, regression trees are conducted using CART software from Salford Systems (www.salfordsystems.com). For variable selection, this software provides "variable importance scores." The variable that receives a 100 score indicates the most influential variable for prediction, followed by other variables based on their relative importance to the most important one. However, there are some different options for calculating the scores, and selecting the threshold of the scores to identify important variables may be subjective.

2.2.1.3 Multiple testing procedure based on the false discovery rate (FDR)

Variable selection using FDR usually divides a dataset into c groups based on a categorical response variable. For each predictor variable ($\boldsymbol{x}_i$), we test for differences in the c samples, using a t-test or F-test. For an n-dimensional problem, a collection of hypothesis tests and the corresponding *p*-values $\{p_i\}_{i=1}^{n}$, where p_i is the *p*-value of testing the null hypothesis for variable $\boldsymbol{x}_i$ (where a rejected null hypothesis corresponds to a significant variable). In the literature, it is standard to choose a *p*-value threshold (α) and declare the variable $\boldsymbol{x}_i$ is significant if and only if the corresponding *p*-value $p_i \leq \alpha$. The FDR is defined as the "expected proportion of false positives among all the hypotheses rejected" (Benjamini & Hochberg, 1995). For a given series of hypotheses (H_i), *p*-values (p_i), and ordered *p*-values ($p_{(i)}$). The general FDR-procedure to identify significant variables is shown as follows.

1. Choose a fixed α, where $0 \leq \alpha \leq 1$.
2. Find $\hat{\imath} = \max[i : p_i \leq \frac{i}{m} \cdot \frac{\alpha}{\pi_0}]$, where $\pi_0 (= \frac{m_0}{m})$ denotes the proportion of true H_i.
3. If $\hat{\imath} \geq 1$, $\Omega =$ {All rejected H_i with $p_\text{i} < p_{(\text{i})}$} with FDR($\Omega$) $\leq \alpha$.

   If $\hat{\imath} = 0$, do not reject any hypothesis since $\Omega = \varnothing$.

In this study, $\alpha = 0.05$ and $\pi_0 = 1$ are prespecified.

2.2.2. Feature Extraction

Feature extraction data mining techniques attempt to create new orthogonal features based on transformations of the original features that can provide useful information for modeling (Kim, 2009). The new orthogonal features are linear combinations of the original features. Feature extraction can be used for both dimension reduction and orthogonalization. Principal component analysis (PCA) and partial least squares (PLS) are the feature extraction techniques used in this dissertation. Brief descriptions of PCA and PLS are given in the following sections.

2.2.2.1 Principal Component Analysis (PCA)

PCA can be seen as a method to compute a new coordinate system formed by the latent variables or principal components (PCs) or scores, which are orthogonal. Typically in practice only a few of the most informative PCs are used. In PCA, correlated original variables (***X***) with *n* rows (samples or observations) and *p* columns (variables) are transformed to uncorrelated (orthogonal) PCs (***Z***) which are linear combinations of ***X*** and are defined in (2.3).

Each consecutive PC is orthogonally chosen in descending order of the proportion of explained variation in $\boldsymbol{X}$.

$$\boldsymbol{Z} = \boldsymbol{XE}\ , \tag{2.3}$$

where $\boldsymbol{E} = [\boldsymbol{E_1}, \boldsymbol{E_2},\dots, \boldsymbol{E_p}]$, $\boldsymbol{Z} = [\boldsymbol{Z_1}, \boldsymbol{Z_2},\dots, \boldsymbol{Z_p}]$.

The eigenvectors of the covariance matrix of $\boldsymbol{X}$ are $\boldsymbol{E} = [\boldsymbol{E_1},\boldsymbol{E_2}, \dots,\boldsymbol{E_p}]$, with corresponding ordered eigenvalues ($\boldsymbol{\lambda_1}>\boldsymbol{\lambda_2}>\dots>\boldsymbol{\lambda_p}$), where $\boldsymbol{\lambda_i}$ represents the variance of $\boldsymbol{Z_i}$. Therefore, the first PC, $\boldsymbol{Z_1}$, accounts for the most variation in the original data $\boldsymbol{X}$. The second PC, $\boldsymbol{Z_2}$, is orthogonal to the first, and explains the next largest variation in the data, and so forth. If the original data $\boldsymbol{X}$ has p dimensions, PCA produces p PCs. The PCs describe the latent structure of $\boldsymbol{X}$ and can be used as regressors to predict a response in the regression model.

2.2.2.2 Partial Least Squares (PLS)

The model structures of PLS and PCA are very similar, except that the new orthogonal variables (PLS components, $\boldsymbol{Z}$) are chosen to maximize the covariance between $\boldsymbol{X}$ (predictors) and $\boldsymbol{Y}$ (responses). PLS can be considered as a compromise between PCA, which finds maximum variance in modeling $\boldsymbol{X}$, and ordinary least squares, which finds maximum correlation in modeling $\boldsymbol{Y}$. The covariance of $\boldsymbol{X}$ and $\boldsymbol{Y}$ combines high variance of $\boldsymbol{X}$ and high correlation with $\boldsymbol{Y}$. The PLS components $\boldsymbol{Z}$ are obtained by searching for a weight vector w that maximizes the covariance between the scores of $\boldsymbol{X}$ and $\boldsymbol{Y}$ shown in (2.4), then regressing $\boldsymbol{Z}$ on $\boldsymbol{X}$ and $\boldsymbol{Y}$ by (2.5)-(2.6), and finally the prediction model $\boldsymbol{Y}$ using the original $\boldsymbol{X}$ can be defined by (2.7). $\boldsymbol{P}$ and $\boldsymbol{Q}$ are loading matrices, and $\boldsymbol{E}$ and $\boldsymbol{F}$ are residual matrices. PLS components $\boldsymbol{Z}$ can be extracted from many algorithms but in this study, PLS based on Wold, Sjöström, and Eriksson (2001) was used, where each PLS component $\boldsymbol{Z}$ and weight w are orthogonal ($\boldsymbol{Z_i}^{\mathrm{T}}\boldsymbol{Z_j}=0$, $\boldsymbol{w_i}^{\mathrm{T}}\boldsymbol{w_j}=0$; $i \neq j$).

$$\boldsymbol{Z} = \boldsymbol{Xw}\ , \tag{2.4}$$

$$\boldsymbol{X} = \boldsymbol{ZP}^{\mathrm{T}} + \boldsymbol{E}\ , \tag{2.5}$$

$$\boldsymbol{Y} = \boldsymbol{ZQ}^{\mathrm{T}} + \boldsymbol{F}\ , \tag{2,6}$$

$$\boldsymbol{Y}_{hat} = \boldsymbol{ZQ}^{\mathrm{T}} = \boldsymbol{Xw}\ \boldsymbol{Q}^{\mathrm{T}} = \boldsymbol{X}\ \boldsymbol{B}_{hat}\ , \tag{2.7}$$

where $\boldsymbol{B}_{hat} = \boldsymbol{w}\,\boldsymbol{Q}^{\mathrm{T}}$.

In general, PLS is better for prediction than PCA because the new orthogonal predictors $\boldsymbol{Z}$ are selected by incorporating information in $\boldsymbol{Y}$.

CHAPTER 3

COMPARISON OF METHODOLOGIES

One of the main reasons for this research is to enable the use of ideal experimental designs for a DACE based SDP solution method when the state variables are highly correlated. The Atlanta ground-level ozone pollution problem from Yang et al. (2009) is selected as our case study because ozone state variables at different monitoring stations and at different time-periods are highly correlated. In addition, the air quality computer model used in the Atlanta ozone problem, called the Atlanta Urban Airshed Model (UAM), is computationally impractical to use directly in the SDP implementation. Therefore, more efficient approaches are studied.

In this chapter, the Atlanta ozone pollution case study is introduced in section 3.1 including spatial and temporal representation of the Atlanta ground-level ozone problem, state and decision variables, objective function and constraints for SDP implementation, and some details about the UAM model. In section 3.2, various metamodels of the UAM that incorporate feature selection and feature extraction data mining techniques are proposed, evaluated, and selected to be used in the next chapter.

3.1 Atlanta Ozone Pollution Problem Case Study

Natural ozone that exists in the upper atmosphere (stratosphere) is good for our earth. This ozone protects the earth from harmful UV rays. However, ozone that is generated at ground-level is a harmful pollutant because ground-level ozone irritates the human eyes and nose and damages vegetation. Ground-level ozone is not directly emitted, but is formed by the chemical reactions of volatile organic compounds (VOCs) and nitrogen oxides (NO_x) in sunlight. Hence, ozone rises during the day and falls at night. Therefore, in order to control ground-level ozone, it is necessary to control emissions of NO_x and VOC. However Atlanta is “NO_x-limited,” which means that targeting VOC emissions is not effective. Hence, for this case study, we focus on NO_x emissions and in the remainder of this dissertation, emissions refer to NO_x emissions. To control NO_x, we have to control the sources of NO_x, which include both point and non-point sources. Power plants and heavy industry that produce a lot of emissions are considered as point sources of NO_x emissions, while other sources, such as small industry and automobiles, are considered as non-point sources.

Figure 3.1 shows a spatial representation of the Atlanta area using the UAM's 40 x 40 grid covering a 160 x 160 kilometer square region of the metropolitan area. Yang et al. (2007) aggregated the 40 x 40 grid into a 5 x 5 grid to represent the non-point source emissions for the Atlanta metropolitan area. In this region, there are a total of 102 point sources. Ozone level is monitored by four Photochemical Assessment Monitoring Stations (PAMS) located at Conyers, S. Dekalb, Tucker, and Yorkville because only these four stations are monitored were the U.S. EPA on the date of the studied ozone episode occurring over July 29 – August 1, 1987.

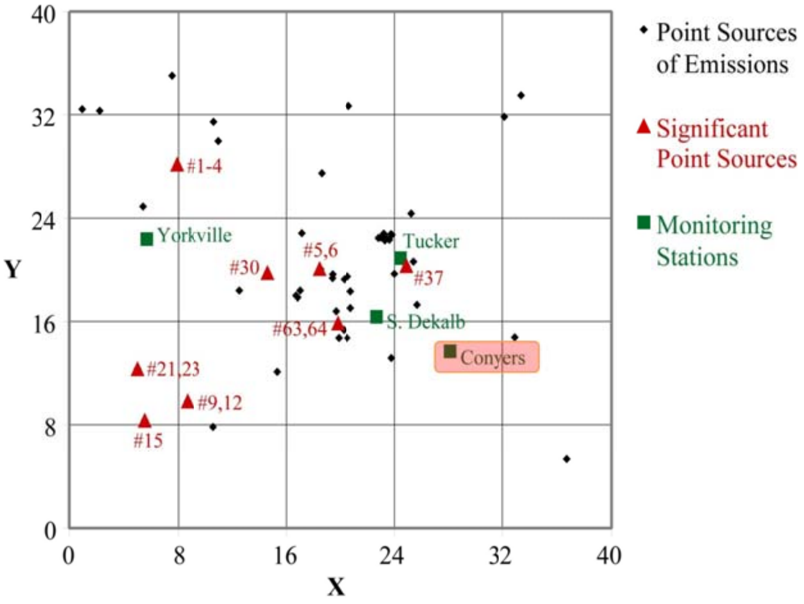

Figure 3.1 Illustration of the emission sources of the Atlanta ozone problem (Yang et al., 2007).

The objective of the Atlanta ozone pollution problem is to minimize the cost of preventing ozone from exceeding the US EPA standard limit, which was 0.12 parts per million in this research (and more recently has been decreased, see http://www.epa.gov/air/criteria.html). To reduce ozone concentrations, emission controls are applied to specific areas and times. Since ozone rises during the daytime when the sun is present, only time periods from 4 a.m. to 7 p.m. are considered as potential time periods for reducing emissions. For the ozone pollution SDP approach, five 3-hour time periods are defined: time period 0 is from 4 a.m. to just before 7 a.m., time period 1 is from 7 a.m. to just before 10 a.m., time period 2 is from 10 a.m. to just before 1 p.m., time period 3 is from 1 p.m. to just before 4 p.m., and time period 4 is from 4 p.m. to just before 7 p.m. Time period 0 is an initialization period. The SDP stages (t) are based on time periods 1 through 4.

3.1.1. State Variables and Decision Variables

At time stage t, the known state variables describe the status of all the factors at the beginning of SDP stage t that may have an impact on ozone concentrations. A sequence of decisions must be made in the four time stages to minimize the total cost to achieve ozone attainment goals. According to the SDP formulation in Chapter 2, state and decision variables of the Atlanta ozone problem can be defined as follows.

State variables ($\boldsymbol{x}_t$) at time t include all historical information on ozone concentrations and NO_x emissions at various spatial locations across the metropolitan Atlanta area. In other words, the initial set of potential state variables for SDP stage t includes information related to ozone air chemistry occurring from time periods 0 though t - 1.

Decision variables ($\boldsymbol{u}_t$) are the actions to be chosen in SDP stage t to control the amount of emissions at various locations and times over the course of the day in order to minimize the reduction of emissions needed to prevent an ozone exceedance.

3.1.2. Objectives and Constraints

The main goal of the Atlanta ozone pollution problem is to maintain the ozone level to satisfy the US EPA standard limit. Although the current ground-level ozone standard has been changed, in this study, the one-hour EPA ozone standard of 0.12 ppm still has been used in order to compare the SDP results with Yang et al. (2009). According to Yang et al., the objective in each of the SDP stage was set up using following criteria.

(1) If the ozone levels are unable to satisfy the EPA standard, then find the control policy to minimize the ozone levels.

(2) If the ozone levels can satisfy the EPA standard, then find the control policy using the least expected cost.

Instead of using strict constraints, Yang et al. use a penalty approach to prioritize more on satisfying the EPA standard. The objective cost function $c_t(\cdot)$ can be divided into two parts, the emission reduction cost function $c_e(\cdot)$ and the penalty cost function $c_{max}(\cdot)$. The SDP objective cost function in each stage *t* (*t* = 1,2,3,…,*T*) can be formulated as follows:

$$c_t(\boldsymbol{x}_t, \boldsymbol{u}_t, \boldsymbol{\varepsilon}) \; = \; \alpha \textstyle\sum_{u_t^i \in \boldsymbol{u}_t} W_t^i c_e\left(u_t^i\right) \; + \; \beta \textstyle\sum_S c_{max}(O_t^S) \;, \tag{3.1}$$

where $c_e(\cdot)$ is the quantic function (3.2) of decision variable u_t^i in $\boldsymbol{u}_t$ and corresponds to the fraction of emission reduced at the emission source i. Let W_t^i be a scaling factor for the emission source i. $c_{max}(\cdot)$ is the quartic function (3.3) of the predicted maximum ozone level O_t^S at monitoring station *S*. In order to satisfy both objective criteria defined above, the α and β values should be chosen such that the penalty cost dominates the emission reduction cost when the maximum ozone levels exceed the EPA limit.

$$c_e(u) \; = \; \begin{cases} 0\,, & u \; \leq 0, \\ 4u^3 - 4u^4\,, & 0 \; < \; u \; < 0.5, \\ u - 0.25\,, & u \; \geq 0.5, \end{cases} \tag{3.2}$$

In the emission reduction cost function (3.2), u is the fraction of the nominal emissions to be reduced and is defined as $u_t^i = (M_t^i - E_t^i)/M_t^i$, where M_t^i is the nominal emission (base case) at source i in time period t, and E_t^i is the corresponding amount of the emission reduction. Because different emission sources may have different amounts of nominal emission, the emission reduction cost for each source i should be scaled using the corresponding scaling factor W_t^i which can be defined as $W_t^i = M_t^i/M$, where M is the total nominal emissions summed over all M_t^i for each time period.

$$c_{max}(x) = \begin{cases} 0\,, & x \leq 0.118, \\ 2.5 \times 10^{11}(x-0.118)^3 - 6.25 \times 10^{13}(x-0.118)^4\,, & 0.118 < x < 0.12, \\ 10^6(x-0.119)\,, & x \geq 0.12. \end{cases} \quad (3.3)$$

In the penalty cost function (3.3), x is the maximum ozone level in ppm for each of the monitoring stations.

For the SDP constraints, the lower and upper limits of emission amounts of a particular source and time period were provided by Dr. Michael Chang at the Georgia Institute of Technology. The nominal emission value is the upper limit of emissions or the maximum amount of emissions realized in the UAM without any control actions. Therefore, the lower and upper bounds of the state and decision variables are also specified by UAM data.

3.1.3. Atlanta Urban Airshed Model (UAM)

At each SDP stage, an air quality model, such as the Atlanta UAM, is needed to evaluate the emission action strategies to determine resulting ozone concentration based on state and decision variables. The UAM may be utilized as a state transition function ($\boldsymbol{x}_{t+1}$) to predict the initial ozone state variables for the next SDP stage.

The UAM is an advanced three-dimensional photochemical air quality grid model that encompasses a 160 x 160 kilometer square region containing the Atlanta metropolitan area. In the 1990's, It was widely used in support of the Clean Air Act Amendments 1990 (CAAA-90) for non-attainment areas to demonstrate their ozone control implementation plans (Georgia state's SIP 2001). Advanced photochemical air quality models help government decision-makers simulate air pollution emissions, chemical reactions, and atmospheric transport in order to evaluate the performance of emission control strategies.

However, direct use of the UAM model in the SDP implementation to calculate ozone concentrations and state transitions is impractical because it is computational expensive and requires very large amount of input data. Therefore, a more efficient model is needed to be utilized as a surrogate for the UAM model within the SDP implementation. Following the work of Yang et al. (2007), this dissertation develops a surrogate model or metamodel of the UAM to be used as a prediction model for ozone concentrations based on relationships between emissions and ozone. The process of developing the metamodels is discussed in section 3.2.

The error terms in the metamodels are used to estimate the stochastic components ε in SDP. It is assumed that these errors follow a normal distribution with mean zero and variance σ. Therefore, the variances σ are estimated by the mean square errors (MSE) of the metamodels. Additionally, all stochastic components in the system are assumed to be independent. Instead of using a continuous normal distribution directly in SDP, the two-point discrete distribution based on the standard normal variable (Z) from Chen et al. (1999) was used and shown in following table.

Table 3.1 Estimated distribution of the errors.

z	$P[Z = z]$
-1	0.5
1	0.5

3.2 Metamodel of UAM

In Yang et al. (2007), the Atlanta UAM model was used as a computer model for generating data on the relevant air chemistry. They studied one of the worst cases in ozone history in urban Atlanta, occurring over July 29 – August 1, 1987, where the episode began on July 31 and peaked on August 1. Yang et al. (2007) and Yang et al. (2009) focused on July 31 with the logic that if the first day of the episode could be controlled, then there might be hope for the controlling the second day. The UAM includes meteorological conditions and nominal emissions as input for this ozone episode. A 500-point Latin Hypercube experimental design was used to scale emissions in different grid regions, different point sources, and different times from zero up to the nominal (maximum) level. These runs were input into the UAM and the resulting ozone concentrations across the 40 x 40 UAM model grid were collected and then aggregated into the 5 x 5 grid. Figure 3.2 shows the metamodeling process that uses the input emissions from experimental design and the ozone output from the UAM to construct statistical models as metamodel surrogates of the UAM. In adaptive DP (ADP), the metamodels are then used to represent the ozone state transition from stage to stage in a DACE based SDP implementation.

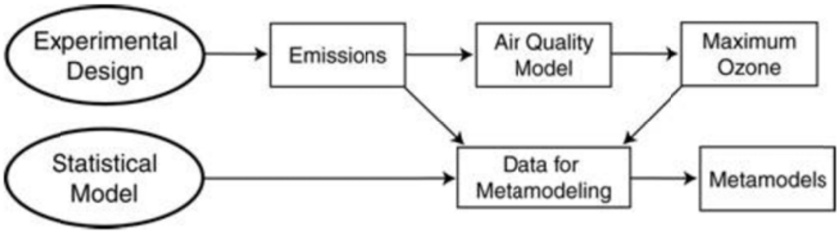

Figure 3.2 Process of developing metamodel (Yang et al., 2007).

Because the state transition function development is an integral part of the ADP process, it is important to conduct dimension reduction for high-dimensional problems, so as to enable better computationally efficiency. In this dissertation, the statistical metamodeling approach is studied in the presence of a highly correlated state space. In this section, various data mining techniques are proposed, including feature selection to reduce dimension and feature extraction to handle multicollinearity. These techniques are evaluated for implementation in the DACE based SDP.

3.2.1. Evaluation Study on Orthogonalized Metamodel Development

In extremely high-dimensional problems with more than 100 state variables, directly conducting DACE based SDP would require an extremely large experimental design. Generally, not all of these state variables are important. Hence, data mining feature selection techniques provide important dimension reduction to reduce computation. Additionally, when the state variables are highly correlated, the ideal experimental design space will not represent the highly correlated state space. To handle this issue, the state space can be orthogonalized by using a feature extraction data mining technique before conducting DACE.

Feature selection data mining techniques are used to reduce the size of the DP problem by identifying the important subset of features. The feature selection techniques used in this study include stepwise regression (Hocking, 1976), regression trees (Breiman et al., 1984), and FDR (Benjamini & Hochberg, 1995).

Feature extraction data mining techniques are used for both dimension reduction and orthogonalization by transforming the original features into new orthogonal features and extracting the useful information for modeling. Principal Component Analysis (PCA) and Partial Least Squares (PLS) are the feature extraction techniques used in this research.

In an evaluation study, 19 modeling approaches are proposed which are shown in Table 3.2. Most of approaches start with a feature selection procedure to reduce the dimension of the original problem, such as using stepwise regression, FDR, or regression trees. Then orthogonalization and dimension reduction are performed using PCA or PLS. For example, approach A-3, first used stepwise regression on the original dataset to select a significant subset of state variables, then used PCA on the selected subset to make them orthogonal, and finally conducted stepwise regression again of the original response on the orthogonal predictors (PCs) to select a final subset of significant PCs.

Table 3.2 Proposed Data Mining Modeling Approaches.

Approach	Pre-Feature Selection	Feature Extraction	Post-Feature Selection
A-1	Stepwise Regression		
A-2	Stepwise Regression	PCA	
A-3	Stepwise Regression	PCA	Stepwise Regression
A-4	Stepwise Regression	PLS	
B-1	FDR w / (2)Categorized Response		
B-2	FDR w / (2)Categorized Response	PCA	
B-3	FDR w / (2)Categorized Response	PCA	Stepwise Regression
B-4	FDR w / (2)Categorized Response	PLS	
C-1	FDR w / Continuous Response		
C-2	FDR w / Continuous Response	PCA	
C-3	FDR w / Continuous Response	PCA	Stepwise Regression
C-4	FDR w / Continuous Response	PLS	
D-1	Regression Tree		
D-2	Regression Tree	PCA	
D-3	Regression Tree	PCA	Stepwise Regression
D-4	Regression Tree	PLS	
E-1	-	PAM Sites – PCA	Stepwise Regression
E-2	-	PCA	Stepwise Regression
F	-	PLS	

3.2.2. Evaluating the Metamodels

Each proposed approach is evaluated on the Atlanta ozone data described above (500-Latin Hypercube design points with ozone concentrations from the UAM) to predict ozone levels for time stage 1 to time stage 4. Table 3.3 shows the numbers of variables involved in the Atlanta ozone SDP problem after the mining phase in Yang et al. (2007). In each stage, the metamodel uses both state and decision variables as initial predictors. It should be noted that the original dimension of the SDP state space prior to the mining phase is over 500.

For the Atlanta ozone problem, non-point sources of emissions are controlled separately in the 5 x 5 grid areas. These comprise 25 non-point source decision variables.

Initially, there are a total of 102 point sources, but after the mining phase in Yang et al. (2007) only 15 were statistically significant; thus, the number of point source decision variables maintained in this study is 15. In each time stage, there are 40 potential decision variables that the decision-maker must control. These decision variables are kept and considered as state variables in the next time stage. Past monitored ozone level information from the four PAMS sites are additional state variables, so the numbers of potential state variables occurring in each time period are 44 variables. For example in time stage 4, the state variables entering stage 4 include all previous ozone levels at all stations and all previous NO_x emissions, i.e., ozone levels and emissions from time periods 0, 1, 2, and 3 yield 176 state variables. The 40 decision variables are the reductions in NO_x emissions for each grid region (5 x 5 = 25) and 15 point sources in time period 4.

Table 3.3 Number of Predictors for the Atlanta Ozone Problem.

	State Space (x_t) (Past Ozone & NO_x)	**Decision Space (u_t)** (NO_x emission)	**Total # Predictors**
Stage-1	44 (40 + 4)	40 (5 x 5 + 15)	84
Stage-2	88 (44 x 2)	40	128
Stage-3	132 (44 x 3)	40	172
Stage-4	176 (44 x 4)	40	216

In the evaluation study, all of the proposed metamodels were constructed separately by time stage to predict only the ozone level at the Conyers monitoring station using the initial dataset shown in Table 3.3. Each modeling approach was evaluated using following performance measures.

- Model R^2 measures how well the model fit to the data.
- Number of variables left in the model represents ability to reduce dimension.
- Variance Inflation Factor (VIF) indicates degree of multicollinearity.
- Percent of prediction error (%Error) based on 10-fold cross-validation to measures model prediction accuracy.

All evaluation results of the proposed metamodeling approach can be seen in Appendix A. However the results for the Conyers station at stage 4 are shown in the Table 3.4. The results show that approaches that start with stepwise regression have higher R^2 and lower error, but they are not the best in term of dimension reduction. FDR and regression trees are very good in dimension reduction but they are less accurate. The approach that incorporates feature extraction methods, including PCA and PLS, are able to handle multicollinearity, indicated by VIFs equal to 1, which means that the approach provides an uncorrelated state space. Because the main goal in this study is to create an uncorrelated state space with better accuracy and a minimal dimension metamodel, approaches with VIF greater than 1 are first removed and then the rest of the approaches are ranked and selected in the next section.

Table 3.4 Results of Various Modeling Scenarios for the metamodel of Conyers stage 4.

Approaches		**R^2**	**Vars. left in model**	**VIF**	**% Error**
A-1	Stepwise	0.9841	26	(1.04 - 44.9)	0.76287
A-2	Stepwise-PCA	0.9841	26	1	0.76287
A-3	Stepwise-PCA-Stepwise	0.9841	25	1	0.76405
A-4	**Stepwise-PLS**	**0.9841**	**9**	**1**	**0.76289**
B-1	FDR	0.9628	9	(1.05 - 56.15)	1.09164
B-2	FDR_PCA	0.9628	9	1	1.09164
B-3	FDR_PCA_StepwiseReg	0.9627	8	1	1.08940
B-4	FDR_PLS	0.9627	7	1	1.09064
C-1	conFDR	0.9548	9	(1.003 - 1.185)	1.25593
C-2	conFDR_PCA	0.9548	9	1	1.25593
C-3	conFDR_PCA_Stepwise	0.9548	9	1	1.25593
C-4	conFDR_PLS	0.9548	4	1	1.25641
D-1	Tree	0.9676	12	(1.01 - 12.10)	1.03436
D-2	Tree_PCA	0.9676	12	1	1.03436
D-3	Tree_PCA_Stepwise	0.9675	11	1	1.03789
D-4	Tree_PLS	0.9676	9	1	1.03437
E-1	PCA-Stepwise	0.9864	167	1	1.03480
E-2	PAMsSites-PCA-Stepwise	0.9836	26	(1.03 - 6.31)	0.78045
F	PLS	0.9877	7	1	1.09891

3.2.3. Selecting Metamodel

After eliminating the approaches that do not meet our main criteria of creating an uncorrelated state space, there are 14 modeling approaches left. These approaches are ranked from the best to the worst separately by the three other criteria which are shown in Table-3.5. The left table is ranked by the number of variables in the model, which indicates dimension reduction ability. The middle table is ranked by percent prediction error, and the last table is ranked by model R^2.

The desired modeling approach should be accurate with fewer dimensions. Even though conFDR-PLS is very good in dimension reduction, it is the worst for prediction accuracy. Overall, stepwise regression with PLS seemed to perform well across all criteria (dimension reduction, orthogonality, and accuracy).Since an objective of the study is an orthogonal model, it was decided to keep Stepwise-PCA and Stepwise-PLS for later study.

Table 3.5 Ranking Results of the Scenarios for the metamodel of Conyers stage 4.

Approaches*	Vars. left in model	Approaches*	% Error	Approaches*	R^2
conFDR_PLS	4	**Stepwise-PCA**	**0.76287**	PLS	0.9877
FDR_PLS	7	**Stepwise-PLS**	**0.76289**	PCA-Stepwise	0.9864
PLS	7	Stepwise-PCA-Stepwise	0.76405	**Stepwise-PCA**	**0.9841**
FDR_PCA_Stepwise	8	Tree_PCA	1.03436	Stepwise-PCA-Stepwise	0.9841
Stepwise-PLS	**9**	Tree_PLS	1.03437	**Stepwise-PLS**	**0.9841**
FDR_PCA	9	PCA-Stepwise	1.03480	Tree_PCA	0.9676
conFDR_PCA	9	Tree_PCA_Stepwise	1.03789	Tree_PLS	0.9676
conFDR_PCA_Stepwise	9	FDR_PCA_Stepwise	1.08940	Tree_PCA_Stepwise	0.9675
Tree_PLS	9	FDR_PLS	1.09064	FDR_PCA	0.9628
Tree_PCA_Stepwise	11	FDR_PCA	1.09164	FDR_PLS	0.9627
Tree_PCA	12	PLS	1.09891	FDR_PCA_Stepwise	0.9627
Stepwise-PCA-Stepwise	25	conFDR_PCA	1.25593	conFDR_PCA	0.9548
Stepwise-PCA	**26**	conFDR_PCA_Stepwise	1.25593	conFDR_PCA_Stepwise	0.9548
PCA-Stepwise	167	conFDR_PLS	1.25641	conFDR_PLS	0.9548

*** VIF > 1 are removed.**

*** Ordered by better to worse**

The results of this study were published in Ariyajunya, Chen, and Kim (2010).

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CHAPTER 4

METAMODEL AND STATE TRANSITION FUNCTIONS DEVELOPMENT

In the SDP formulation in Chapter 2, the state transition function is the function that describes how the state of the system evolves from the current time stage to the next. This function represents the dynamics of a system as a function of state and decision variables and uncertainty. The state transition function can be stationary, i.e., the same for all stages, or it can be non-stationary, i.e., changing from stage to stage. Typically, in the DP literature, the state transition is known. This dissertation employs adaptive DP (ADP) to address the more challenging case of non-stationary state transitions and estimation of unknown system dynamics via data mining statistical models. The state transition function is generally represented by (4.1),

$$\boldsymbol{x}_{t+1} = \boldsymbol{f}_t\ (\boldsymbol{x}_t, \boldsymbol{u}_t, \boldsymbol{\varepsilon})\ , \tag{4.1}$$

where at the beginning of time stage *t*+1, the state of the system ($\boldsymbol{x}_{t+1}$) is determined by the state ($\boldsymbol{x}_t$) at time *t*, the decision ($\boldsymbol{u}_t$) that made at time *t*, and random variable ($\boldsymbol{\varepsilon}$).

In this chapter, a general procedure for developing state transition functions are described for two different situations (low and high multicollinearity) in section 4.1, and then in section 4.2, three test cases for state transition modeling are demonstrated for the Atlanta ozone pollution case study.

4.1 State Transition Function Modeling

In this research, it is assumed that the state transition function is unknown, so it is necessary to estimate state transition functions by utilizing real data from the system itself or perhaps from a simulation of the system dynamics. Even if a computer simulation model is available for complex system, like an airshed, it may be too computationally impractical to directly embed within an SDP implementation. For the DACE based SDP solution method, this issue is further complicated by the presence of multicollinearity of the state space; however, statistical data mining methods can help. The degree of multicollinearity is defined by the variance inflation factor (VIF) from regression modeling (Kutner, Nachtsheim, & Neter, 2005). The general rule of thumb is that VIFs greater than 4 need further investigation, while VIFs greater than 10 indicates serious multicollinearity that requires correction (Kutner et al., 2005). In this research, low and high multicollinearity are the cases where VIFs are less than 4 and VIFs are greater than 10, respectively. The general state transition function modeling procedure for ADP is given for two multicollinearity cases in the next section.

4.1.1 Low Multicollinearity Case

For a given SDP problem that does not have serious multicollinearity issues, the state transition model can be developed as follows (see Yang et al., 2007).

1. Initialization Phase: Identify the stages (t = 1, 2, 3, …, T), state variables, and decision variables of the system including the modeling space (boundary of state and decision variables).

2. Data Collection: For each time stage t, collect data on system dynamics as it evolves through the time stages, and collect data on system performance (i.e., metrics related to cost or benefit objectives). This may be based on purely observational data or may be collected via controlled experiments. When a computer simulation is available, controlled experiments, i.e., a DACE process, are possible. For example, for the Atlanta ozone case study, Yang et al. (2007) used experimental design to control the initial state of the system and the decision variables in each stage, and subsequent states evolved via the simulation.

3. Mining Phase: Utilize feature selection data mining techniques to eliminate state and decision variables that clearly do not influence state transitions or system performance. This is a dimension reduction step. Further dimension reduction may occur in the next phase.

4. Modeling Phase: Construct statistical prediction models of the future state outputs and system performance as a function of the current state and decision design inputs shown previously in (4.1). Uncertainty modeled from the statistical analysis is combined with the prediction models to incorporate random disturbances in the state transition and system performance. These stochastic prediction models serve as state transition functions and metrics for cost or benefit objectives in the SDP implementation. If the system dynamics are simulated by a complex computer model, these models are also referred to as a surrogate models or metamodels of the complex computer model. This phase may involve additional data collection on only those variables selected by the Mining Phase, so as to enable more accurate modeling. Yang et al. (2007) implemented two phases of data collection.

For a high dimensional SDP problem, the Mining Phase is important for reducing the dimensionality of the problem. The developed state transition models are employed directly within ADP process that employs a DACE based experimental design to discretize the state space. Since ideal experimental designs assume the controlled variables can be varied independently, in DACE based SDP, this implies the state variables are assumed to be uncorrelated. If the state variables exhibit low multicollinearity, then ideal experimental designs can still be applied in practice.

4.1.2 High Multicollinearity Case

If the state variables have high multicollinearity, then ideal experimental designs for direct discretization of the state space are inappropriate. Classical regression analysis methods recommend assessing variance inflation factors (VIFs) to evaluate the impact of multicollinearity in a specific regression model (Kutner et al., 2005). High VIFs indicate that the variances of the parameter estimators are inflated due to the high multicollinearity, leading to undesirable models. Careful variable selection can potentially yield regression models with low VIFs that mitigate the impact of the high multicollinearity in the data.

An alternate approach proposed and developed in this dissertation is to modify the representation of the state variables. By transforming the state variables to an orthogonalized set, ideal experimental designs can now be applied to the orthogonalized state variables. In this case, the state transition modeling in the previous section must be modified to incorporate orthogonalized state variables. To achieve orthogonalization, feature extraction data mining techniques are used to transform the state space into one in which the state variables are uncorrelated. In addition, feature selection data mining techniques, including those used by Yang et al. (2007) and Shih et al (2006), are used to reduce the dimension of the state space. This integrated feature extraction and feature selection problem to handle high dimensions with multicollinearity is shown as follows. Phases 1, 2, and 3 are the same as before,

4. Orthogonalization Phase: Orthogonalize the selected state variables ($\boldsymbol{x}_t$) into orthogonal state variables ($\boldsymbol{z}_t$) using a feature extraction technique. This phase may involve additional data collection on only those variables selected by the Mining Phase, so as to enable more accurate modeling. For the analysis in this dissertation, only the second (larger) data set from Yang et al. (2007) is employed.

5. Modeling Phase: Backward from stage $T - 1$ to 1, construct statistical prediction models of $\boldsymbol{z}_{t+1}$ and system performance as a function of $\boldsymbol{z}_t$ and decision variables ($\boldsymbol{u}_t$). Uncertainty modeled from the statistical analysis is combined with the prediction models to incorporate random disturbances ($\boldsymbol{\varepsilon}$) in the state transition and system performance. The stochastic state transition function is shown in (4.2).

$$\boldsymbol{z}_{t+1} = \boldsymbol{f}_t\ (\boldsymbol{z}_t, \boldsymbol{u}_t, \boldsymbol{\varepsilon}). \tag{4.2}$$

Because the $\boldsymbol{z}_t$ are orthogonalized state variables, ideal experimental designs employed within a DACE based SDP solution method are now appropriate. Decision variables were not orthogonalized because they are not part of the experimental design process. In addition, for optimization purposes, it was considered more practical to maintain the decision variables in their original form.

4.2 Test Cases for State Transition Metamodeling for the Atlanta Ozone Pollution Problem

In the SDP implementation of Yang et al. (2007), the metamodels are used to predict ozone concentrations and evaluate control strategies. Ozone concentrations are both state variables and metrics for system performance in this case. Because the system dynamics late in the day depend on the system states early in the day, ozone concentrations and emissions from multiple time periods and locations/sources are maintained among the state variables as the system evolves. The ozone state variables are highly correlated, across both time and location. The main objective of this study is to address multicollinearity in the SDP state space. Three test cases for state transition modeling for the Atlanta ozone study are demonstrated.

The purpose of these test cases is to test the impact of different state transition and cost metamodels within SDP. In SDP, these metamodels are used to predict future behavior of the system (e.g. ozone). If the state variables are orthogonal, then the metamodels are valid over the entire state space. However, if the state variables are correlated, then the metamodels are only valid within the correlated space. Because SDP can attempt to predict behavior using any part of the state space, extrapolation (and poor prediction) can occur. For a state space with high multicollinearity, it is possible to craft a low multicollinearity metamodel using a subset of the state variables by carefully tracking VIFs. For such metamodels, extrapolation may not be a problem, depending on the level of muliticollinearity.

All test cases are based on the same Atlanta ozone problem which is known for a highly correlated state space. The difference in these cases is how they address multicollinearity. The High-VIF test case does not address multicollinearity and allows high VIF metamodels. The Low-VIF test case addresses the multicollinearity problem by carefully crafting regression models to obtain low VIF metamodels. The orthogonalized cases including the Stepwise-PCA and the Stepwise-PLS test cases address multicollinearity by orthogonalization. These test cases of the High-VIF, the Low-VIF, and the orthogonalized cases are demonstrated in Sections 4.2.1, 4.2.2, and 4.2.3, respectively.

4.2.1 High-VIF Test Case

In this section, high-VIF state transition models are deliberately developed to represent a worst case outcome of using the low multicollinearity modeling process in the presence of high multicollinearity. The High-VIF model forces all ozone state variables in the model. Stepwise regression for feature selection is applied only to select emission variables.

The summary of the High-VIF ozone models is shown in Table 4.1. For example, the High-VIF ozone model for the Yorkville site at time stage 1 (ykM3p1), has all four ozone state variables occurring in time period 0 (cyM3p0, skM3p0, tkM3p0, and ykM3p0), then stepwise regression selects 13 emission variables, for a total of 17 variables are included in the ykM3p1 model, The highest VIF for this model is 62.1101, which is very high.

Table 4.1 Summary of the High-VIF Ozone State Transition Functions.

Max Ozone Reg. Model	# Forced Vars.	# Selected Vars.	# Total Vars. in model	Model R-Square	Root MSE	Max VIF
cyM3p1	4	7	11	0.2682	0.000686	1.08587
skM3p1	4	11	15	0.9864	0.000642	17.85896
tkM3p1	4	5	9	0.9612	0.001240	62.00896
ykM3p1	4	13	17	0.9945	0.000022	62.16101
cyM3p2	8	9	17	0.9937	0.000336	30.21039
skM3p2	8	10	18	0.2642	0.005560	69.71315
tkM3p2	8	10	18	0.6370	0.002700	69.4942
ykM3p2	8	20	28	0.9993	0.000023	163.6091
cyM3p3	12	14	26	0.9846	0.000649	76.98236
skM3p3	12	28	40	0.9920	0.001020	75.97847
tkM3p3	12	17	29	0.9747	0.001060	74.85089
ykM3p3	12	15	27	0.9994	0.000032	1366.4426
cyM3p4	16	24	40	0.9847	0.001270	95.77446
skM3p4	16	26	42	0.9930	0.000895	86.51176
tkM3p4	16	43	59	0.9891	0.000789	92.46303
ykM3p4	16	32	48	0.9994	0.000017	374.81606

4.2.2 Low-VIF Test Case

Yang et at. (2007) constructed ozone state transition functions using a regression modeling approach for which most of the models achieved R^2 greater than 0.90 but VIF values in 3 of the 16 models are very high (VIF > 20), indicating serious multicollinearity in those models. To reduce VIFs in the models without incorporating an orthogonalization approach, these ozone state transition models should be revised. Table 4.2 shows summary results of all 16 ozone state transition functions for four PAMS sites and four time periods. Labeling rules for emission and ozone variables shown in Table 4.2 are the variable labels used in the computer codes. The first two letters in each variable label stand for the type of emission source, with “sq” standing for square region source from the 5 x 5 grid in Figure 3.1, and “pt” standing for point sources. If the type is “sq”, then the following two numbers concatenated with an underscore indicate the coordinates of square region in the 5 x 5 grid. If the type is “pt”, then the following number indicates the index of the point source. The letter “p” followed by a number identifies the time period. For example, “sq4_2p1” is the emission quantity within square (4,2) occurring in time period 1, and “pt4p3” is the point source index number 4 occurring in time period 3. Ozone variables are labeled similarly, where the first two letters indicate PAMS sites (cy = Conyers, sk = South DeKalb, tk = Tucker, and yk = Yorkville). For example, “cyM3p1” is the maximum ozone (M3) at the Conyers site in time period 1.

From Table 4.2, the VIF values of the ozone models tkM3p2, ykM3p2, and ykM3p3 are 23.69, 106.64, and 407.03 respectively which indicate serious multicollinearity that needs correction. In addition, some predictors in the model, namely tkM3p1 and tkM3p2, are not significant, as indicated by the p-values of 0.1750 and 0.2335, respectively, so these models also require correction. The models (tkM3p1, tkM3p2, ykM3p2, and ykM3p3) are revised and the results are shown in Table 4.3. The high-VIF models (tkM3p2, ykM3p2, and ykM3p3) are corrected by identifying the highly correlated group of predictors in the models, and then removing some of them, refitting and re-evaluating the models. The process is repeated if VIFs greater than 4 still remain. The tkM3p1 model was revised by using stepwise regression to select only statistically significant predictors at a significance level of 0.05.

Table 4.2 Summary of Ozone State Transition Functions from Yang et al (2007).

Max Ozone Reg. Model	Model R-Square	Root MSE	Max p-value	Max VIF	# Vars. in model	Variables in the model						
cyM3p1	0.2646	0.000685	0.0224	1.01485	7	sq4_2p1	sq2_3p0	sq1_3p1	sq2_5p0	sq1_4p1	sq3_1p1	pt4p1
skM3p1	0.9855	0.000659	0.0072	1.00748	7	sq3_3p1	sq4_3p1	sq4_3p0	pt64p0	skM3p0	sq5_3p0	sq1_2p1
tkM3p1	0.9607	0.001250	**0.1750**	1.03554	7	sq4_3p1	sq3_3p1	tkM3p0	pt5p1	sq4_4p1	ykM3p0	skAMp0
ykM3p1	0.9942	0.000023	0.0027	1.01581	7	sq1_3p1	sq2_3p0	sq1_3p0	sq2_3p1	sq1_4p1	pt30p0	pt64p0
cyM3p2	0.9935	0.000338	0.0056	1.24377	7	sq4_2p1	sq4_2p2	cyM3p1	sq4_2p0	sq3_2p1	sq5_4p1	sq3_2p2
skM3p2	0.1954	0.005750	0.0364	1.03064	7	sq3_3p2	pt15p0	sq4_4p0	pt63p0	sq3_5p1	sq5_4p1	skM3p1
tkM3p2	0.6080	0.002770	**0.2335**	**23.69384**	7	sq4_3p1	skM3p1	tkM3p1	sq4_3p2	pt5p0	sq4_3p0	sq3_5p1
ykM3p2	0.9992	0.000025	<.0001	**106.64782**	7	ykM3p1	sq1_4p1	sq1_4p2	sq1_3p2	sq1_3p1	sq1_3p0	sq2_3p0
cyM3p3	0.9808	0.000709	<.0001	1.01795	7	sq3_2p1	sq3_2p2	sq4_2p3	sq3_2p0	cyM3p2	skM3p1	sq3_2p3
skM3p3	0.9692	0.001940	<.0001	1.02966	7	sq3_3p2	sq3_3p3	sq3_3p1	sq3_3p0	sq3_2p3	sq3_2p2	pt6p1
tkM3p3	0.9536	0.001410	<.0001	1.3483	7	sq3_3p2	sq3_3p1	skM3p2	sq4_3p2	sq3_3p3	sq4_3p3	tkM3p2
ykM3p3	0.9990	0.000041	<.0001	**407.03335**	7	ykM3p2	ykM3p1	sq1_3p2	sq1_3p1	sq1_4p2	sq1_3p3	sq1_4p1
cyM3p4	0.9625	0.001920	0.0021	3.44082	7	sq3_2p3	cyM3p3	tkM3p3	sq3_2p2	skM3p3	sq3_3p1	sq4_2p3
skM3p4	0.9801	0.001460	<.0001	1.57076	7	skM3p3	sq3_3p3	sq3_3p4	sq3_2p3	sq3_2p2	pt6p3	pt5p2
tkM3p4	0.9308	0.001880	<.0001	1.56751	7	sq3_3p3	sq3_3p4	sq3_4p2	sq3_4p1	skM3p3	sq2_4p2	sq2_4p1
ykM3p4	0.9624	0.000130	<.0001	1.01661	7	sq1_4p4	sq1_4p3	sq1_4p2	sq1_3p4	pt4p3	sq1_4p1	pt3p3

Table 4.3 Summary of Revised Ozone State Transition Functions.

Max Ozone Reg. Model	Model R-Square	Root MSE	Max p-value	Max VIF	# Vars. in model	Variables in the model						
tkM3p1	0.9603	0.001250	0.0259	1.01605	5	sq4_3p1	sq3_3p1	tkM3p0	pt5p1	sq4_4p1		
tkM3p2	0.6069	0.002770	0.0052	1.02819	6		skM3p1	tkM3p1	sq4_3p2	pt5p0	sq4_3p0	sq3_5p1
ykM3p2	0.9987	0.000031	<.0001	1.01281	6		sq1_4p1	sq1_4p2	sq1_3p2	sq1_3p1	sq1_3p0	sq2_3p0
ykM3p3	0.9978	0.000059	<.0002	2.33132	5	ykM3p2		sq1_3p2		sq1_4p2	sq1_3p3	sq1_4p1

4.2.3 Orthogonalized Test Case

To handle multicollinear state spaces, various metamodeling methods were developed and evaluated in the previous chapter. Two candidates (Stepwise-PCA and Stepwise-PLS) that perform well across all criteria were selected to develop the transition metamodels for the Atlanta ozone problem.

4.2.3.1 Stepwise-PCA Model

This modeling approach uses stepwise regression to reduce dimensionality and then uses PCA for orthogonalization to handle multicollinearity in the state space. In the ozone pollution problem (refer to Yang et al., 2007), the ozone level at site (*S*) occurring in time *t* is defined as O_t^S. The modeling process is described as follow.

1. For each ozone model, stepwise regression is used to select the statistically significant state and decision variables.

2. In each stage (t), the union of selected state variables $(\boldsymbol{x}_t)$ and the union of selected decision variables $(\boldsymbol{u}_t)$ from the four ozone models are taken separately to determine the set of variables that are maintained in each SDP stage.

3. The state variables in each stage $(\boldsymbol{x}_t)$ are transformed into orthogonal state variables $(\boldsymbol{z}_t)$ by PCA.

4. The orthogonal state transition model is constructed backward from the last time stage (T) to time stage 1. For the last stage (T), only ozone variables (O_T^S) are modeled as a function of the orthogonal state variables $(\boldsymbol{z}_T)$ and decision variables $(\boldsymbol{u}_T)$ by stepwise regression. After adding uncertainty ε, the model can expressed as in (4.3):

$$O_T^S \;=\; \boldsymbol{g}_T\,(\boldsymbol{z}_T, \boldsymbol{u}_T) + \varepsilon\,. \tag{4.3}$$

5. For stage $t = T$ - 1 to 1, the ozone variables O_t^S, and the orthogonal state variables of the next stage $\boldsymbol{z}_{t+1}$ are separately modeled as a function of the orthogonal state variables

$(\boldsymbol{z}_t)$ and the decision variables $(\boldsymbol{u}_t)$ by stepwise regression. The state variables of the next stage $(\boldsymbol{z}_{t+1})$ are modeled only if they are required by the next stage to predict the ozone level (O_{t+1}^S). Finally, after adding uncertainty, the Stepwise-PCA models for stage t are represented by (4.4) and (4.5):

$$O_t^S \;=\; \boldsymbol{g}_t\,(\boldsymbol{z}_t, \boldsymbol{u}_t) + \varepsilon\,, \tag{4.4}$$

$$\boldsymbol{z}_{t+1} = \boldsymbol{f}_t^z(\boldsymbol{z}_t, \boldsymbol{u}_t) + \varepsilon\,. \tag{4.5}$$

The Stepwise-PCA model seems to include a lot more state variables than the original Yang et al. (2007) and the Low-VIF models, so it was decided not implement the Stepwise-PCA model in the Atlanta ozone problem. Only the Stepwise-PLS model is implemented for the orthogonalized case.

4.2.3.2 Stepwise-PLS Model

The Stepwise-PLS modeling process starts with the same procedure used in the Stepwise-PCA approach, which is using stepwise regression to select important variables. However, the orthogonalization process uses PLS instead of PCA. Since PLS performs fitting and transformation simultaneously during the modeling process, state $(\boldsymbol{x}_t)$ and decision $(\boldsymbol{u}_t)$ variables cannot be separately addressed in PLS-model fitting. Since it is desired to orthogonalize only the state variables, the modeling process of the state transition with PLS in each stage is divided into two phases. First, ozone variables are modeled as a function of orthogonalized state variables. Second, the residuals from the first phase are modeled as a function of the decision variables. The following procedures are the Stepwise-PLS modeling process.

1. For each ozone model, stepwise regression is used to select the statistically significant state and decision variables.

2. In each stage (t), the union of the selected state variables $(\boldsymbol{x}_t)$ and the union of the selected decision variables $(\boldsymbol{u}_t)$ from the four ozone models are taken separately to determine the set of variables that must be maintained in each SDP stage.

3. The orthogonal state transition model is constructed backward from the last time stage (T) to time stage 1. For the last stage (T):

Phase (1): Only ozone variables $(\boldsymbol{O}_T)$ are modeled as a function of the orthogonal state variables $(\boldsymbol{z}_T)$ by PLS. Only the subset of $\boldsymbol{z}_T$ that minimizes the predicted residual sum of squares (PRESS) based on Voet's test (van der Voet, 1994) are maintained. After adding uncertainty, the first phase model is shown in (4.6)

$$\boldsymbol{O}_T{}^{(1)} = \boldsymbol{g}_T^{(1)}(\boldsymbol{z}_T) + \varepsilon. \tag{4.6}$$

Phase (2): The residuals of the last stage model $\{\boldsymbol{O}_T - \hat{\boldsymbol{g}}_T^{(1)}(\boldsymbol{z}_T)\}$ are modeled as a function of the decision variables $(\boldsymbol{u}_T)$ by stepwise regression. The second phase model is defined as $\boldsymbol{O}_T{}^{(2)}$ and is shown in (4.7) after adding uncertainty:

$$\boldsymbol{O}_T{}^{(2)} = \boldsymbol{g}_T^{(2)}(\boldsymbol{u}_T) + \varepsilon. \tag{4.7}$$

The final ozone state transition model for the last stage $(\boldsymbol{O}_T)$ is represented by (4.9)

$$\boldsymbol{O}_T = \boldsymbol{O}_T{}^{(1)} + \boldsymbol{O}_T{}^{(2)}, \tag{4.8}$$

$$\boldsymbol{O}_T = \hat{\boldsymbol{g}}_T(\boldsymbol{z}_T, \boldsymbol{u}_T) = \hat{\boldsymbol{g}}_T^{(1)}(\boldsymbol{z}_T) + \hat{\boldsymbol{g}}_T^{(2)}(\boldsymbol{u}_T)\ . \tag{4.9}$$

4. For stages $t = T$ - 1 to 1:

Phase (1): The ozone variables $(\boldsymbol{O}_t)$ and future orthogonal state variables $(\boldsymbol{z}_{t+1})$ are simultaneously modeled as a function of the current orthogonal state variables $(\boldsymbol{z}_t)$ by PLS. Only the subset of $\boldsymbol{z}_t$ that minimizes the predicted residual sum of squares (PRESS) based on

Voet's test (van der Voet, 1994) are selected. The future orthogonal state variables $(\boldsymbol{z}_{t+1})$ are modeled only if they are required by the next stage to predict $(\boldsymbol{O}_{t+1}^{S})$ and $(\boldsymbol{z}_{(t+1)+1})$. After adding uncertainty, the first phase models are shown in (4.10) and (4.11):

$$\boldsymbol{O}_t^{\ (1)} = \boldsymbol{g}_t^{(1)}(\boldsymbol{z}_t) + \varepsilon\,, \tag{4.10}$$

$$\boldsymbol{z}_{t+1}^{(1)} = \boldsymbol{f}_t^{z^{(1)}}(\boldsymbol{z}_t) + \varepsilon\,. \tag{4.11}$$

Phase (2): Residuals from both models $\{\boldsymbol{O}_t - \hat{\boldsymbol{g}}_t^{(1)}(\boldsymbol{z}_t)\}$ and $\{\boldsymbol{z}_{t+1} - \hat{\boldsymbol{f}}_t^{z^{(1)}}(\boldsymbol{z}_t)\}$ are separately modeled as a function of decision variables $(\boldsymbol{u}_t)$ by stepwise regression and these residual models are defined as $\boldsymbol{O}_t^{\ (2)}$ and $\boldsymbol{z}_{t+1}^{(2)}$ respectively. The second phase models are shown in (4.12) and (4.13) after adding uncertainty:

$$\boldsymbol{O}_t^{\ (2)} = \boldsymbol{g}_t^{(2)}(\boldsymbol{u}_t) + \varepsilon\,, \tag{4.12}$$

$$\boldsymbol{z}_{t+1}^{(2)} = \boldsymbol{f}_t^{z^{(2)}}(\boldsymbol{u}_t) + \varepsilon\,. \tag{4.13}$$

The final ozone model $(\boldsymbol{O}_t\ )$ and final state transition function $(\boldsymbol{z}_{t+1})$ are represented by (4.14) and (4.15), respectively:

$$\boldsymbol{O}_t = \hat{\boldsymbol{g}}_t\,(\boldsymbol{z}_t, \boldsymbol{u}_t) = \hat{\boldsymbol{g}}_T^{(1)}(\boldsymbol{z}_t) + \hat{\boldsymbol{g}}_T^{(2)}(\boldsymbol{u}_t)\,, \tag{4.14}$$

$$\boldsymbol{z}_{t+1} = \hat{\boldsymbol{f}}_t^{z}(\boldsymbol{z}_t, \boldsymbol{u}_t) = \hat{\boldsymbol{f}}_t^{z^{(1)}}(\boldsymbol{z}_t) + \hat{\boldsymbol{f}}_t^{z^{(2)}}(\boldsymbol{u}_t)\,. \tag{4.15}$$

Table 4.4 – Table 4.7 show summary results of Stepwise-PLS modeling for Atlanta ozone problem. The Stepwise-PLS metamodel in matrix form can be seen in Appendix B.

Most of the ozone models, R^2 are greater than 0.9. The ozone models (cyM3p1, skM3p2, and tkM3p2) achieve R^2 less than 0.7 but they are comparable with the ozone models in Yang et al. (2007). All VIF values in PLS-Phase (1) model are equal to 1 indicated that all state variables in the models are orthogonal. The modeling of ozone model and state transition functions in stage-4 (Table 4.4), the union set of the stepwise selected state and decision variables are considered as initial predictors xt4 and ut4 respectively. There are initially 81 state variables and 14 decision variables. PLS select 9 orthogonal state variables (Zpls4_1 – Zpls4_9) in Phase (1), and stepwise regression selects a maximum of 3 decision variables in Phase (2). Those 9 selected orthogonal state variables need to be maintained and modeled as a function of xt3 and ut3 in stage-3. In stage-1 (Table 4.7), there are 25 selected orthogonal state variables, which is the maximum number of state variables selected by Stepwise-PLS. Hence, the effective dimension of the SDP in this ADP process is 25.

Table 4.4 Summary of the Stepwise – PLS Ozone and State Transition Functions for Stage-4.

Response Var.	Initial Predictor Variables			Phase-(1) + Phase-(2) Model					Phase-(1) PLS (Multiple-Response)				Phase-(2) Residual of PLS			
Max. Ozone/ Transition	# Initial xt4	# Initial ut4	# Initial Vars.	# Selected zt4 (1)	# Selected ut4 (2)	# Selected Vars.	Model R-Square	Root MSE	# Selected zt4 (1)	Model R-Square	Root MSE	VIF	# Selected ut4 (2)	Model R-Square	Root MSE	VIF (Max)
cyM3p4	81	14	95	9	2	11	0.9795	0.00142	9	0.97467	0.001579	1	2	0.1885	0.00141	1.00012
skM3p4					3	12	0.9858	0.00123		0.97967	0.001474		3	0.2996	0.00122	1.00741
tkM3p4					3	12	0.9469	0.00165		0.67084	0.004103		3	0.8388	0.00164	1.01707
ykM3p4					2	11	0.9231	0.00019		0.64664	0.000398		2	0.7823	0.00018	1.00161

Table 4.5 Summary of the Stepwise – PLS Ozone and State Transition Functions for Stage-3.

Response Var.	Initial Predictor Variables			Phase-(1) + Phase-(2) Model					Phase-(1) PLS (Multiple-Response)				Phase-(2) Residual of PLS			
Max. Ozone/ Transition	# Initial xt3	# Initial ut3	# Initial Vars.	# Selected zt3 (1)	# Selected ut3 (2)	# Selected Vars.	Model R-Square	Root MSE	# Selected zt3 (1)	Model R-Square	Root MSE	VIF	# Selected ut3 (2)	Model R-Square	Root MSE	VIF (Max)
cyM3p3	77	27	104	14	3	17	0.9430	0.00124	14	0.8850	0.00175	1	3	0.5061	0.00122	1.00425
skM3p3					2	16	0.9318	0.00291		0.6789	0.00630		2	0.7875	0.00287	1.00065
tkM3p3					2	16	0.9156	0.00191		0.8988	0.00209		2	0.1651	0.00189	1.00489
ykM3p3					1	15	0.9735	0.00021		0.9732	0.00021		1	0.0096	0.00020	1.00000
Zpls4_1					12	26	0.9667	0.33071		0.7433	0.90653		12	0.8702	0.32593	1.03301
Zpls4_2					14	28	0.9493	0.32087		0.6464	0.83484		14	0.8565	0.31621	1.03135
Zpls4_3					17	31	0.9480	0.26542		0.4443	0.85260		17	0.9065	0.26154	1.04211
Zpls4_4					19	33	0.9664	0.24974		0.6429	0.79780		19	0.9058	0.24607	1.04548
Zpls4_5					17	31	0.9325	0.33760		0.4684	0.93046		17	0.8730	0.33266	1.04183
Zpls4_6					17	31	0.9562	0.25509		0.7810	0.56055		17	0.8002	0.25136	1.04830
Zpls4_7					19	33	0.9364	0.29066		0.6743	0.64474		19	0.8047	0.28639	1.05556
Zpls4_8					19	33	0.9291	0.31745		0.7252	0.61243		19	0.7418	0.31278	1.05501
Zpls4_9					21	35	0.9546	0.25957		0.6779	0.67630		21	0.8591	0.25574	1.06805

Table 4.6 Summary of the Stepwise – PLS Ozone and State Transition Functions for Stage-2.

Response Var.	Initial Predictor Variables			Phase-(1) + Phase-(2) Model					Phase-(1) PLS (Multiple-Response)				Phase-(2) Residual of PLS			
Max. Ozone/ Transition	**# Initial xt2**	**# Initial ut2**	**# Initial Vars.**	**# Selected zt2 (1)**	**# Selected ut2 (2)**	**# Selected Vars.**	**Model R-Square**	**Root MSE**	**# Selected zt2 (1)**	**Model R-Square**	**Root MSE**	**VIF**	**# Selected ut2 (2)**	**Model R-Square**	**Root MSE**	**VIF (Max)**
cyM3p2	56	30	86	23	2	25	0.9348	0.00109	23	0.55289	0.002849	1	2	0.8541	0.00106	1.00093
skM3p2					4	27	0.2847	0.00554		0.15302	0.005999		4	0.1553	0.00541	1.00877
tkM3p2					2	25	0.6466	0.00268		0.63524	0.002719		2	0.0313	0.00262	1.00009
ykM3p2					3	26	0.9690	0.00016		0.70699	0.000480		3	0.8943	0.00015	1.00483
Zpls3_1					17	40	0.9294	0.38581		0.65160	0.841894		17	0.7975	0.37649	1.05335
Zpls3_2					16	39	0.9493	0.32188		0.70498	0.763294		16	0.8281	0.31412	1.04602
Zpls3_3					17	40	0.9392	0.39000		0.51961	1.076335		17	0.8734	0.38059	1.04338
Zpls3_4					19	42	0.9469	0.33551		0.66695	0.823492		19	0.8406	0.32737	1.07408
Zpls3_5					23	46	0.9715	0.22046		0.69152	0.707544		23	0.9076	0.21507	1.08048
Zpls3_6					21	44	0.9557	0.26637		0.68448	0.694804		21	0.8595	0.25988	1.05347
Zpls3_7					22	45	0.9595	0.27725		0.62603	0.822364		22	0.8916	0.27048	1.07646
Zpls3_8					20	43	0.9653	0.23755		0.56770	0.820498		20	0.9197	0.23178	1.06902
Zpls3_9					22	45	0.9464	0.29718		0.66180	0.729094		22	0.8415	0.28993	1.06717
Zpls3_10					22	45	0.9406	0.30363		0.59807	0.771066		22	0.8521	0.29622	1.06380
Zpls3_11					27	50	0.9662	0.21978		0.65908	0.678261		27	0.9010	0.21436	1.08611
Zpls3_12					25	48	0.9534	0.24363		0.59064	0.702705		25	0.8861	0.23764	1.08157
Zpls3_13					24	47	0.9683	0.20054		0.71087	0.589871		24	0.8902	0.19563	1.07075
Zpls3_14					24	47	0.9486	0.29720		0.61231	0.795624		24	0.8675	0.28991	1.08480

Table 4.7 Summary of the Stepwise – PLS Ozone and State Transition Functions for Stage-1.

Response Var.	**Initial Predictor Variables**			**Phase-(1) + Phase-(2) Model**					**Phase-(1) PLS (Multiple-Response)**				**Phase-(2) Residual of PLS**			
Max. Ozone/ Transition	**# Initial xt1**	**# Initial ut1**	**# Initial Vars.**	**# Selected zt1 (1)**	**# Selected ut1 (2)**	**# Selected Vars.**	**Model R-Square**	**Root MSE**	**# Selected zt1 (1)**	**Model R-Square**	**Root MSE**	**VIF**	**# Selected ut1 (2)**	**Model R-Square**	**Root MSE**	**VIF (Max)**
cyM3p1	32	29	61	25	5	30	0.2759	0.00070	25	0.06424	0.000787	1	5	0.2262	0.00068	1.00398
skM3p1					2	27	0.9184	0.00159		0.07675	0.005351		2	0.9116	0.00155	1.00333
tkM3p1					3	28	0.9149	0.00188		0.04726	0.006260		3	0.9106	0.00183	1.00249
ykM3p1					4	29	0.9551	0.00007		0.07803	0.000294		4	0.9513	0.00006	1.00713
Zpls2_1					18	43	0.9612	0.29832		0.12089	1.391971		18	0.9558	0.29047	1.05031
Zpls2_2					12	37	0.9276	0.41252		0.23702	1.321665		12	0.9050	0.40179	1.03773
Zpls2_3					20	45	0.9826	0.20116		0.85759	0.562857		20	0.8777	0.19584	1.06349
Zpls2_4					20	45	0.9511	0.33884		0.16524	1.370479		20	0.9415	0.32988	1.05859
Zpls2_5					23	48	0.9724	0.20212		0.29045	1.000064		23	0.9611	0.19674	1.06132
Zpls2_6					22	47	0.9483	0.29226		0.27594	1.067945		22	0.9286	0.28449	1.05204
Zpls2_7					23	48	0.9554	0.24048		0.42128	0.845325		23	0.9230	0.23408	1.05578
Zpls2_8					26	51	0.9768	0.17808		0.42978	0.858858		26	0.9594	0.17331	1.06798
Zpls2_9					23	48	0.9831	0.14942		0.53723	0.761896		23	0.9634	0.14544	1.06528
Zpls2_10					23	48	0.9833	0.15368		0.55119	0.776067		23	0.9627	0.14959	1.06242
Zpls2_11					25	50	0.9761	0.17277		0.24187	0.946389		25	0.9684	0.16815	1.05964
Zpls2_12					24	49	0.9688	0.20216		0.33873	0.907207		24	0.9529	0.19676	1.05637
Zpls2_13					25	50	0.9527	0.24015		0.69686	0.591502		25	0.8439	0.23374	1.06605
Zpls2_14					24	49	0.9739	0.17679		0.31980	0.879453		24	0.9616	0.17207	1.06654
Zpls2_15					24	49	0.9443	0.25277		0.44521	0.777570		24	0.8997	0.24603	1.05913
Zpls2_16					25	50	0.9842	0.13632		0.64515	0.629220		25	0.9555	0.13268	1.06491
Zpls2_17					22	47	0.9648	0.19580		0.60793	0.637968		22	0.9102	0.19060	1.06042
Zpls2_18					18	43	0.6782	0.54311		0.37516	0.742330		18	0.4851	0.52880	1.04190
Zpls2_19					25	50	0.9844	0.13428		0.52856	0.719374		25	0.9670	0.13070	1.06517
Zpls2_20					23	48	0.9672	0.19380		0.56545	0.687585		23	0.9244	0.18865	1.06291
Zpls2_21					25	50	0.9583	0.22100		0.52436	0.726800		25	0.9124	0.21509	1.06282
Zpls2_22					23	48	0.9741	0.17066		0.52709	0.710687		23	0.9451	0.16612	1.06148
Zpls2_23					19	44	0.9145	0.30748		0.42800	0.779354		19	0.8506	0.29936	1.03533

CHAPTER 5

COMPUTATIONAL RESULTS

The continuous-state SDP problem for the Atlanta ozone problem has been solved using an algorithm shown in Figure 2.1 (Chen et al., 1999). To address multicollinearity in SDP state spaces, three types of state transition function modeling were discussed in section 4.2, namely state transition metamodels with high VIFs, low VIFs, or othogonalized using a procedure such as Stepwise-PLS model. Table 5.1 summarizes the numbers of state as well as decision variables for these three types of metamodels, as implemented in the Atlanta ozone SDP problem. The list of state and decision variables for each metamodel type can be seen in Appendix C. Lower and upper bounds for all state and decision variables are shown in Appendix D.

Table 5.1 Summary of Number of State and Decision Variables for All Methods.

Stage	**Variables**	**# Initial Variables.**	**State Transition Modeling Methods**			
			Yang	**Low-VIF**	**High-VIF**	**Stepwise-PLS**
Stage-4	**# Decision variables**	40	3	3	12	7
	# State variables	**176**	**19**	**19**	**92**	**9**
	# Total variables	216	22	22	104	16
Stage-3	**# Decision variables**	40	9	9	30	25
	# State variables	**132**	**23**	**21**	**82**	**14**
	# Total variables	172	32	32	112	39
Stage-2	**# Decision variables**	40	9	9	31	28
	# State variables	**88**	**25**	**23**	**59**	**23**
	# Total variables	128	34	34	90	51
Stage-1	**# Decision variables**	40	17	17	29	29
	# State variables	**44**	**17**	**16**	**34**	**25**
	# Total variables	84	34	34	63	54

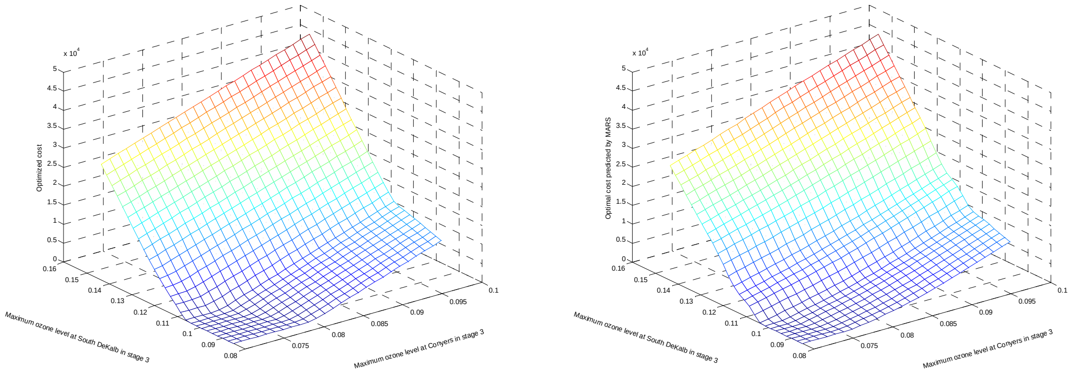
Previous metamodels by Yang et al (2009) have a slightly different set of state variables than the Low-VIF model, but the decision variables are identical. The High-VIF model includes the most of both state and decision variables. All variables included in the Yang et al. and Low-VIF models are a subset of the variables in the High-VIF and Stepwise-PLS models. The dimension of an SDP problem is determined by the maximum number of state variable across all stages; therefore, the SDP dimensions for Yang et al, Low-VIF, High-VIF, and Stepwise-PLS are 25, 23, 92, and 25, respectively.

SDP implementations for all state transition modeling methods are described in Section 5.1. After using a backward SDP solution method to approximate the future value functions, a forward SDP re-optimization in a "real-time" simulation is used to re-solve for the optimal decisions. Re-optimization has been found to be more accurate (Tejada-Guibert, Johnson, & Stedinger, 1993) and is described in Section 5.2. Computational results on optimal control policy are presented for 50 random hypothetical scenarios and the Atlanta base case are shown in Section 5.3. Finally, verification of each of these metamodels is given in Section 5.4.

5.1 Backward DP Solution for the Future Value Function of the Atlanta Ozone Problem

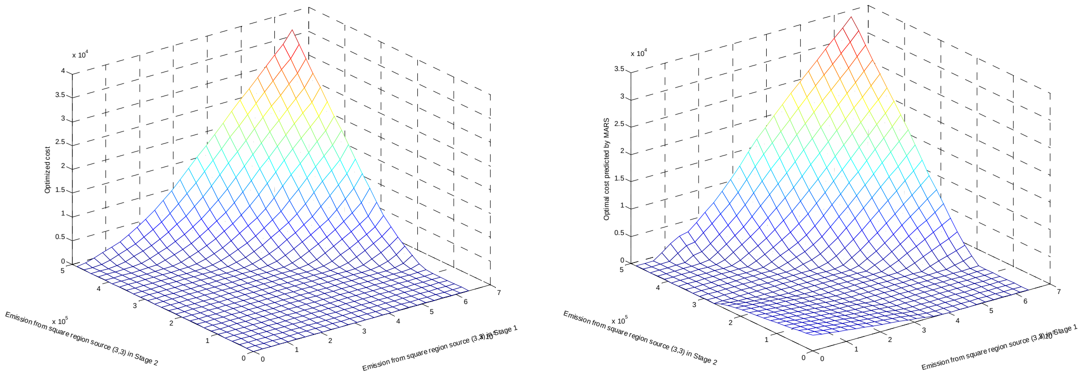
The backward DP solution method solves the problem starting from the last stage and moves backward until all stages have been solved, as described in Figure 2.1. Following Yang et al. (2009), a low-discrepancy sequence by Sobol´ (1967) was employed to discretize state space, and multivariate adaptive regression splines (MARS) models were used to approximate future value functions of the Atlanta ozone problem. The 2000 designed points from the Sobol´ sequences were generated using the Sobol´ dataset generator obtained from the website: http://people.sc.fsu.edu/~jburkardt/cpp_src/sobol_dataset/sobol_dataset.html. At each design point, a non-linear programming was used to solve for an optimal solution and a commercial optimization library (NAG E04) was utilized as the optimization module in solving the SDP for the Atlanta ozone problem. The three different types of modeling methods for the state transition function, from Section 4.2, are implemented in the Atlanta ozone problem separately.

In each stage, the solution of the backward SDP process is the MARS approximation of the future value functions for each stage. For visualization purposes, a 3D mesh plot of each future value function and the corresponding MARS approximation in each stage are generated, but only two state variables can be plotted and the other variables are fixed at the midpoint of their possible range. Mesh plots in Figures 5.1 – 5. 4 illustrate the future value functions and their MARS approximations for the Atlanta ozone SDP problem using the Low-VIF metamodels. The plots show that the MARS approximations seem to mimic the future value function appropriately. Unlike the previous study (Yang et al., 2009), which allows MARS approximations to fall negative, in this study the negative MARS values are truncated to zero because a negative cost is not realistic. Since the NAG optimization module requires convexity of the objective function, the mesh plots of the future value functions in stage 1 (Figure 5.4) and stage 2 (Figure 5.3) exhibit a non-convexity issue. To address the potential for local optima, multiple starting points are implemented with the optimization module to achieve better optimal costs. Although the use of many starting points increases the chance of getting close to the global optimal cost, this study is limited to two starting points (midpoint and lower bound) and an additional ten random points within the ranges for computational reasons. Figure 5.5 – 5.8 compare the optimal costs when using multiple starting points. The use of multiple starting points tends to achieve better optimal costs than using only one starting (middle) point, especially in stage 1 and stage 2. Adding ten random points tends to improve optimal costs more on average. Therefore in this SDP implementation, the optimization module includes the two plus ten random starting points for stage 1 and stage 2.



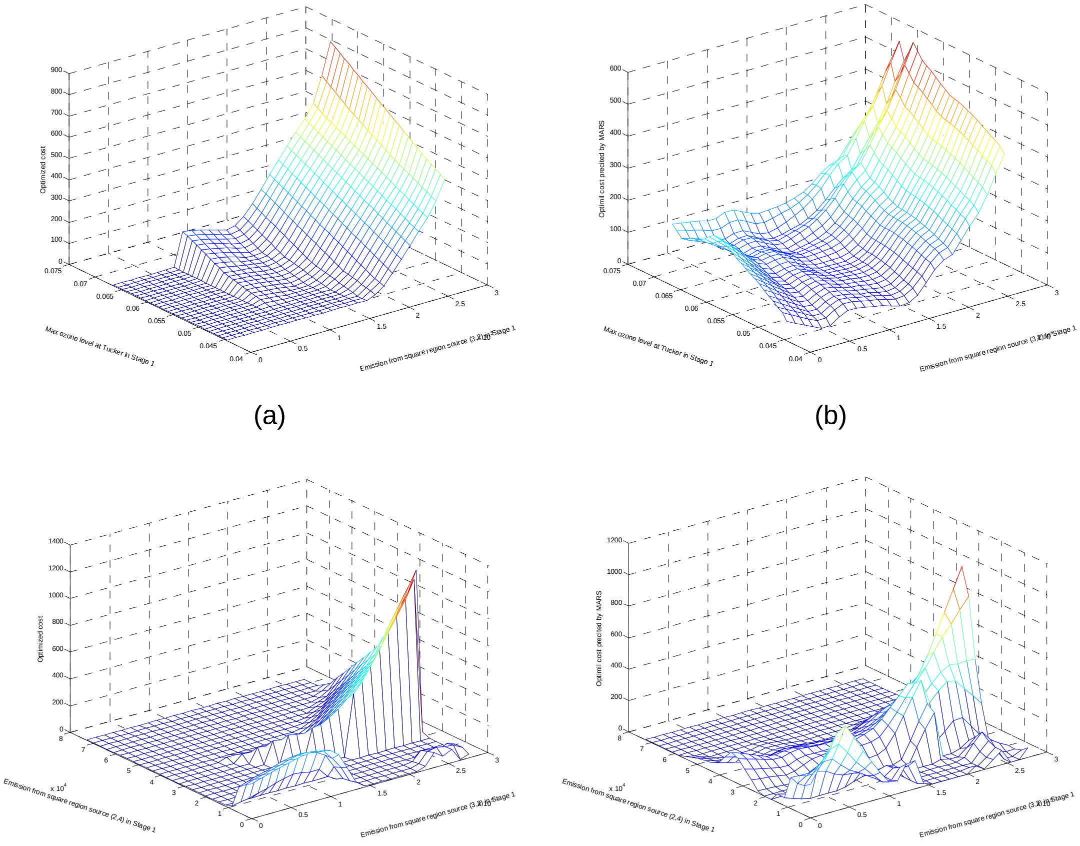
(a) (b)

Figure 5.1 Future value function (a) and MARS approximation (b) using Low-VIF model for stage 4.



(a) (b)

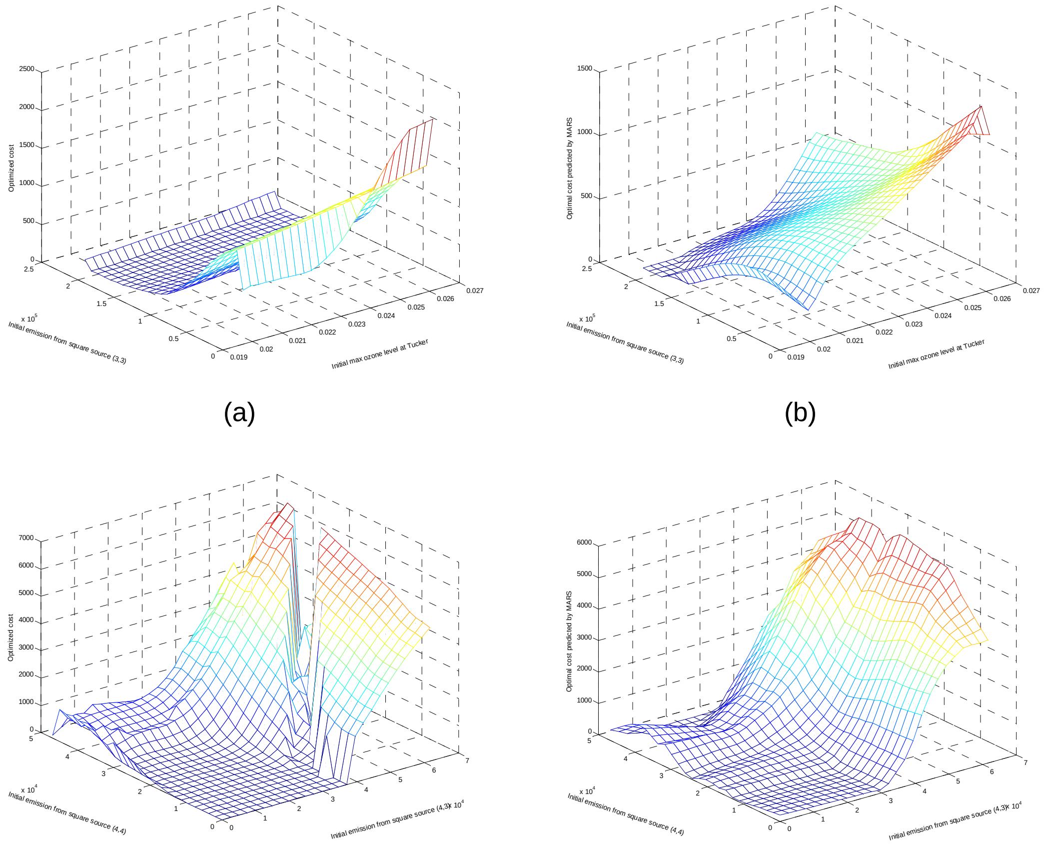
Figure 5.2 Future value function (a) and MARS approximation (b) using Low-VIF model for stage 3.



(a) (b)

(c) (d)

Figure 5.3 Future value function (a, c) and MARS approximation (b, d) using Low-VIF model for stage 2.



(a) (b)

(c) (d)

Figure 5.4 Future value function (a, c) and MARS approximation (b, d) using Low-VIF model for stage 1.

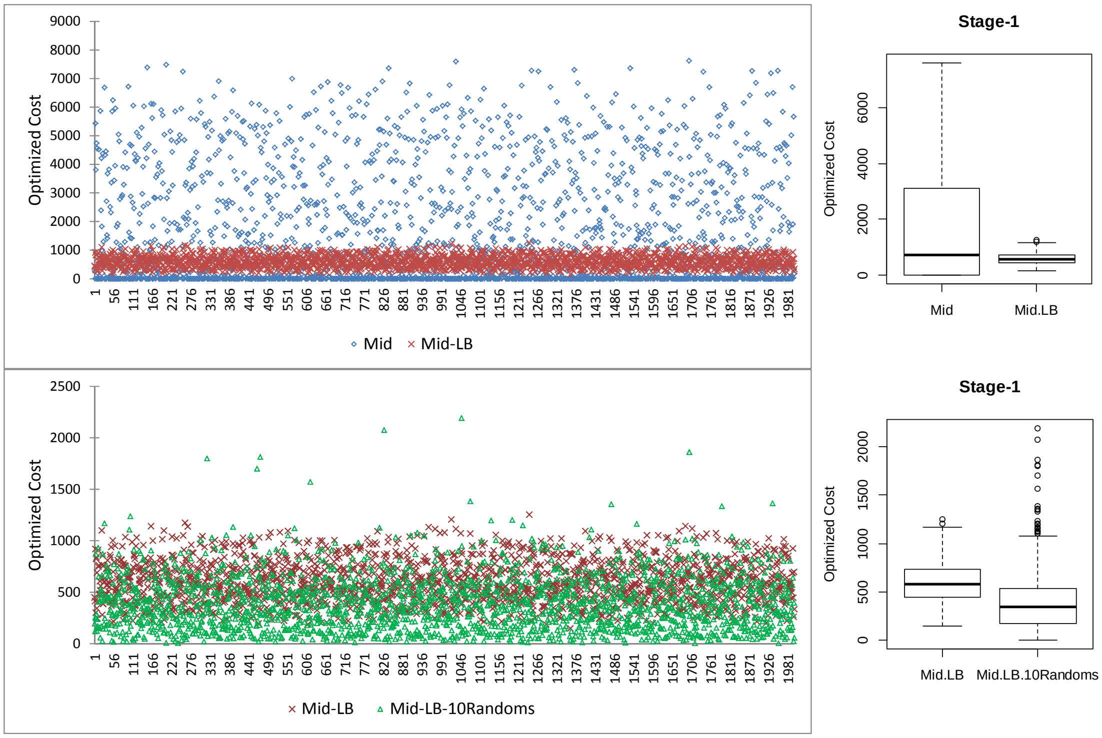


Figure 5.5 Solved optimal cost using multiple starting points for stage 1.

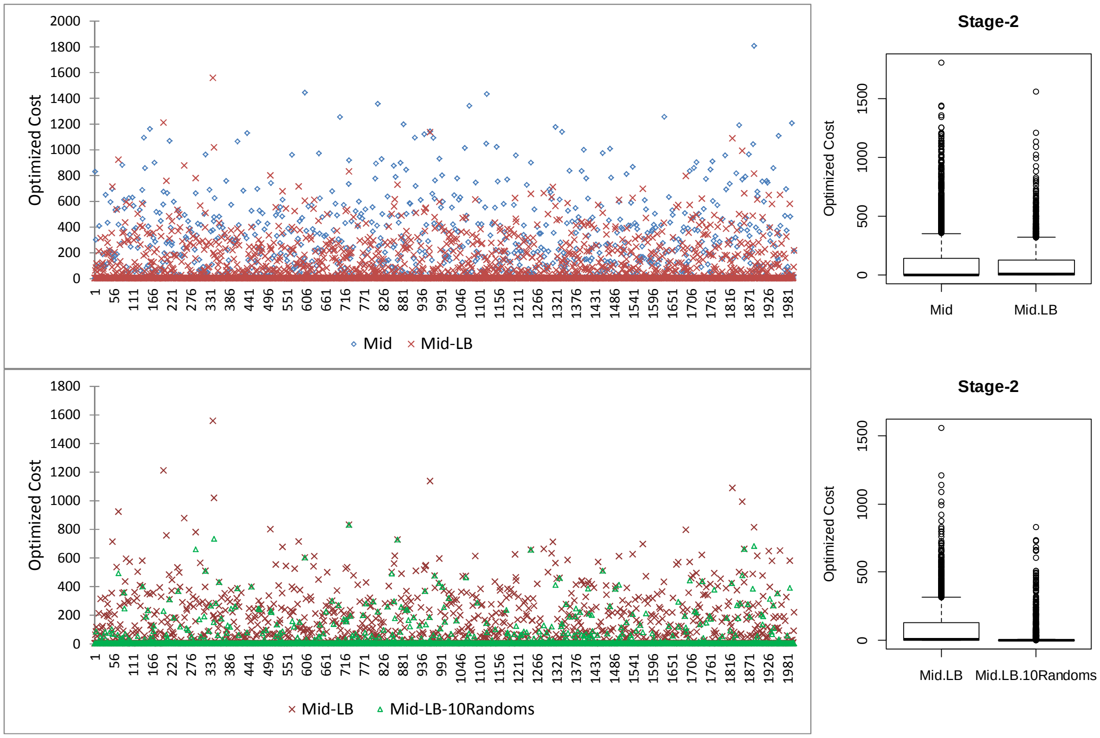


Figure 5.6 Solved optimal cost using multiple starting points for stage 2.

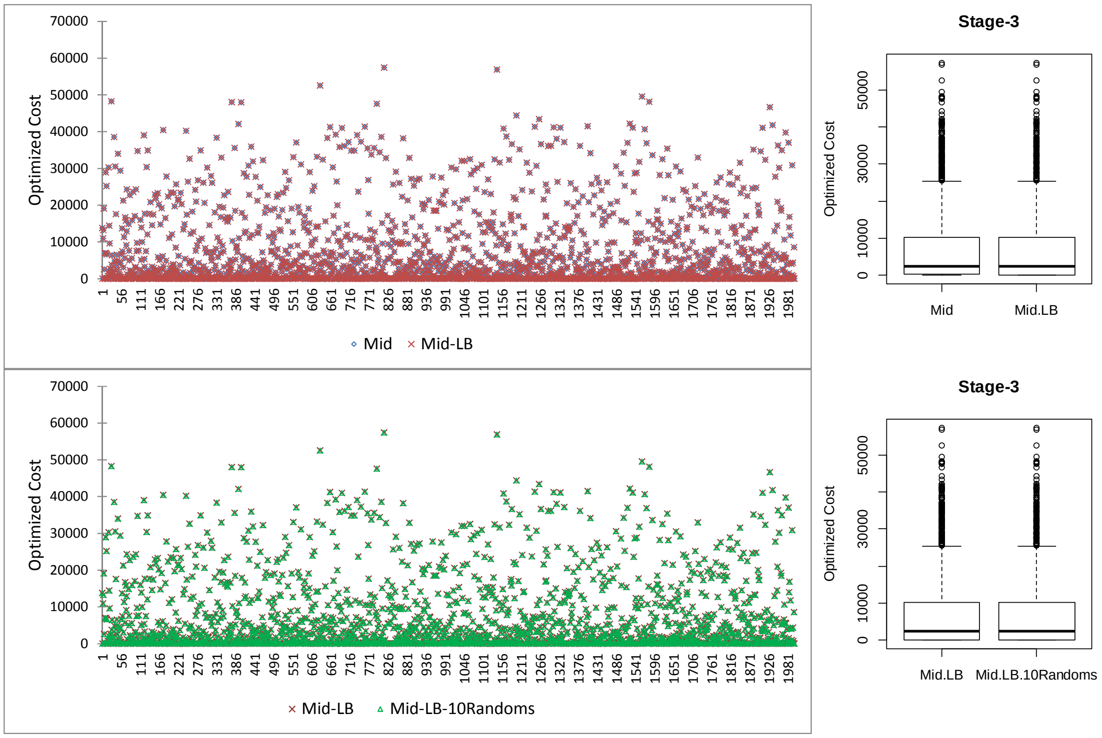


Figure 5.7 Solved optimal cost using multiple starting points for stage 3.

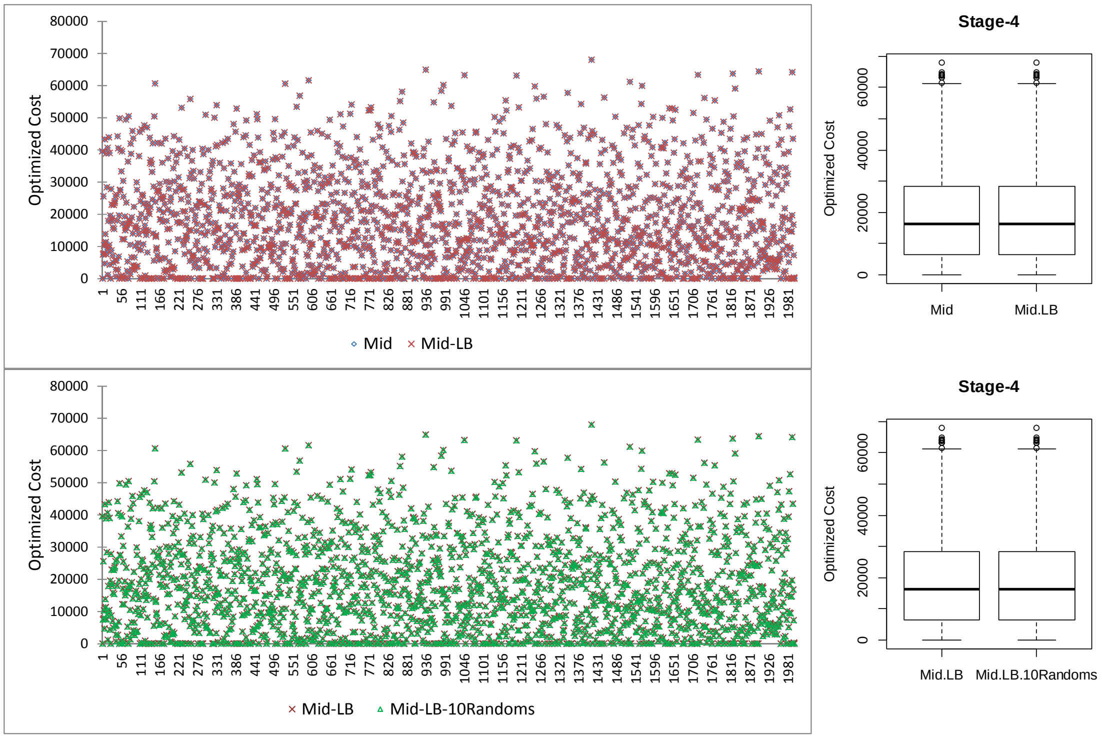


Figure 5.8 Solved optimal cost using multiple starting points for stage 4.

In addition to the non-convex optimization issue, two ozone models had previously been identified in Yang et al., (2007) to be poor models. Specifically, the ozone model for S.Dekalb at time period 2 (skM3p2) achieved an R^2 of only 19.54%. This model had been refined by Yang et al. using MARS, which achieved a very good R^2 of 98.58%, as shown in Figure 5.9. The MARS state transition model for skM3p2 shows that ozone may be reduced by increasing emissions at grid square (3,3) in time period 1 (sq3_3p1). However, this type of action is undesirable in air quality control. In order to eliminate such undesirable actions, all negative coefficients in the ozone metamodels are truncated to zero in this SDP implementation.

All SDP runs are implemented on a 2.6 GHz dual-processor workstation with 3 GB of memory, and common setup can be seen in Table 5.2. Running time and the MARS approximation of the future value function in each stage are summarized in Table 5.3. These MARS approximations will be used later in the next section to find the optimal policies in the "real-time" forward simulation.

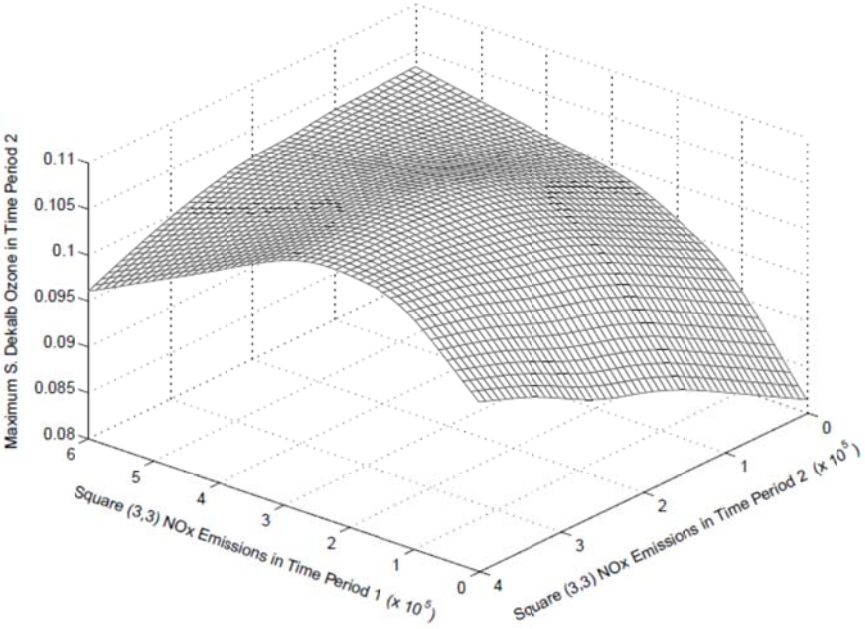


Figure 5.9 Transition function metamodel for skM3p2 using MARS (Yang et al., 2007).

Table 5.2 SDP implementation setup for all runs.

DOE for state spaces discretization	2000-Point Sobol' Sequence
Ozone threshold	0.12 ppm (modeled in penalty functions)
Negative coefficients in ozone models.	Truncated to zero
MARS approximation algorithm	MARS ASR-II
Maximum basis functions for MARS	2000
Maximum order of interaction in MARS	2
Number of knots	35
Non-linear optimization library	NAG Fortran Mark 15
Starting point in optimization (stage 1 and stage 2)	Midpoint, Lower Bound, and 10 Random Points.
Starting point in optimization (stage 3 and stage 4)	Midpoint and Lower Bound.
Running environment	Workstation with dual 2.6G AMD AtIon processors and 3GB memory; CentOS 4.9 gcc version 3.4.6 20060404 (Red Hat 3.4.6-9)

Table 5.3 Number of MARS basis functions and running times.

Metamodel	Stage	Number of State Vars.	Number of Decision Vars.	Number of Basis functioin selected by MARS	Fitting MARS (hh:mm:ss)	Solving SDP (hh:mm:ss)	Total Running time (hh:mm:ss)
Low-VIF	**Stage-1**	**16**	**17**	394	0:53:31	1:07:57	2:01:28
Low-VIF	**Stage-2**	**23**	**9**	1853	50:09:49	0:16:44	50:26:33
Low-VIF	**Stage-3**	**21**	**9**	104	0:02:47	0:05:21	0:08:08
Low-VIF	**Stage-4**	**19**	**3**	90	0:02:30	0:00:32	0:03:02
				Total time (hh:mm:ss)	**51:08:37**	**1:30:34**	**52:39:11**
High-VIF	**Stage-1**	**34**	**29**	1296	30:01:51	0:59:32	31:01:23
High-VIF	**Stage-2**	**59**	**31**	300	1:01:09	4:40:24	5:41:33
High-VIF	**Stage-3**	**82**	**30**	227	0:54:26	0:23:25	1:17:51
High-VIF	**Stage-4**	**92**	**12**	182	1:57:53	0:02:24	2:00:17
				Total time (hh:mm:ss)	**33:55:19**	**6:05:45**	**40:01:04**
Stepwise-PLS	**Stage-1**	**25**	**29**	1354	24:27:20	29:49:16	54:16:36
Stepwise-PLS	**Stage-2**	**23**	**28**	964	7:57:58	27:54:13	35:52:11
Stepwise-PLS	**Stage-3**	**14**	**25**	215	0:07:14	4:32:07	4:39:21
Stepwise-PLS	**Stage-4**	**9**	**7**	72	0:00:32	0:03:58	0:04:30
				Total time (hh:mm:ss)	**32:33:04**	**62:19:34**	**94:52:38**

5.2 Forward Re-optimization for Optimal Control Policy of the Atlanta Ozone Problem

In this study, the forward re-optimization technique is chosen to solve for the optimal control policy (Tejada-Guibert et al., 1993). The re-optimization algorithm is delineated in Figure 5.10. Given the initial state vector for stage 1 ($\boldsymbol{x}_1$), the re-optimization algorithm solves for the optimal control policy ($\boldsymbol{u}_t$) forward stage by stage until all stages have been solved. As demonstrated for this ozone problem, the optimal control policy for given initial emissions and ozone levels occurring prior to time period 1 is the decision on how emissions should be reduced at specific locations and times over the course of the day.

1. For stage $t = 1,\ldots,T\text{-}1$
    a. Solve $\tilde{V}_t(x_t) = \min\limits_{u_t} E\left\{c_t(\boldsymbol{x}_t, u_t, \boldsymbol{\varepsilon}_t) + \hat{V}_{t+1}\big(f_t(\boldsymbol{x}_t, u_t, \boldsymbol{\varepsilon}_t)\big)\right\}$ for $\boldsymbol{u}_t$
    b. Calculate $\boldsymbol{x}_{t+1} = f_t(\boldsymbol{x}_t, u_t, \boldsymbol{\varepsilon}_t)$
2. For stage T, solve $\tilde{V}_T(x_T) = \min\limits_{u_T} E\left\{c_T(\boldsymbol{x}_T, u_T, \boldsymbol{\varepsilon}_T)\right\}$ for $\boldsymbol{u}_T$

Figure 5.10 Re-optimization algorithm for solving for the optimal control policy (Yang et al., 2009).

Since 4 time periods have been considered in the Atlanta ozone problem, the optimal control decision will consist of 4 decision vectors ($\boldsymbol{u}_1, \boldsymbol{u}_2, \boldsymbol{u}_3, \boldsymbol{u}_4$) for a given initial state vector ($\boldsymbol{x}_1$).

5.3 Comparing Results

The SDP implementation using the three different metamodel types are evaluated for two cases on the initial state vector. The first case assumes the Atlanta base case scenario that initiates the first day of the ozone episode on July 31, 1987. The second case considers 50 random initial scenarios.

5.3.1 Base Case Results

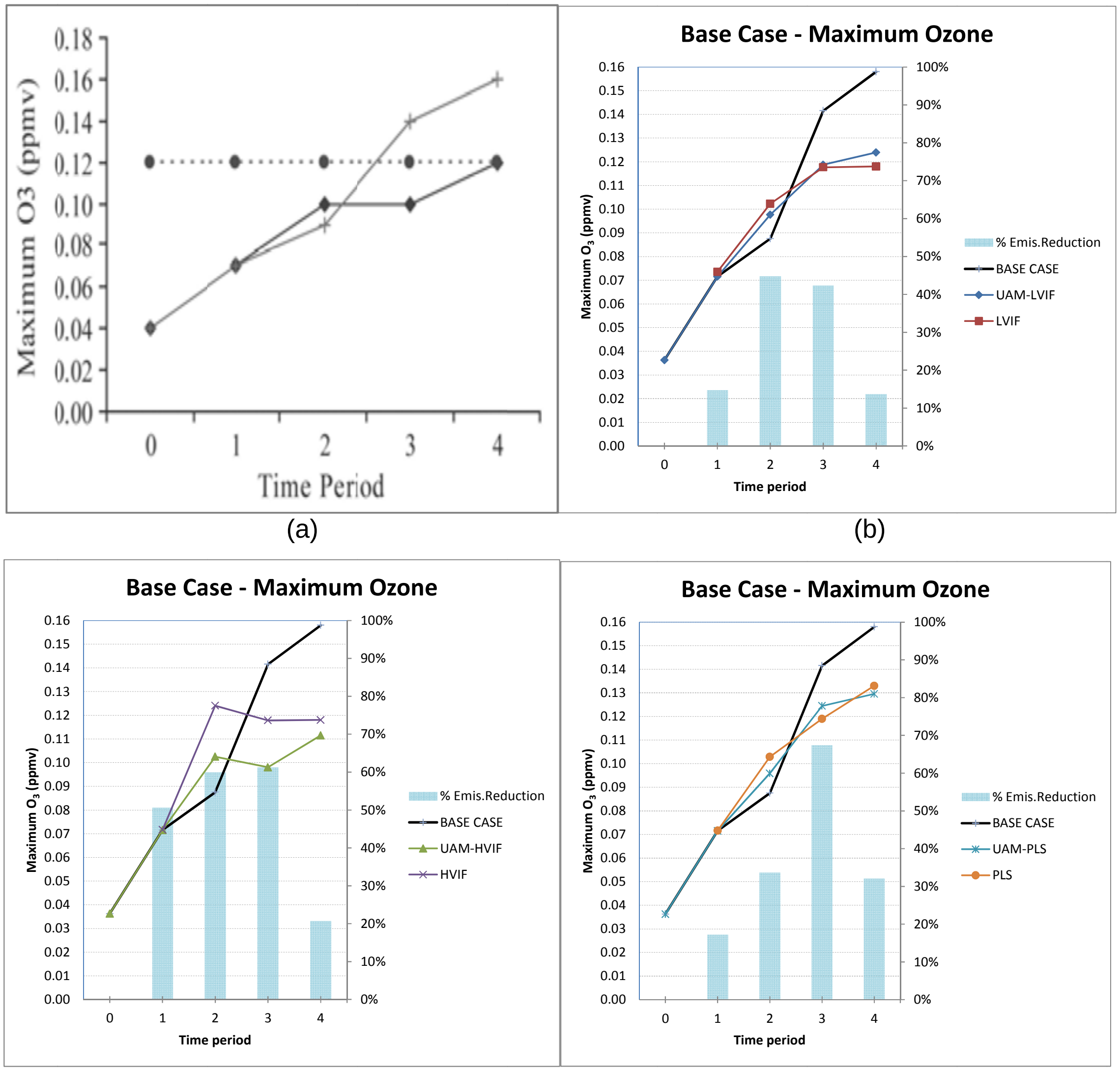
The initial emissions and ozone levels entering the first time period are taken from the nominal values on July 31, 1987 and the re-optimizaion algorithm is executed to determine optimal control decisions. Then, this optimized policy is simulated in the Atlanta urban airshed model (UAM) to calculate the ozone level as a best representation of the actual ozone level.

Emission reductions from the optimal control policies for the base case using different metamodels are illustrated in Figure 5.12 – 5.15 and summarized in Table 5.4. The optimal control policy using the Low-VIF metamodels requires a lower daily total of emission reduction of 27.66%, followed by the Stepwise-PLS metamodels that require 36.63%, and the High-VIF metamodels that require the most of reduction of 47.03%. In general, all three require emission reduction mostly in time periods 2 and 3 (from 10AM to 4PM).

The resulting maximum ozone level trajectory using both the metamodels and the UAM are shown in Figure 5.11. The primary y-axis on the left side indicates the maximum ozone level, and the secondary y-axis on the right (side) indicates the percentage of emission reduction. The “BASE CASE” line represents the maximum ozone level when no control action has been taken. The “UAM-LVIF,” “UAM-HVIF,” and “UAM-PLS” lines represent the actual ozone level simulated by the UAM when using the optimal control policy from the Low-VIF, High-VIF, and Stepwise-PLS metamodels, respectively. The “LVIF,” “HVIF,” and “PLS” lines represent the ozone level predicted by the Low-VIF, High-VIF, and Stepwise-PLS metamodels, respectively. According to Figure 5.11, the High-VIF metamodels are the least accurate models and always overestimate the maximum ozone levels; as a result they require more emission reduction than necessary. The Low-VIF metamodels seem to perform the best but slightly underestimate the ozone levels, which can cause lower emission reductions than necessary in time periods 3 and 4. The Stepwise-PLS metamodels perform better than the High-VIF models but slightly overestimate the ozone levels in time periods 2 and 4, which may lead to a more (stringent) emission reduction policy in time period 3.

Table 5.4 Base case emission reduction on the optimal policies.

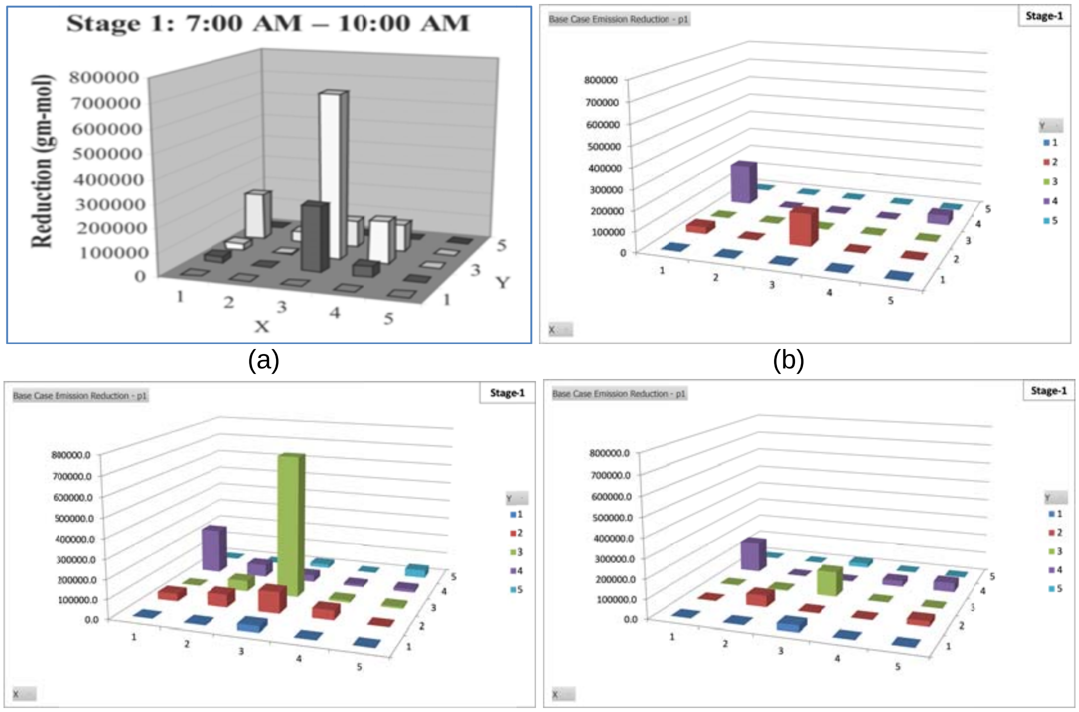
Base Case	Low-VIF		High VIF		Stepwise - PLS	
	Emission Reduction (gm-mol)	% Reduction	Emission Reduction (gm-mol)	% Reduction	Emission Reduction (gm-mol)	% Reduction
Stage-1	**446,941.4**	**14.77%**	**1,531,936.0**	**50.63%**	**520,937.7**	**17.22%**
Stage-2	**1,147,042.2**	**44.81%**	**1,535,720.7**	**60.00%**	**862,915.9**	**33.71%**
Stage-3	**1,101,894.7**	**42.35%**	**1,594,932.6**	**61.30%**	**1,754,379.6**	**67.42%**
Stage-4	**422,009.0**	**13.68%**	**639,188.0**	**20.71%**	**990,565.7**	**32.10%**
Daily Total	**3,117,887.4**	**27.66%**	**5,301,777.3**	**47.03%**	**4,128,798.9**	**36.63%**



(a) (b)

(c) (d)

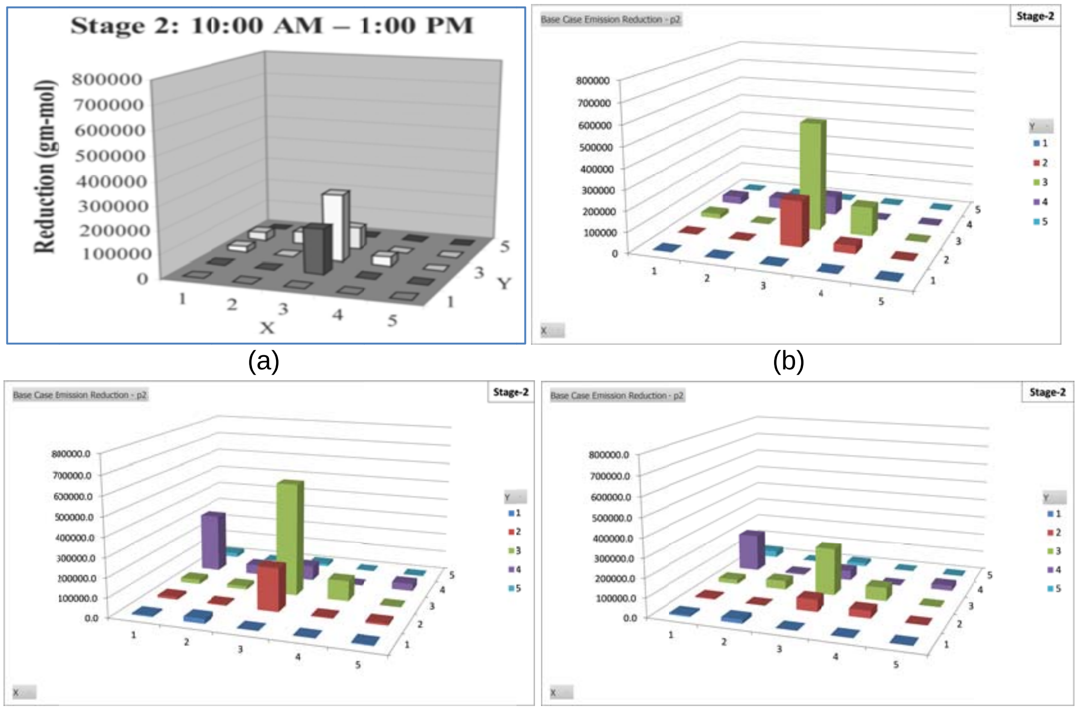
Figure 5.11 Maximum ozone levels and emission reductions for the base case optimal policies using (a) Yang et al., (2009), (b) Low-VIF, (c) High-VIF, and (d) Stepwise-PLS metamodels.



(a) (b)

(c) (d)

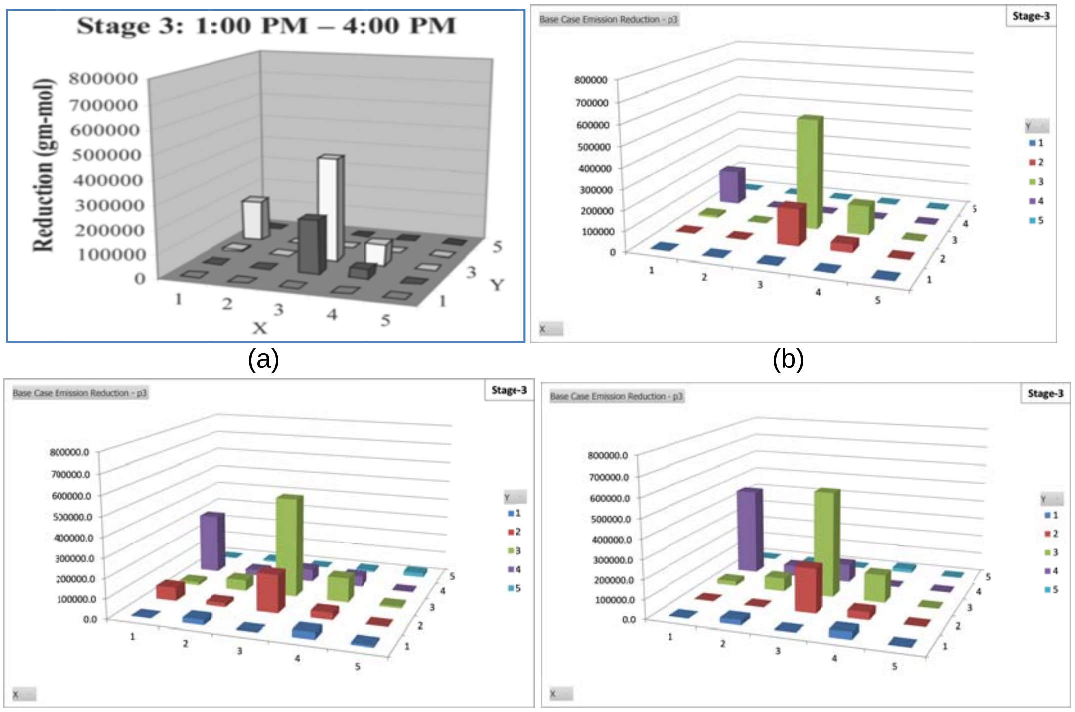
Figure 5.12 Emission reductions in each grid square for the base case optimal policies (stage 1) using (a) Yang et al., (2009), (b) Low-VIF, (c) High-VIF, and (d) Stepwise-PLS metamodels.



(a) (b)

(c) (d)

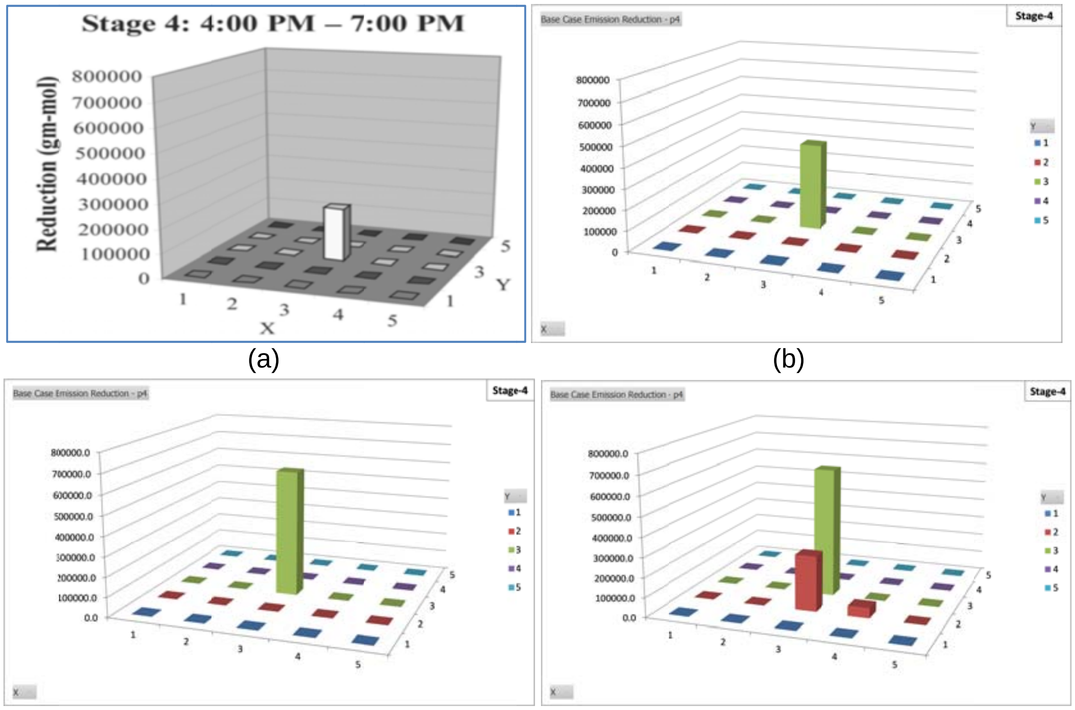
Figure 5.13 Emission reductions in each grid square for the base case optimal policies (stage 2) using (a) Yang et al., (2009), (b) Low-VIF, (c) High-VIF, and (d) Stepwise-PLS metamodels.



(a) (b)

(c) (d)

Figure 5.14 Emission reductions in each grid square for the base case optimal policies (stage 3) using (a) Yang et al., (2009), (b) Low-VIF, (c) High-VIF, and (d) Stepwise-PLS metamodels.



(a) (b)

(c) (d)

Figure 5.15 Emission reductions in each grid square for the base case optimal policies (stage 4) using (a) Yang et al., (2009), (b) Low-VIF, (c) High-VIF, and (d) Stepwise-PLS metamodels.

5.3.2 The 50 Hypothetical Scenario Results

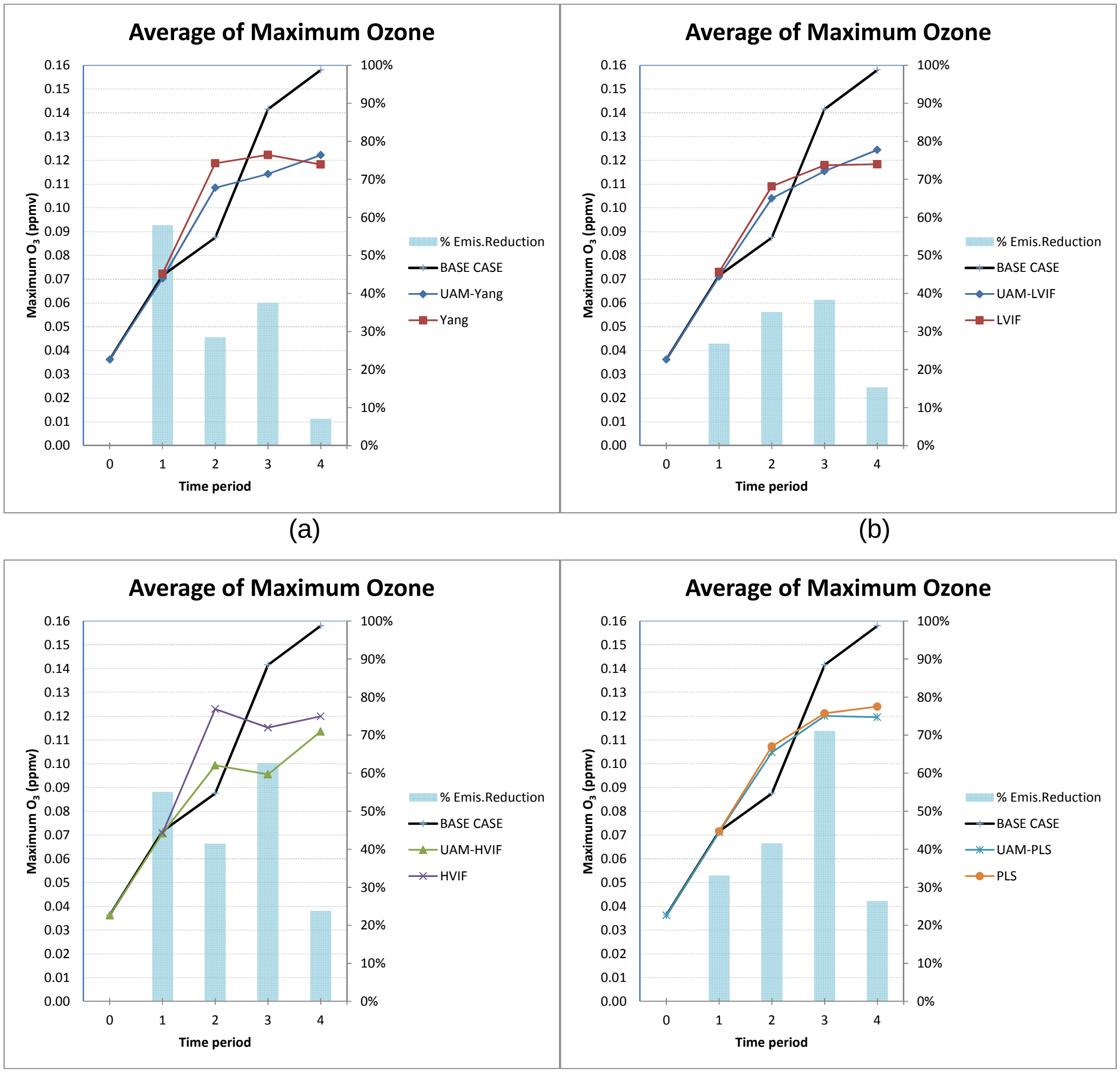
The base case results represent only one specific situation and its optimal policy is optimized for only the base case. To illustrate how the dynamic nature of SDP handles different situations, 50 hypothetical scenarios are generated and tested. To generate the 50 hypothetical scenarios, the 50 initial emissions are randomly generated based on the ranges of emissions from the base case, then these initial emissions are used as the inputs to run UAM in order to obtain the 50 initial ozone levels. The data for the 50 hypothetical scenarios can be seen in Appendix E.

The optimal control policies for the 50 hypothetical scenarios are obtained by the same procedure used in the base case, and their solutions corresponding to the Low-VIF, High-VIF, and Stepwise-PLS metamodels are shown in Appendix F, G, and H, respectively. The average emission reduction of the optimal control policies using the different metamodels are illustrated in Figure 5.17 – 5.20 and summarized in Table 5.5. The emission reduction requirements for the optimal control policies averaged across the 50 scenarios are comparable to that required by the base case.

The average maximum ozone level trajectory from both the metamodels and the UAM are shown in Figure 5.16. In the 50 scenarios, on average, the High-VIF model still performs the worst, and the Stepwise-PLS seems to perform close to the Low-VIF model. The major difference between the Low-VIF and the Stepwise-PLS models occurs in time period 4, in which maximum ozone level is underestimated by the Low-VIF model, but overestimated by the Stepwise-PLS model. The maximum ozone level in time period 4 using the Low-VIF model is actually over the EPA limit of 0.12 ppm, indicating that the optimal control policy in time periods 3 and 4 from using the Low-VIF model may not be enough to maintain ozone within the regulatory required limit. Therefore, emission reduction on locations that are excluded from the Low-VIF model but required in the Stepwise-PLS model may be considered as the potential locations that require more (stringent) emission reduction in order to reduce the maximum ozone level.

Table 5.5 Average optimal emission reduction across 50 hypothetical scenarios.

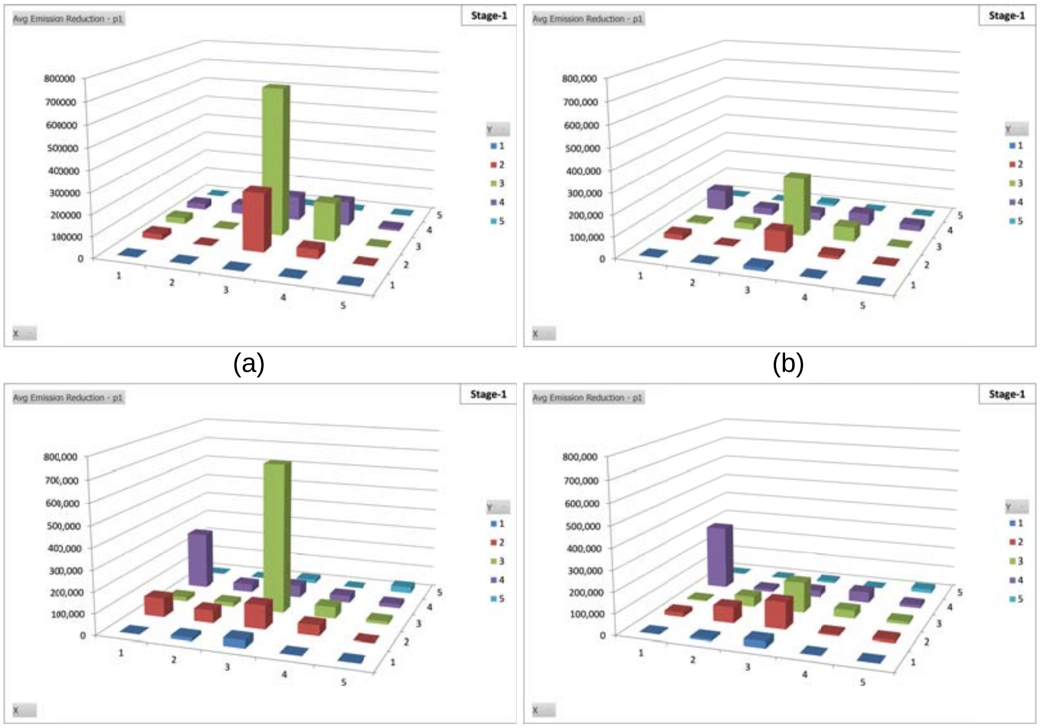
50 Scenarios	Yang et al. (2009)		Low-VIF		High VIF		Stepwise - PLS	
	Average of Emission Reduction (gm-mol)	% Average Reduction	Average of Emission Reduction (gm-mol)	% Average Reduction	Average of Emission Reduction (gm-mol)	% Average Reduction	Average of Emission Reduction (gm-mol)	% Average Reduction
Stage-1	1,754,435.9	57.99%	811,481.7	26.82%	1,667,498.8	55.11%	1,001,731.1	33.11%
Stage-2	728,402.8	28.46%	900,083.1	35.16%	1,060,932.1	41.45%	1,065,100.0	41.61%
Stage-3	977,187.9	37.55%	997,836.3	38.35%	1,630,609.9	62.67%	1,850,742.3	71.13%
Stage-4	218,629.4	7.08%	473,427.0	15.34%	735,351.2	23.83%	813,879.3	26.37%
Daily Total	3,678,656.0	32.63%	3,182,828.0	28.23%	5,094,392.0	45.19%	4,731,452.7	41.97%



(a) (b)

(c) (d)

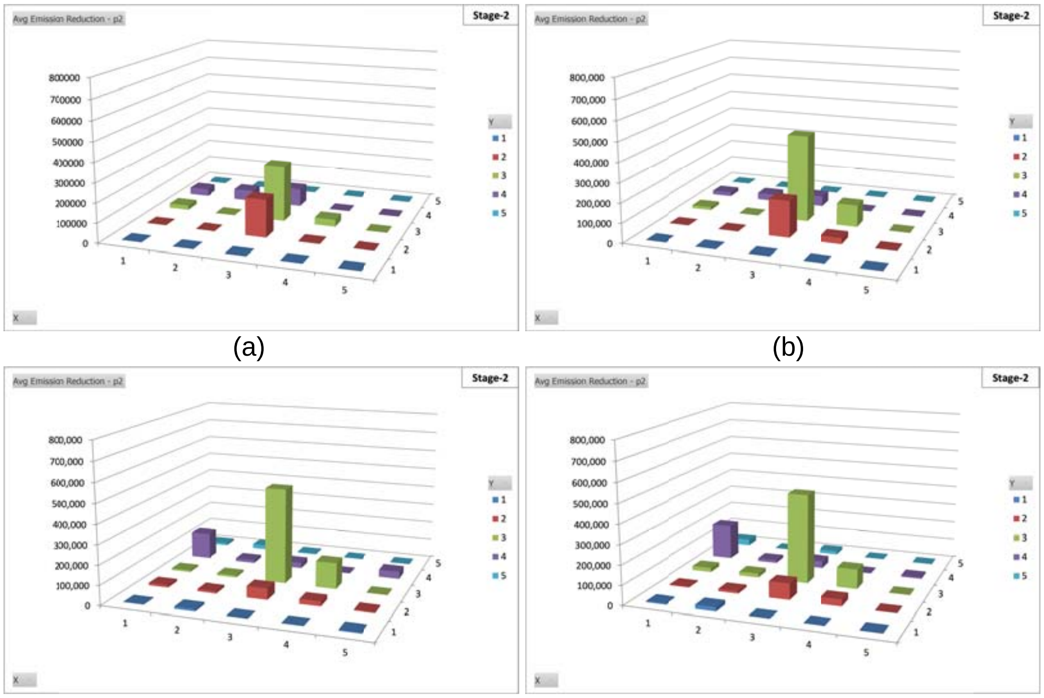
Figure 5.16 Maximum ozone levels and optimal emission reductions for the 50 scenarios using (a) Yang et al., (2009), (b) Low-VIF, (c) High-VIF, and (d) Stepwise-PLS metamodels.



(a) (b)

(c) (d)

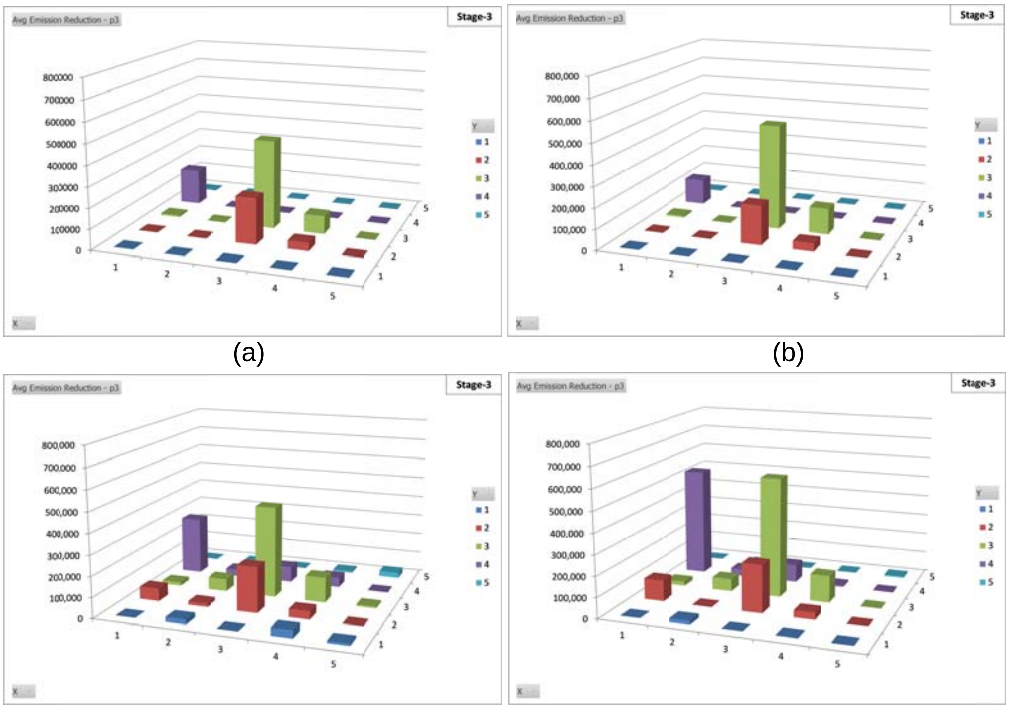
Figure 5.17 Average optimal emission reductions in each grid square for the 50 scenarios(stage 1) using (a) Yang et al., (2009), (b) Low-VIF, (c) High-VIF, and (d) Stepwise-PLS metamodels.



(a) (b)

(c) (d)

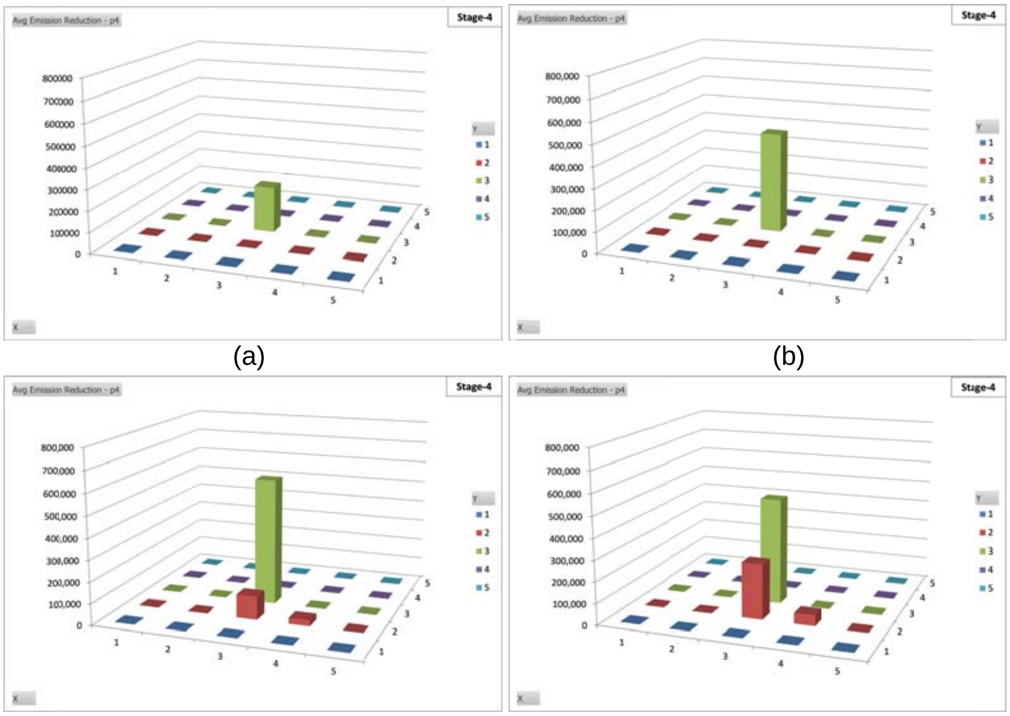
Figure 5.18 Average optimal emission reductions in each grid square for the 50 scenarios (stage 2) using (a) Yang et al., (2009), (b) Low-VIF, (c) High-VIF, and (d) Stepwise-PLS metamodels.



(a) (b)

(c) (d)

Figure 5.19 Average optimal emission reductions in each grid square for the 50 scenarios (stage 3) using (a) Yang et al., (2009), (b) Low-VIF, (c) High-VIF, and (d) Stepwise-PLS metamodels.



(a) (b)

(c) (d)

Figure 5.20 Average optimal emission reductions in each grid square for the 50 scenarios (stage 4) using (a) Yang et al., (2009), (b) Low-VIF, (c) High-VIF, and (d) Stepwise-PLS metamodels.

5.4 Verification of the Metamodels

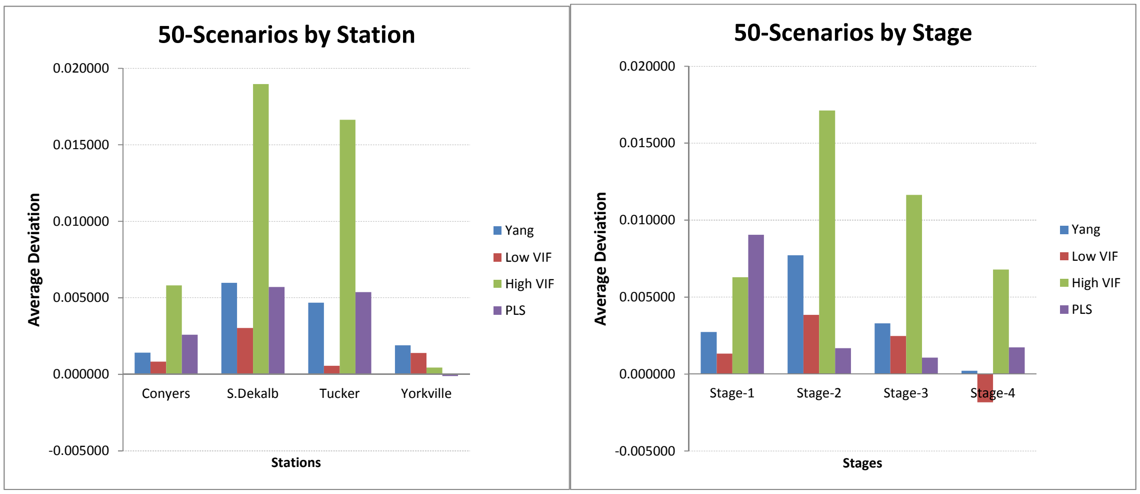
The most desirable optimal policy for the Atlanta ozone problem is the policy that requires the minimum emission reductions necessary to maintain maximum ozone level within the EPA standard. However, the computational results of the ADP process are affected by the accuracy of the metamodels because they are included in SDP as state transition functions. The best optimal policy results from the SDP implementations alone may not be enough to justify the best overall results. Therefore, the accuracy of the metamodels should be examined. the first, the deviations between the metamodels and the UAM is examined for the optimal control policies. Second, the deviations under random control policies are also examined.

5.4.1 Deviation of Metamodels on the Optimal Control Policy

The optimal control policies of the 50 hypothetical scenarios from section 5.3.2 were simulated in the UAM to obtain the maximum ozone levels and then were compared with the maximum ozone levels predicted by metamodels. The deviation of maximum ozone levels in each monitoring station between the metamodel predictions and the values from UAM are calculated, and the average absolute deviation is shown in Figure 5.23 and Figure 5.24. The deviations are also summarized by station and by stage in Figure 5.21 and Figure 5.22.

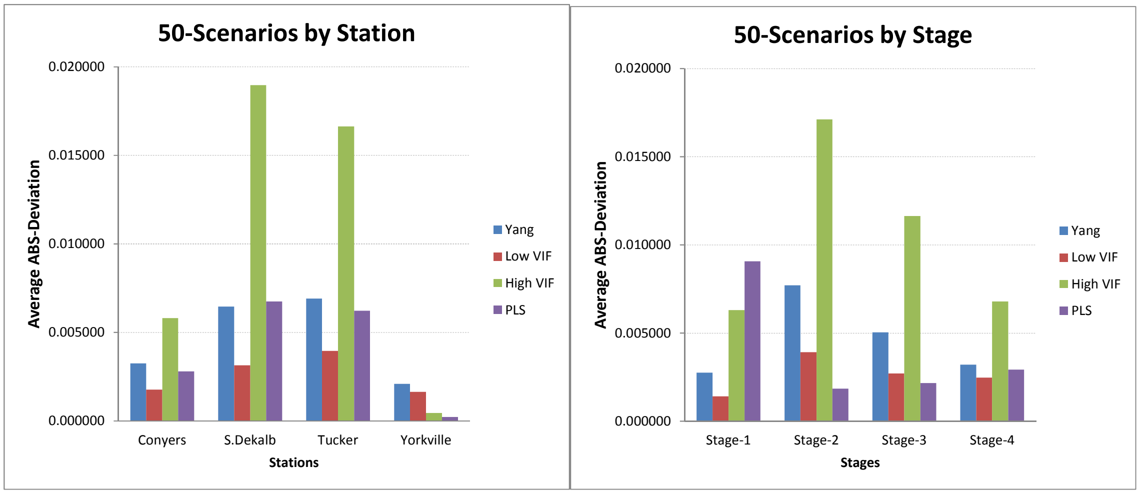
The deviation results show that the Low-VIF model is the most accurate model, followed by the Stepwise-PLS model and then the High-VIF model. Deviations of the Stepwise-PLS models are mostly comparable to the Low-VIF models. However, some ozone models in time period 1 (skM3p1 and tkM3p1) using the Stepwise-PLS method deviate from UAM more than other methods.

The maximum ozone level occurs in stage-4. The results for stage-4 show that the Low-VIF model always underestimates ozone at Tucker, by -5.09% on average, and underestimates ozone at Conyers by -1.08% on average. The Stepwise-PLS model, on average, overestimates ozone at Tucker and Conyers by 0.21% and 5.19%, respectively. This will affect the optimal emission reduction policy as discussed earlier in section 5.3.



(a) (b)

Figure 5.21 Summary of deviation between metamodels and UAM for the 50 scenarios using optimal policies by station (a) and by stage (b).



(a) (b)

Figure 5.22 Summary of ABS-deviation between metamodels and UAM for the 50 scenarios using optimal policies by station (a) and by stage (b).

	Yang	Low VIF	High VIF	PLS
cyM3p1	0.001214	0.001700	0.003307	0.001103
skM3p1	0.003151	0.000666	0.004609	0.017018
tkM3p1	0.004632	0.000984	0.017194	0.018028
ykM3p1	0.001960	0.001952	0.000088	0.000051
cyM3p2	0.001078	0.001690	0.002864	0.001129
skM3p2	0.016498	0.007214	0.041986	0.003414
tkM3p2	0.010486	0.005082	0.023524	0.002223
ykM3p2	0.002800	0.001438	0.000114	-0.000032
cyM3p3	-0.003193	0.001304	0.007512	0.002036
skM3p3	0.005151	0.003382	0.018035	0.001406
tkM3p3	0.008059	0.002505	0.019656	0.001057
ykM3p3	0.003199	0.002690	0.001348	-0.000199
cyM3p4	0.006580	-0.001352	0.009556	0.006088
skM3p4	-0.000891	0.000858	0.011234	0.000987
tkM3p4	-0.004463	-0.006341	0.006138	0.000205
ykM3p4	-0.000395	-0.000476	0.000229	-0.000301
Average (overall)	0.003492	0.001456	0.010462	0.003388

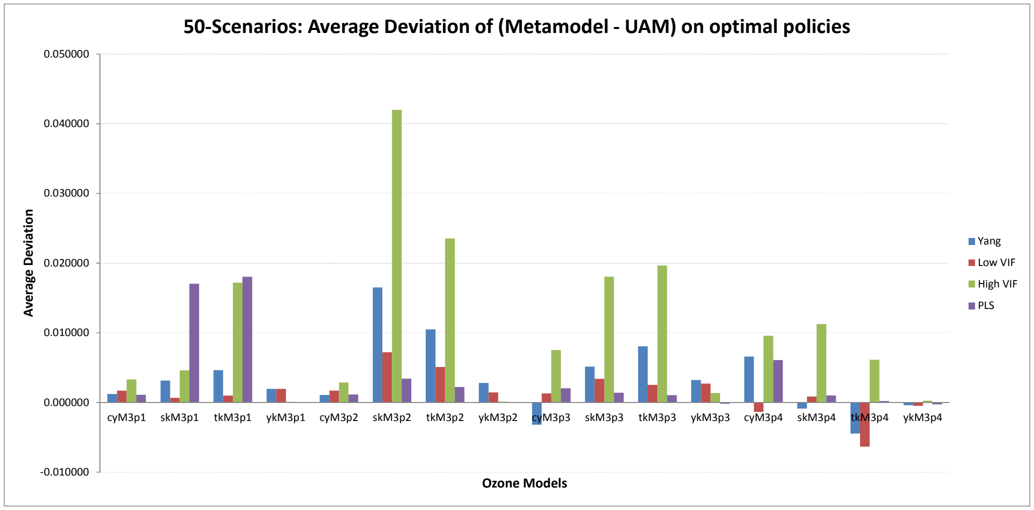


Figure 5.23 Average deviation between metamodels and UAM for the 50 scenarios using optimal policies.

	Yang	Low VIF	High VIF	PLS
cyM3p1	0.001238	0.001700	0.003307	0.001142
skM3p1	0.003164	0.000842	0.004609	0.017018
tkM3p1	0.004632	0.001144	0.017194	0.018028
ykM3p1	0.001960	0.001952	0.000088	0.000060
cyM3p2	0.001078	0.001690	0.002864	0.001449
skM3p2	0.016498	0.007439	0.041986	0.003522
tkM3p2	0.010486	0.005082	0.023524	0.002290
ykM3p2	0.002800	0.001438	0.000114	0.000126
cyM3p3	0.003692	0.001531	0.007512	0.002307
skM3p3	0.005200	0.003386	0.018035	0.003391
tkM3p3	0.008059	0.003231	0.019656	0.002640
ykM3p3	0.003199	0.002690	0.001348	0.000311
cyM3p4	0.006999	0.002167	0.009556	0.006287
skM3p4	0.000954	0.000899	0.011234	0.003083
tkM3p4	0.004463	0.006341	0.006138	0.001926
ykM3p4	0.000395	0.000476	0.000229	0.000401
Average (overall)	0.004676	0.002626	0.010462	0.003999

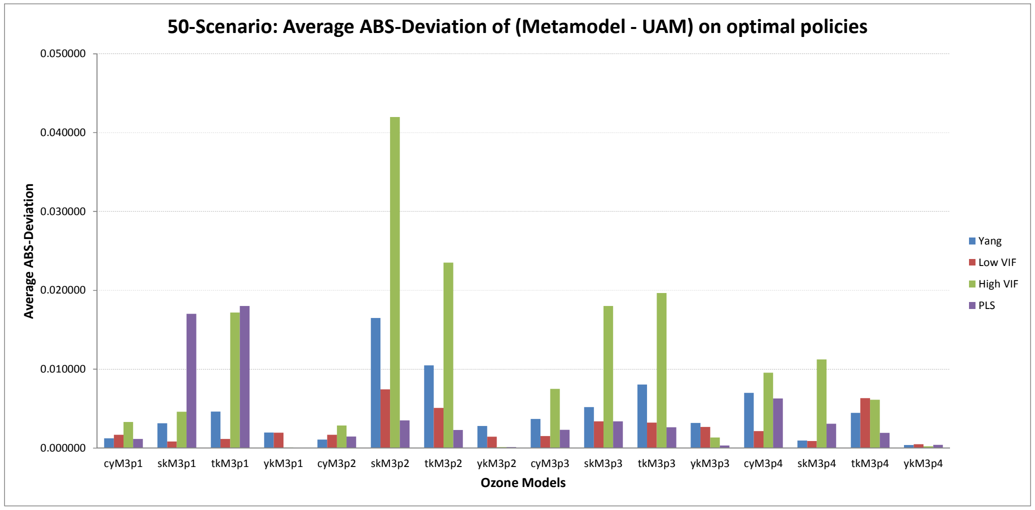


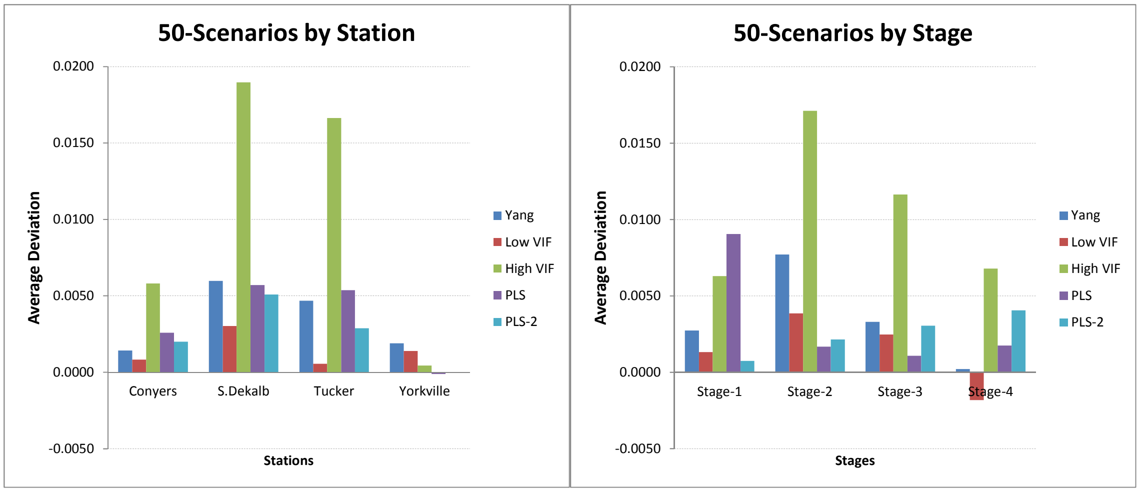
Figure 5.24 Average ABS-deviation between metamodels and UAM for the 50 scenarios using optimal policies.

5.4.2 Deviation of Metamodels on the Random Control Policy

Unlike section 5.4.1 that examines the accuracy of the metamodels for only the specific case of the optimal policy, this section will verify the metamodels to cover entire modeling space by using randomly chosen emission reductions. Using the same verification procedure, the random control policies of the 50 hypothetical scenarios from section 5.3.2 are simulated in the UAM and then compared with the predicted ozone from the metamodels. In addition to the deviation for the optimal policy, “PLS-2” shows the random policy results from the Stepwise-PLS metamodel that includes negative coefficients in ozone model computation.

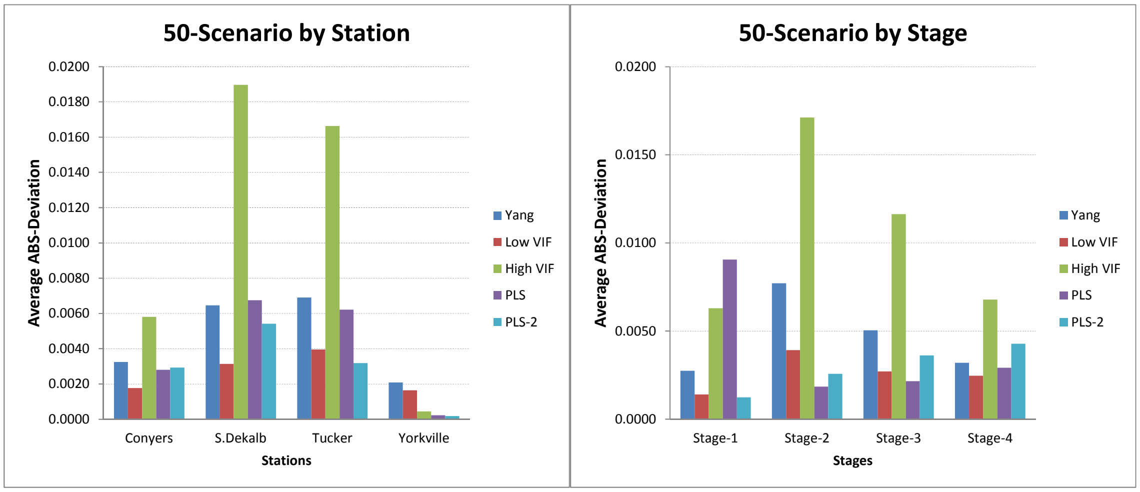
The deviation of maximum ozone level in each of the monitoring stations between the metamodel predictions and the values from the UAM are calculated, and the average absolute deviation results can be seen in Figure 5.27 and Figure 5.28. The deviations are also summarized by station and by stage in Figure 5.25 and Figure 5.26.

The deviation results using random control policies are mostly in agreement with the results using optimal policies. Additionally, allowing negative coefficients in the Stepwise-PLS model does improve the accuracy of the model, especially for the skM3p1 and tkM3p1 ozone models, which previously had high deviations.



(a) (b)

Figure 5.25 Summary of deviations between metamodels and UAM for the 50 scenarios using random policies by station (a) and by stage (b).



(a) (b)

Figure 5.26 Summary of ABS-deviation between metamodels and UAM for the 50 scenarios using random policies by station (a) and by stage (b).

	Yang	Low VIF	High VIF	PLS	PLS-2
cyM3p1	0.00121	0.00170	0.00331	0.00110	-0.00072
skM3p1	0.00315	0.00067	0.00461	0.01702	0.00177
tkM3p1	0.00463	0.00098	0.01719	0.01803	0.00183
ykM3p1	0.00196	0.00195	0.00009	0.00005	0.00006
cyM3p2	0.00108	0.00169	0.00286	0.00113	0.00074
skM3p2	0.01650	0.00721	0.04199	0.00341	0.00553
tkM3p2	0.01049	0.00508	0.02352	0.00222	0.00223
ykM3p2	0.00280	0.00144	0.00011	-0.00003	0.00008
cyM3p3	-0.00319	0.00130	0.00751	0.00204	0.00048
skM3p3	0.00515	0.00338	0.01803	0.00141	0.00716
tkM3p3	0.00806	0.00251	0.01966	0.00106	0.00462
ykM3p3	0.00320	0.00269	0.00135	-0.00020	-0.00008
cyM3p4	0.00658	-0.00135	0.00956	0.00609	0.00752
skM3p4	-0.00089	0.00086	0.01123	0.00099	0.00590
tkM3p4	-0.00446	-0.00634	0.00614	0.00020	0.00282
ykM3p4	-0.00040	-0.00048	0.00023	-0.00030	-0.00002
Average (overall)	0.00349	0.00146	0.01046	0.00339	0.00250

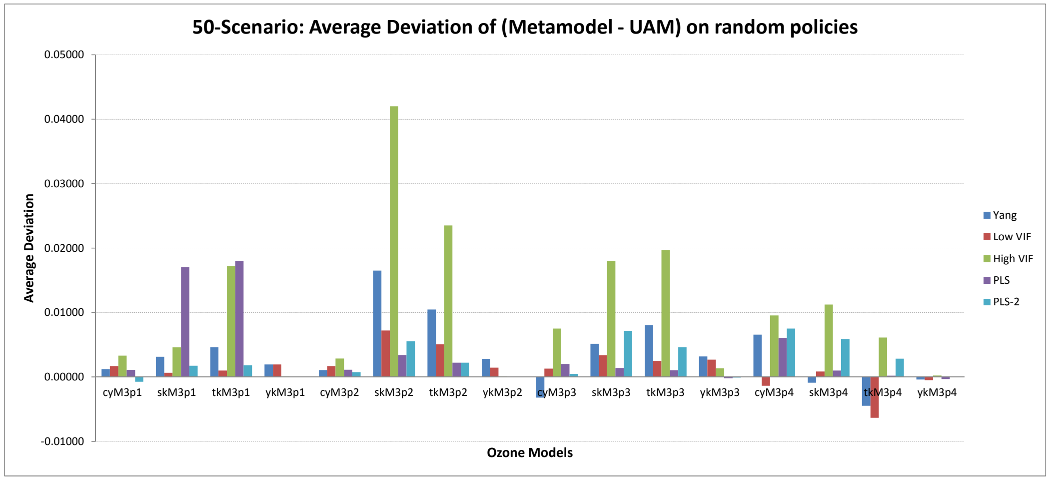


Figure 5.27 Average deviation between metamodels and UAM for the 50 scenarios using random policies.

	Yang	Low VIF	High VIF	PLS	PLS-2
cyM3p1	0.001238	0.001700	0.003307	0.001142	0.000843
skM3p1	0.003164	0.000842	0.004609	0.017018	0.002024
tkM3p1	0.004632	0.001144	0.017194	0.018028	0.002051
ykM3p1	0.001960	0.001952	0.000088	0.000060	0.000076
cyM3p2	0.001078	0.001690	0.002864	0.001449	0.001397
skM3p2	0.016498	0.007439	0.041986	0.003522	0.005998
tkM3p2	0.010486	0.005082	0.023524	0.002290	0.002713
ykM3p2	0.002800	0.001438	0.000114	0.000126	0.000165
cyM3p3	0.003692	0.001531	0.007512	0.002307	0.001901
skM3p3	0.005200	0.003386	0.018035	0.003391	0.007505
tkM3p3	0.008059	0.003231	0.019656	0.002640	0.004744
ykM3p3	0.003199	0.002690	0.001348	0.000311	0.000292
cyM3p4	0.006999	0.002167	0.009556	0.006287	0.007573
skM3p4	0.000954	0.000899	0.011234	0.003083	0.006138
tkM3p4	0.004463	0.006341	0.006138	0.001926	0.003221
ykM3p4	0.000395	0.000476	0.000229	0.000401	0.000191
Average (overall)	0.00468	0.00263	0.01046	0.00400	0.00293

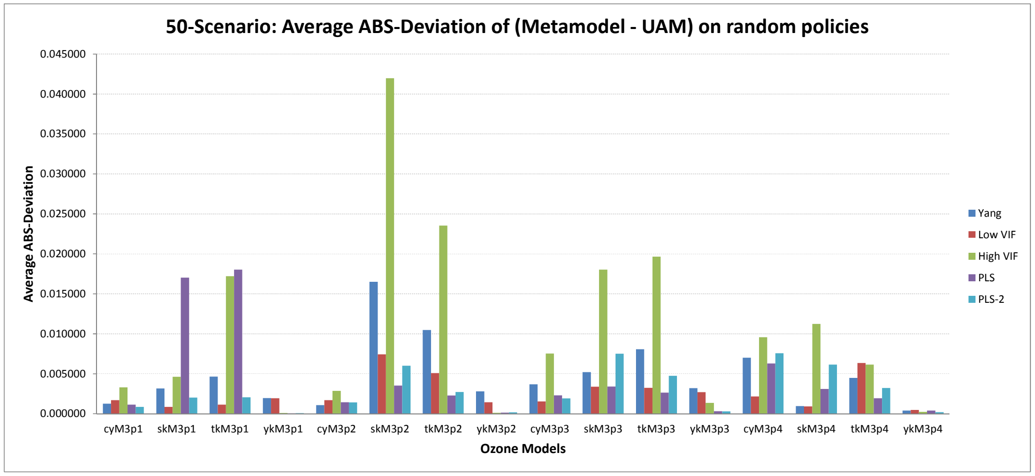


Figure 5.28 Average ABS-deviation between metamodels and UAM for the 50 scenarios using random policies.

CHAPTER 6

CONCLUSIONS AND FUTURE RESEARCH

6.1 Conclusions

In this dissertation, highly correlated state spaces in the high-dimensional continuous-state SDP solution methods were explored. The Atlanta ground-level ozone pollution problem from Yang et al. (2009) was selected as our case study because ozone state variables at different monitoring stations and at different time-periods are highly correlated. The Atlanta Urban Airshed Model (UAM) is computationally impractical to be used directly in the SDP as the state transition function. Therefore, in the ADP process, three types of statistical metamodels were developed as surrogates of the UAM, High-VIF models, Low-VIF models, and orthogonalized Stepwise-PLS models. All cases were developed on the Atlanta ozone pollution case study with highly multicollinear state variables.

If the high multicollinearity in the data is ignored, then metamodels with high VIFs are possible. High-VIF models were deliberately generated to test this worst case. The previous metamodeling from Yang et al. (2007) had some high-VIF models. With careful revision Low-VIF models could be developed. Finally, Stepwise-PLS metamodeling transforms the state variables to a set of orthogonalized variables, eliminating the problem of multicollinearity.

All three types of metamodels, Low-VIF, High-VIF, and Stepwise-PLS, were implemented in the SDP for the base case of the Atlanta case study and for 50 random initial scenarios. According to the implementation results, Table 6.1 provides a summary of the advantages (pros) and disadvantages (cons) the different metamodels for this multicollinear SDP problem.

Table 6.1 Pros and Cons for Transition Metamodels.

Transition Metamodel	Pros	Cons
High-VIF	• N/A	• High-VIF state space. • Least accurate metamodels. • Always overestimated the ozone level. • Required too much emission reduction.
Low-VIF	• Low-VIF state space. • Most accurate metamodels. • Required lower emission reduction. • Lower computational time.	• Slightly underestimated the ozone level. in time period 4. • Actual ozone level (UAM) in time period 4 slightly violated EPA limit on average. • Excluding these highly correlated variables from the model can give the false impression that these excluded variables are unimportant. • The modeling requires special effort to yield low VIF metamodels.
Stepwise-PLS	• State space is orthogonal. • Slightly less accurate than the Low-VIF model. • Required comparable emission reduction to the Low-VIF model (except in time period 3). • The PLS approach allows important variables to be maintained in the state, even if they are correlated. • The Stepwise-PLS approach can be automated.	• Slightly overestimated the ozone level in time period 4. • More computational effort.

The results show that the High-VIF model is less accurate than other models and always overestimates the maximum ozone level. Consequently, its subsequent optimal policies may require too much emission reduction. The SDP optimal policy using the Low-VIF metamodel tends to require lower emission reduction than using any other metamodels. Even though the Low-VIF model is the most accurate, the predicted maximum ozone level in time period 4 using the Low-VIF model, on average, is slightly underestimated and the actual ozone is above the EPA limit of 0.12 ppm, indicating an minor ozone exceedance. Parameters in the cost objective can be modified to provide more margin of error to better prevent this. The optimal control policies when using the Stepwise-PLS model require comparable amounts of emission reduction to the Low-VIF model except in time period 3, in which more emission reduction was required due to overestimation of the ozone level for the Stepwise-PLS model in time period 4.

In the Low-VIF modeling case, one is essentially avoiding combinations of variables that are highly correlated. Excluding these highly correlated variables from the model can give the false impression that these excluded variables are unimportant. The PLS approach allows important variables to be maintained in the state, even if they are correlated. In terms of automated nature of the modeling process, the Low-VIF modeling requires special effort to yield low VIF metamodels. By contrast, the Stepwise-PLS approach can be automated.

For solving a SDP problem with a multicollinear state space, the comparison results suggest that the Low-VIF models should be considered first, primarily due to the SDP computational effort. An orthogonalization type method, such as the Stepwise-PLS model, should be considered when accurate Low-VIF models cannot be constructed, or an automated process is desired.

6.2 Future Research

As discussed earlier in Chapter 5, there are at least two issues that should be addressed more appropriately in solving the current SDP problem. The first issue was the presence of non-convexity in the MARS future value function approximations. In theory, the future value function is convex and the objective function of the optimization should be convex. However, due to nonconvexities generated by interaction terms in the MARS model, the approximated future value function can be non-convex. This complicates the optimization, which requires multiple starts in an attempt to seek the global optimum, Shih (2006) and Shih et al. (2012) developed convex versions of MARS. Use of these convex versions would eliminate the need to solve a non-convex optimization. Alternately, Martinez, Martinez, Rosenberger, and Chen (2011) developed a global optimization method for a non-convex piecewise linear MARS function. In future work, the methods by Shih et al. and Martinez et al. may be able to address the optimization issues for the Atlanta ozone pollution case study.

Another important issue is the metamodels. As explained in Yang et al. (2007), the inaccurate metamodels are due to curvature in the relationship when NO_x is high. Ozone generation is low when NO_x concentrations are dominant, but allowing such relationships to be represented in the state transition metamodels could allow the optimization to reduce ozone by increasing NO_x emissions, which is clearly undesirable. To alleviate this issue in this dissertation, all negative coefficients associated with decision variables are truncated to zero but this approach degrades the accuracy of our models, especially, when the key decision variables have been truncated. For the future work, a monotonic ozone transition function without negative coefficients should be explored. For example, we may modify MARS to select only basis functions with non-negative coefficients.

In addition to addressing these issues, when it is difficult to obtain low VIF models, the Stepwise-PLS approach should be employed. The Stepwise-PLS model has been shown to be a good potential model to handle multicollinear state spaces. However, the Stepwise-PLS is slightly less accurate than the Low-VIF model. To improve the Stepwise-PLS approach a modeling approach that permits interactions between the decision variables ($\boldsymbol{u}$) and the state variables ($\boldsymbol{x}$) should be explored.

APPENDIX A

EVALUATION RESULTS OF VARIOUS MODELING SCENARIOS FOR THE METAMODEL OF UAM AT CONYERS STATION

Table A.1 Results of Various Modeling Scenarios for the metamodel of Conyers stage 1.

Approaches		R^2	Vars. left in model	VIF	% Error
A-1	Stepwise	0.2646	7	(1.0006 - 1.0137)	1.08925
A-2	Stepwise-PCA	0.2646	7	1	1.08925
A-3	Stepwise-PCA-Stepwise	0.2597	4	1	1.09229
A-4	**Stepwise-PLS**	**0.2636**	**1**	**1**	**1.08741**
B-1	FDR	0.2219	3	(1.003 - 1.008)	1.10580
B-2	FDR_PCA	0.2219	3	1	1.10580
B-3	FDR_PCA_StepwiseReg	0.2208	2	1	1.10352
B-4	FDR_PLS	0.2205	1	1	1.10384
C-1	conFDR	0.1894	1	1	1.13779
C-2	conFDR_PCA	0.1894	1	1	1.13779
C-3	conFDR_PCA_Stepwise	0.1894	1	1	1.13779
C-4	conFDR_PLS	0.1894	1	1	1.13779
D-1	Tree	0.1937	2	1.00061	1.13840
D-2	Tree_PCA	0.1937	2	1	1.13840
D-3	Tree_PCA_Stepwise	0.1937	2	1	1.13840
D-4	Tree_PLS	0.1936	1	1	1.13890
E-1	PCA-Stepwise	0.2476	20	1	1.15553
E-2	PAMsSites-PCA-Stepwise	0.2646	7	(1.002 - 1.014)	1.08925
F	PLS	0.3048	1	1	1.18912

Table A.2 Ranking Results of the Scenarios for the metamodel of Conyers stage 1.

Approaches*	Vars. left in model
Stepwise-PLS	**1**
FDR_PLS	1
conFDR_PCA	1
conFDR_PCA_Stepwise	1
conFDR_PLS	1
Tree_PLS	1
PLS	1
FDR_PCA_StepwiseReg	2
Tree_PCA	2
Tree_PCA_Stepwise	2
FDR_PCA	3
Stepwise-PCA-Stepwise	4
Stepwise-PCA	7
PCA-Stepwise	20

Approaches*	% Error
Stepwise-PLS	**1.08741**
Stepwise-PCA	1.08925
Stepwise-PCA-Stepwise	1.09229
FDR_PCA_StepwiseReg	1.10352
FDR_PLS	1.10384
FDR_PCA	1.10580
conFDR_PCA	1.13779
conFDR_PCA_Stepwise	1.13779
conFDR_PLS	1.13779
Tree_PCA	1.13840
Tree_PCA_Stepwise	1.13840
Tree_PLS	1.13890
PCA-Stepwise	1.15553
PLS	1.18912

Approaches*	R^2
PLS	0.3048
Stepwise-PCA	0.2646
Stepwise-PLS	**0.2636**
Stepwise-PCA-Stepwise	0.2597
PCA-Stepwise	0.2476
FDR_PCA	0.2219
FDR_PCA_StepwiseReg	0.2208
FDR_PLS	0.2205
Tree_PCA	0.1937
Tree_PCA_Stepwise	0.1937
Tree_PLS	0.1936
conFDR_PCA	0.1894
conFDR_PCA_Stepwise	0.1894
conFDR_PLS	0.1894

*** VIF > 1 are removed.**

*** Ordered by better to worse**

Table A.3 Results of Various Modeling Scenarios for the metamodel of Conyers stage 2.

Approaches		R^2	Vars. left in model	VIF	% Error
A-1	Stepwise	0.9937	10	(1.009 - 1.260)	0.33001
A-2	Stepwise-PCA	0.9937	10	1	0.33001
A-3	Stepwise-PCA-Stepwise	0.9937	10	1	0.33001
A-4	**Stepwise-PLS**	**0.9934**	**3**	**1**	**0.34289**
B-1	FDR	0.9894	3	(1.01 - 1.23)	0.45582
B-2	FDR_PCA	0.9894	3	1	0.45582
B-3	FDR_PCA_Stepwise	0.9894	3	1	0.45582
B-4	FDR_PLS	0.9894	1	1	0.45582
C-1	conFDR	0.9900	6	(1.01302 - 1.24359)	0.45066
C-2	conFDR_PCA	0.9900	6	1	0.45066
C-3	conFDR_PCA_Stepwise	0.9900	6	1	0.45066
C-4	conFDR_PLS	0.9897	3	1	0.45497
D-1	Tree	0.9894	4	(1.00064 - 1.23411)	0.45593
D-2	Tree_PCA	0.9894	4	1	0.45593
D-3	Tree_PCA_Stepwise	0.9894	4	1	0.45593
D-4	Tree_PLS	0.9894	3	1	0.45652
E-1	PCA-Stepwise	0.9946	110	1	0.42443
E-2	PAMsSites-PCA-Stepwise	0.9935	14	(1.02 - 2.11)	0.34485
F	PLS	0.9947	10	1	0.43429

Table A.4 Ranking Results of the Scenarios for the metamodel of Conyers stage 2.

Approaches*	Vars. left in model
FDR_PLS	1
Stepwise-PLS	**3**
FDR_PCA	3
FDR_PCA_Stepwise	3
conFDR_PLS	3
Tree_PLS	3
Tree_PCA	4
Tree_PCA_Stepwise	4
conFDR_PCA	6
conFDR_PCA_Stepwise	6
Stepwise-PCA	10
Stepwise-PCA-Stepwise	10
PLS	10
PCA-Stepwise	110

Approaches*	% Error
Stepwise-PCA-Stepwise	0.33001
Stepwise-PCA	0.33001
Stepwise-PLS	**0.34289**
PCA-Stepwise	0.42443
PLS	0.43429
conFDR_PCA	0.45066
conFDR_PCA_Stepwise	0.45066
conFDR_PLS	0.45497
FDR_PCA_Stepwise	0.45582
FDR_PLS	0.45582
FDR_PCA	0.45582
Tree_PCA_Stepwise	0.45593
Tree_PCA	0.45593
Tree_PLS	0.45652

Approaches*	R^2
PLS	0.9947
PCA-Stepwise	0.9946
Stepwise-PCA	0.9937
Stepwise-PCA-Stepwise	0.9937
Stepwise-PLS	**0.9934**
conFDR_PCA	0.9900
conFDR_PCA_Stepwise	0.9900
conFDR_PLS	0.9897
FDR_PLS	0.9894
Tree_PLS	0.9894
FDR_PCA	0.9894
FDR_PCA_Stepwise	0.9894
Tree_PCA	0.9894
Tree_PCA_Stepwise	0.9894

*** VIF > 1 are removed.**

*** Ordered by better to worse**

Table A.5 Results of Various Modeling Scenarios for the metamodel of Conyers stage 3.

Approaches		R^2	Vars. left in model	VIF	% Error
A-1	Stepwise	0.9847	21	(1.02 - 1.10)	0.51086
A-2	Stepwise-PCA	0.9847	21	1	0.51086
A-3	Stepwise-PCA-Stepwise	0.9846	20	1	0.51669
A-4	**Stepwise-PLS**	**0.9846**	**3**	**1**	**0.52170**
B-1	FDR	0.9659	3	(1.004 - 1.011)	0.75258
B-2	FDR_PCA	0.9659	3	1	0.75258
B-3	FDR_PCA_Stepwise	0.9659	3	1	0.75258
B-4	FDR_PLS	0.9652	1	1	0.75727
C-1	conFDR	0.9727	7	(1.00281 - 1.01647)	0.72409
C-2	conFDR_PCA	0.9727	7	1	0.72409
C-3	conFDR_PCA_Stepwise	0.9727	7	1	0.72409
C-4	conFDR_PLS	0.9727	2	1	0.72316
D-1	Tree	0.9659	4	(1.00605 - 1.01342)	0.75327
D-2	Tree_PCA	0.9659	4	1	0.75327
D-3	Tree_PCA_Stepwise	0.9659	3	1	0.74759
D-4	Tree_PLS	0.9659	2	1	0.75677
E-1	PCA-Stepwise	0.9871	135	1	0.71002
E-2	PAMsSites-PCA-Stepwise	0.9848	21	(1.01 - 1.32)	0.50636
F	PLS	0.9879	11	1	0.71337

Table A.6 Ranking Results of the Scenarios for the metamodel of Conyers stage 3.

Approaches*	Vars. left in model
FDR_PLS	1
conFDR_PLS	2
Tree_PLS	2
Stepwise-PLS	**3**
FDR_PCA	3
FDR_PCA_Stepwise	3
Tree_PCA_Stepwise	3
Tree_PCA	4
conFDR_PCA	7
conFDR_PCA_Stepwise	7
PLS	11
Stepwise-PCA-Stepwise	20
Stepwise-PCA	21
PCA-Stepwise	135

Approaches*	% Error
Stepwise-PCA	0.51086
Stepwise-PCA-Stepwise	0.51669
Stepwise-PLS	**0.52170**
PCA-Stepwise	0.71002
PLS	0.71337
conFDR_PLS	0.72316
conFDR_PCA	0.72409
conFDR_PCA_Stepwise	0.72409
Tree_PCA_Stepwise	0.74759
FDR_PCA	0.75258
FDR_PCA_Stepwise	0.75258
Tree_PCA	0.75327
Tree_PLS	0.75677
FDR_PLS	0.75727

Approaches*	R^2
PLS	0.9879
PCA-Stepwise	0.9871
Stepwise-PCA	0.9847
Stepwise-PLS	**0.9846**
Stepwise-PCA-Stepwise	0.9846
conFDR_PCA	0.9727
conFDR_PCA_Stepwise	0.9727
conFDR_PLS	0.9727
FDR_PCA	0.9659
FDR_PCA_Stepwise	0.9659
Tree_PCA	0.9659
Tree_PCA_Stepwise	0.9659
Tree_PLS	0.9659
FDR_PLS	0.9652

*** VIF > 1 are removed.**

*** Ordered by better to worse**

Table A.7 Results of Various Modeling Scenarios for the metamodel of Conyers stage 4.

Approaches		**R^2**	**Vars. left in model**	**VIF**	**% Error**
A-1	Stepwise	0.9841	26	(1.04 - 44.9)	0.76287
A-2	Stepwise-PCA	0.9841	26	1	0.76287
A-3	Stepwise-PCA-Stepwise	0.9841	25	1	0.76405
A-4	**Stepwise-PLS**	**0.9841**	**9**	**1**	**0.76289**
B-1	FDR	0.9628	9	(1.05 - 56.15)	1.09164
B-2	FDR_PCA	0.9628	9	1	1.09164
B-3	FDR_PCA_StepwiseReg	0.9627	8	1	1.08940
B-4	FDR_PLS	0.9627	7	1	1.09064
C-1	conFDR	0.9548	9	(1.003 - 1.185)	1.25593
C-2	conFDR_PCA	0.9548	9	1	1.25593
C-3	conFDR_PCA_Stepwise	0.9548	9	1	1.25593
C-4	conFDR_PLS	0.9548	4	1	1.25641
D-1	Tree	0.9676	12	(1.01 - 12.10)	1.03436
D-2	Tree_PCA	0.9676	12	1	1.03436
D-3	Tree_PCA_Stepwise	0.9675	11	1	1.03789
D-4	Tree_PLS	0.9676	9	1	1.03437
E-1	PCA-Stepwise	0.9864	167	1	1.03480
E-2	PAMsSites-PCA-Stepwise	0.9836	26	(1.03 - 6.31)	0.78045
F	PLS	0.9877	7	1	1.09891

Table A.8 Ranking Results of the Scenarios for the metamodel of Conyers stage 4.

Approaches*	**Vars. left in model**	**Approaches***	**% Error**	**Approaches***	**R^2**
conFDR_PLS	4	**Stepwise-PCA**	**0.76287**	PLS	0.9877
FDR_PLS	7	**Stepwise-PLS**	**0.76289**	PCA-Stepwise	0.9864
PLS	7	Stepwise-PCA-Stepwise	0.76405	**Stepwise-PCA**	**0.9841**
FDR_PCA_Stepwise	8	Tree_PCA	1.03436	Stepwise-PCA-Stepwise	0.9841
Stepwise-PLS	**9**	Tree_PLS	1.03437	**Stepwise-PLS**	**0.9841**
FDR_PCA	9	PCA-Stepwise	1.03480	Tree_PCA	0.9676
conFDR_PCA	9	Tree_PCA_Stepwise	1.03789	Tree_PLS	0.9676
conFDR_PCA_Stepwise	9	FDR_PCA_Stepwise	1.08940	Tree_PCA_Stepwise	0.9675
Tree_PLS	9	FDR_PLS	1.09064	FDR_PCA	0.9628
Tree_PCA_Stepwise	11	FDR_PCA	1.09164	FDR_PLS	0.9627
Tree_PCA	12	PLS	1.09891	FDR_PCA_Stepwise	0.9627
Stepwise-PCA-Stepwise	25	conFDR_PCA	1.25593	conFDR_PCA	0.9548
Stepwise-PCA	**26**	conFDR_PCA_Stepwise	1.25593	conFDR_PCA_Stepwise	0.9548
PCA-Stepwise	167	conFDR_PLS	1.25641	conFDR_PLS	0.9548

*** VIF > 1 are removed.**

*** Ordered by better to worse**

APPENDIX B

STEPWISE-PLS METAMODELS AND TRANSTION FUNCTION

Stepwise-PLS Metamodels and Transtion Functions (Stage-1).

$$\begin{bmatrix} O_1^C \\ O_1^S \\ O_1^T \\ O_1^Y \\ z_1^2 \\ \vdots \\ z_{23}^2 \end{bmatrix}' = \begin{bmatrix} z_1^1 \\ z_2^1 \\ z_3^1 \\ \vdots \\ z_{25}^1 \end{bmatrix}' \begin{bmatrix} b_1^C & \cdots & b_1^Y & b_1^{z_1^2} & \cdots & b_1^{z_{23}^2} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ b_{25}^C & \cdots & b_{25}^Y & b_{25}^{z_1^2} & \cdots & b_{25}^{z_{23}^2} \end{bmatrix} + \begin{bmatrix} 1 \\ u_1^1 \\ u_2^1 \\ u_3^1 \\ \vdots \\ u_{29}^1 \end{bmatrix}' \begin{bmatrix} a_0^C & \ldots & a_0^Y & a_0^{z_1^2} & \ldots & a_0^{z_{23}^2} \\ a_1^C & \cdots & a_1^Y & a_1^{z_1^2} & \cdots & a_1^{z_{23}^2} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ a_{29}^C & \cdots & a_{29}^Y & a_{29}^{z_1^2} & \cdots & a_{29}^{z_{23}^2} \end{bmatrix} + \begin{bmatrix} \varepsilon_1^C \\ \varepsilon_1^S \\ \varepsilon_1^T \\ \varepsilon_1^Y \\ \varepsilon_1^{z_1^2} \\ \vdots \\ \varepsilon_1^{z_{23}^2} \end{bmatrix}'$$

Stepwise-PLS Metamodels and Transtion Functions (Stage-2).

$$\begin{bmatrix} O_2^C \\ O_2^S \\ O_2^T \\ O_2^Y \\ z_1^3 \\ \vdots \\ z_{14}^3 \end{bmatrix}' = \begin{bmatrix} z_1^2 \\ z_2^2 \\ z_3^2 \\ \vdots \\ z_{23}^2 \end{bmatrix}' \begin{bmatrix} b_1^C & \cdots & b_1^Y & b_1^{z_1^3} & \cdots & b_1^{z_{14}^3} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ b_{23}^C & \cdots & b_{23}^Y & b_{23}^{z_1^3} & \cdots & b_{23}^{z_{14}^3} \end{bmatrix} + \begin{bmatrix} 1 \\ u_1^2 \\ u_2^2 \\ u_3^2 \\ \vdots \\ u_{28}^2 \end{bmatrix}' \begin{bmatrix} a_0^C & \ldots & a_0^Y & a_0^{z_1^3} & \ldots & a_0^{z_{14}^3} \\ a_1^C & \cdots & a_1^Y & a_1^{z_1^3} & \cdots & a_1^{z_{14}^3} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ a_{28}^C & \cdots & a_{28}^Y & a_{28}^{z_1^3} & \cdots & a_{28}^{z_{14}^3} \end{bmatrix} + \begin{bmatrix} \varepsilon_2^C \\ \varepsilon_2^S \\ \varepsilon_2^T \\ \varepsilon_2^Y \\ \varepsilon_2^{z_1^3} \\ \vdots \\ \varepsilon_2^{z_{14}^3} \end{bmatrix}'$$

Stepwise-PLS Metamodels and Transtion Functions (Stage-3).

$$\begin{bmatrix} O_3^C \\ O_3^S \\ O_3^T \\ O_3^Y \\ z_1^4 \\ \vdots \\ z_9^4 \end{bmatrix}' = \begin{bmatrix} z_1^3 \\ z_2^3 \\ z_3^3 \\ \vdots \\ z_{14}^3 \end{bmatrix}' \begin{bmatrix} b_1^C & \cdots & b_1^Y & b_1^{z_1^4} & \cdots & b_1^{z_9^4} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ b_{14}^C & \cdots & b_{14}^Y & b_{14}^{z_1^4} & \cdots & b_{14}^{z_9^4} \end{bmatrix} + \begin{bmatrix} 1 \\ u_1^3 \\ u_2^3 \\ u_3^3 \\ \vdots \\ u_{25}^3 \end{bmatrix}' \begin{bmatrix} a_0^C & \dots & a_0^Y & a_0^{z_1^4} & \dots & a_0^{z_9^4} \\ a_1^C & \cdots & a_1^Y & a_1^{z_1^4} & \cdots & a_1^{z_9^4} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ a_{25}^C & \cdots & a_{25}^Y & a_{25}^{z_1^4} & \cdots & a_{25}^{z_9^4} \end{bmatrix} + \begin{bmatrix} \varepsilon_3^C \\ \varepsilon_3^S \\ \varepsilon_3^T \\ \varepsilon_3^Y \\ \varepsilon_3^{z_1^4} \\ \vdots \\ \varepsilon_3^{z_9^4} \end{bmatrix}'$$

Stepwise-PLS Metamodels and Transtion Functions (Stage-4).

$$\begin{bmatrix} O_4^C \\ O_4^S \\ O_4^T \\ O_4^Y \end{bmatrix}' = \begin{bmatrix} z_1^4 \\ z_2^4 \\ z_3^4 \\ \vdots \\ z_9^4 \end{bmatrix}' \begin{bmatrix} b_1^C & b_1^S & b_1^T & b_1^Y \\ b_2^C & b_2^S & b_2^T & b_2^Y \\ b_3^C & b_3^S & b_3^T & b_3^Y \\ \vdots & \vdots & \vdots & \vdots \\ b_9^C & b_9^S & b_9^T & b_9^Y \end{bmatrix} + \begin{bmatrix} 1 \\ u_1^4 \\ u_2^4 \\ u_3^4 \\ \vdots \\ u_7^4 \end{bmatrix}' \begin{bmatrix} a_0^C & a_0^S & a_0^T & a_0^Y \\ a_1^C & a_1^S & a_1^T & a_1^Y \\ a_2^C & a_2^S & a_2^T & a_2^Y \\ a_3^C & a_3^S & a_3^T & a_3^Y \\ \vdots & \vdots & \vdots & \vdots \\ a_7^C & a_7^S & a_7^T & a_7^Y \end{bmatrix} + \begin{bmatrix} \varepsilon_4^C \\ \varepsilon_4^S \\ \varepsilon_4^T \\ \varepsilon_4^Y \end{bmatrix}'$$

Table B.1 Coefficient Matrix of Stepwise – PLS Metamodel (Phase-1) for Stage-1.

	b_i^C	b_i^S	b_i^T	b_i^Y	$b_i^{z_1^2}$	$b_i^{z_2^2}$	$b_i^{z_3^2}$	$b_i^{z_4^2}$	$b_i^{z_5^2}$	$b_i^{z_6^2}$	$b_i^{z_7^2}$	$b_i^{z_8^2}$	$b_i^{z_9^2}$	$b_i^{z_{10}^2}$
$i = 1$	0.0350572982	-0.0316803730	-0.0050999380	0.0015675277	0.0075060307	0.1519456683	-0.6060468510	0.0673756310	0.0037512673	0.0541239146	0.0737867350	0.0383425216	0.0141850794	-0.0697587180
$i = 2$	0.0062157710	0.0550459674	-0.0439306580	-0.0140485810	-0.0037927860	-0.0359066030	-0.1040012950	-0.1104767130	0.1725466506	0.1679326811	0.1042159539	0.0168711630	-0.2351609690	0.4647825059
$i = 3$	0.0585604446	-0.0580653400	-0.0379455630	-0.0140395880	0.0121335746	0.0863408852	0.0283097198	-0.0699575440	-0.0515827260	0.1601613229	-0.0419341670	-0.2243602850	0.2600823839	0.1821582058
$i = 4$	0.0554318391	-0.0801419770	-0.0747259040	-0.0038638850	-0.0645199360	0.2208568247	0.0964085734	-0.1596226310	-0.2539557820	-0.1608552360	-0.1010459240	0.0943434042	-0.2811550500	-0.0787796190
$i = 5$	0.0870662545	-0.0599396660	0.0247864919	0.0696719849	-0.1283052950	0.1043526535	0.0374969293	0.1168798352	0.0845462551	-0.2076835180	0.3748576094	-0.1636586090	0.2376948874	-0.1601875510
$i = 6$	0.0348666711	-0.0192225140	-0.0637171830	-0.0639707250	0.1292527224	0.0575156720	-0.0337048740	-0.0646025490	0.1718821272	0.0076021352	0.1748437532	-0.2625653450	0.1213102485	0.2084188547
$i = 7$	0.0374660284	-0.1054753350	-0.0020617940	-0.0500656110	0.0363224787	0.1514170312	0.0373867090	0.0645053154	0.1179417323	-0.0879860350	0.2003922049	0.2945580318	0.1901053783	-0.0051720210
$i = 8$	0.0397913936	-0.0311497900	-0.0403261400	-0.0674729710	0.1019549416	0.0312209534	-0.0088341340	-0.0464263400	0.0144452777	-0.0656301260	-0.1521804140	0.0645587950	0.1395814028	-0.0712387900
$i = 9$	0.0491016428	-0.0474684620	0.0403161213	-0.1236323090	0.1078070432	0.0341312097	0.0136690936	0.0808137094	0.0647194577	0.0702112279	0.0523528865	0.2024273713	0.1454915935	-0.0642418070
$i = 10$	0.0450219106	0.0250047293	-0.0050081870	-0.0489623200	0.0787110243	-0.0180657850	-0.0114554660	-0.0213850950	0.0373159176	-0.0763795260	-0.0710280290	0.1669623133	0.0667397974	0.1186027260
$i = 11$	0.0674137043	-0.0217190380	-0.0365736340	0.0648312887	-0.0389282990	0.0689571010	0.0120176080	-0.0439367250	0.1690147309	-0.0037623850	-0.1714403080	0.0278117830	-0.0691827960	-0.0172740260
$i = 12$	0.0342737226	0.0176446282	-0.0289180100	-0.0561304170	0.0229212850	-0.0056220350	0.0051338451	-0.0642097840	-0.0917986840	0.0842531206	0.1206996326	-0.1027388000	0.1075705176	-0.1206335580
$i = 13$	0.0523421814	0.0781673267	-0.0094869120	0.0180170335	-0.1026346760	-0.0747658860	-0.0811362470	-0.0891055910	-0.1554979560	0.1006433469	-0.1599606240	0.1222762236	0.1587168726	-0.0258408940
$i = 14$	0.0924685563	0.0497463588	-0.0077782570	-0.0320557860	0.0256412605	-0.0405151850	-0.0205189850	-0.0251424820	-0.0462706610	-0.0360310930	0.0549699048	-0.0770663560	-0.0297782440	-0.0317700970
$i = 15$	0.0089852760	-0.0590374480	-0.0080297820	-0.1015505050	0.1327001625	0.0942266285	-0.0077316220	0.0422073764	-0.0603551490	-0.0028069850	-0.0611968750	0.1495685455	0.0510097237	0.0658370293
$i = 16$	0.0593151198	-0.1091285870	-0.0047106410	-0.1043534490	0.0537354739	0.1572277509	0.0467110237	0.0540812391	0.0999336830	-0.0088160140	-0.0910579130	0.0429472333	-0.0645901930	-0.0899810260
$i = 17$	0.0770204970	0.0360262840	-0.0075949050	-0.0321557930	0.0337304167	-0.0015193130	-0.0283944010	-0.0900407870	-0.0517806110	-0.1822412020	0.0379351052	0.0325270163	0.0581235666	0.0949806625
$i = 18$	0.0127670760	-0.0236346780	0.1136278397	0.0046084081	-0.0163083930	-0.0269340980	0.0301486183	0.1611197388	-0.0487512290	0.0316764524	0.0113948889	-0.0441838940	0.0341117508	0.0454482742
$i = 19$	0.0225102853	0.0192403926	0.0748295842	0.0340220157	-0.0589068660	-0.0471889700	-0.0354201140	0.0336456567	0.0106739532	-0.1182833490	-0.0704547240	0.0253399893	0.0892148951	0.0640532922
$i = 20$	0.0409461915	0.0675977312	0.0604363842	-0.0598987000	0.0658679135	-0.0976892470	0.0028925513	0.0181614999	0.0538544534	-0.0709418350	0.0008349386	-0.0264519330	-0.0768078070	-0.0697977660
$i = 21$	0.0430474681	-0.0580455670	0.0079488067	0.0296581144	-0.0381546960	0.0824898148	-0.0277292680	0.0210506310	-0.0672443210	-0.0870494890	-0.0302578870	-0.0023180040	-0.0731954720	0.0602904926
$i = 22$	0.0203773938	0.0305128019	-0.0226540860	0.0303491982	-0.0354740120	-0.0413748450	-0.0200549050	-0.0134034450	0.0676285126	0.0122830725	0.0175417326	-0.0105490470	0.0052722538	-0.0326253820
$i = 23$	0.0034073416	-0.0154564820	-0.0024721660	-0.0314850300	-0.0046626260	0.0307807553	-0.0005346600	-0.0155375390	-0.0337956470	0.0022283568	0.0186584869	-0.0360083650	0.0126866158	-0.0545895580
$i = 24$	0.0476928376	0.0167344725	0.0052709354	0.0440732678	0.0027817936	0.0022146268	0.0411131314	-0.0104730960	-0.0154608230	-0.0176821080	-0.0344362260	0.0108585405	0.0176361352	-0.0298120840
$i = 25$	0.0214989325	0.0146429721	0.0039747119	0.0142957723	-0.0136611670	-0.0138307620	-0.0166483050	-0.0137953180	0.0016329669	0.0223353133	0.0045634762	-0.0092755190	0.0119783300	-0.0169274820

Table B.1 Coefficient Matrix of Stepwise – PLS Metamodel (Phase-1) for Stage-1 (Continued).

	$b_i^{z_{11}^2}$	$b_i^{z_{12}^2}$	$b_i^{z_{13}^2}$	$b_i^{z_{14}^2}$	$b_i^{z_{15}^2}$	$b_i^{z_{16}^2}$	$b_i^{z_{17}^2}$	$b_i^{z_{18}^2}$	$b_i^{z_{19}^2}$	$b_i^{z_{20}^2}$	$b_i^{z_{21}^2}$	$b_i^{z_{22}^2}$	$b_i^{z_{23}^2}$
$i = 1$	0.0561254749	0.1319537060	0.0081660302	0.0164588515	-0.0237824790	-0.0105156080	0.0131324899	0.0303540690	0.0423014926	0.0432241783	0.0459749024	0.0128134752	0.0180569688
$i = 2$	-0.0376029340	-0.0243640990	0.0999024541	0.0094260629	-0.0323639990	-0.0623152320	-0.1214954730	-0.0586147080	-0.3921636600	0.0499956254	0.0741865697	0.0977349875	0.0615580666
$i = 3$	0.0161023244	-0.2681017300	0.2673100810	-0.0721116810	-0.1467921630	-0.2088043070	0.0657024114	0.0225346534	0.1520001635	0.1720598074	-0.0008778540	0.2558738889	0.0662522013
$i = 4$	-0.0358807150	0.2064966349	0.3614829921	0.0670079135	0.0022971761	-0.1537969510	-0.2653007280	0.0431383266	-0.0137654410	0.2104439669	0.2016342958	-0.0708699370	-0.1186665120
$i = 5$	0.1121766066	0.0066761892	0.0901203310	-0.1385103620	0.2496446368	0.1546053987	-0.0918802200	-0.1002947110	-0.2386315670	0.1924363863	-0.0291652090	0.2294954146	-0.2526616950
$i = 6$	-0.3297187240	-0.0465947250	0.0072116902	0.2379405578	0.2163582412	0.0531641932	-0.2279954560	0.1869249900	0.2471468595	0.0066067354	0.0394975163	-0.3747090850	-0.2200391480
$i = 7$	-0.0242483250	-0.1233264690	0.0435245385	-0.1312379300	-0.1751099140	-0.2078437420	-0.3009508440	0.0604843723	0.1180326818	-0.4453678590	0.2978467404	0.1371014035	0.0291242199
$i = 8$	0.1468770149	-0.1491809820	-0.3332578620	0.1408372964	0.1263666432	-0.0409757520	-0.4325355060	-0.0605318240	-0.1002379250	0.2765919335	-0.0827433150	0.0138270955	0.2585901509
$i = 9$	-0.0154851470	0.0658310694	0.1960761938	-0.0785184900	0.0338544815	-0.4184471440	0.0917075591	-0.1718513530	0.0125442902	0.1615312854	-0.2999105860	-0.1861039370	0.0166718308
$i = 10$	-0.0246601280	0.0991866107	0.3707608886	-0.1241703670	-0.0036084300	0.4154558922	-0.1872620590	0.1083165142	0.0943229091	-0.0972685850	-0.3816536900	0.1164926952	0.1373415125
$i = 11$	-0.0393868380	-0.0311426190	-0.2325021860	-0.1758234770	-0.1761264600	-0.1901885880	0.0300147535	0.4265209019	-0.0769862470	0.1155579383	-0.2654399840	0.0533947017	-0.2483056090
$i = 12$	0.0526973812	-0.0188597610	0.0735340643	0.2484270383	-0.3532408030	0.0953027701	-0.1260983810	0.0509467710	-0.1195125740	-0.0431253270	-0.0917159320	-0.1078920660	-0.1009436770
$i = 13$	-0.0700868460	-0.0309276300	0.0117976521	0.1491339138	0.1655547322	0.0310595339	0.0000848083	0.1207357865	0.0245806212	-0.0343350850	0.0540243454	0.1786220630	-0.1811777330
$i = 14$	0.1111956888	-0.1561104970	0.1125059661	-0.0226019360	0.1566469455	-0.0629290600	0.0301301540	0.2047252435	-0.0991900150	-0.1520007020	-0.0319810200	-0.1286701270	0.1343006249
$i = 15$	0.1359872058	-0.2024971080	0.0042213607	-0.0605798500	-0.0090124370	0.1512464449	0.0687596518	0.0221796638	-0.0636852080	0.1588399775	0.1185653677	-0.1641555540	-0.1516376830
$i = 16$	-0.1104471540	-0.0294825870	0.0210748918	0.1379554730	0.0629899449	0.0366314287	0.1192201432	-0.0693990660	-0.1522705370	-0.0424264250	-0.0408299560	0.0720244935	0.0211344359
$i = 17$	0.0141468652	0.0281979489	-0.0681298720	0.0673901660	-0.0667535650	0.0087682599	0.1647863296	0.0029204042	0.0571617281	0.0640585156	0.0057567392	0.0505236504	0.0855368401
$i = 18$	-0.0114624970	0.0297564612	-0.0182387400	0.0672764550	0.0054353519	0.0322927709	0.0081072835	0.0245866851	0.0244044124	0.0384632663	0.0126725566	0.0166082736	0.0544749813
$i = 19$	-0.1073594520	0.0203169939	-0.0186426890	-0.0307296690	-0.0063632890	-0.0128157930	0.0123216065	-0.0927948040	-0.1385425310	-0.0232986940	-0.0119919670	-0.1320689120	-0.0677151850
$i = 20$	-0.0359473240	-0.0292249520	-0.0148439640	0.0169925520	-0.0099217700	0.0092459403	-0.0252601090	-0.0437557050	0.0628491097	-0.0023951220	0.0316525151	0.0272805809	-0.0814613800
$i = 21$	0.0146153809	-0.0431273840	-0.0087663720	0.0237219109	-0.0162237150	-0.0737711840	-0.0785451020	-0.0369404310	0.0733818893	0.0223399525	-0.0561436430	-0.0162896260	-0.0380823020
$i = 22$	-0.0296056210	-0.0429783020	0.0048241291	0.0587846090	-0.0299700070	-0.0387888100	-0.0372054720	0.0484344793	-0.0165120010	0.0855144213	0.0102852901	-0.0351847960	0.0144299916
$i = 23$	-0.0509341600	0.0215658117	-0.0656132740	-0.0068133220	0.0355232870	0.0233932954	-0.0589362560	-0.0371819110	-0.0044394720	0.0288082394	0.0713695356	0.0038939614	0.0629180196
$i = 24$	0.0810218146	0.0538180394	0.0178699363	0.0087651708	-0.0089509780	0.0309964350	-0.0405222990	0.0125810150	-0.0416863360	0.0142010050	0.0083586970	0.0533204046	0.0111200163
$i = 25$	0.0506525770	-0.0367278910	-0.0517610060	0.0616777012	0.0687173134	-0.0489051200	0.0319666520	-0.0467197790	-0.0094759940	-0.0003948310	-0.0229523910	-0.0022294820	-0.0030324930

Table B.2 Coefficient Matrix of Stepwise – PLS Metamodel (Phase-2) for Stage-1.

	a_i^C	a_i^S	a_i^T	a_i^Y	$a_i^{z_1^2}$	$a_i^{z_2^2}$	$a_i^{z_3^2}$	$a_i^{z_4^2}$	$a_i^{z_5^2}$	$a_i^{z_6^2}$	$a_i^{z_7^2}$	$a_i^{z_8^2}$	$a_i^{z_9^2}$	$a_i^{z_{10}^2}$
$i = 0$	5.424300E-04	8.360000E-03	7.710000E-03	-5.382200E-04	1.342610E+00	-2.981790E+00	-1.228260E+00	1.207260E+00	1.960800E-01	1.957280E+00	-1.757140E+00	-6.852300E-01	5.555500E-01	-2.124210E+00
$i = 1$	0	0	0	0	5.490000E-06	0	-3.590000E-06	-3.390000E-06	3.070000E-06	-5.340000E-06	-4.600000E-06	2.290000E-06	3.416000E-05	1.445000E-05
$i = 2$	1.089050E-08	0	0	3.213511E-08	-1.432800E-04	1.406000E-05	0	-1.086000E-05	1.289000E-05	-5.440000E-06	-9.240000E-06	-1.405000E-05	2.110000E-06	1.455000E-05
$i = 3$	-5.507220E-09	0	0	6.372570E-10	-1.917000E-05	-3.580000E-06	5.820000E-06	7.810000E-06	-1.819000E-05	1.698000E-05	3.748000E-05	4.202000E-05	-1.240000E-05	0
$i = 4$	0	1.736534E-08	0	0	6.020000E-06	0	1.564000E-05	-4.590000E-06	1.898000E-05	-2.242000E-05	0	7.780000E-06	1.030000E-05	-1.739000E-05
$i = 5$	0	0	0	0	0	0	-5.690000E-06	7.940000E-06	-5.650000E-06	6.630000E-06	-1.484000E-05	3.310000E-06	-1.119000E-05	6.940000E-06
$i = 6$	0	0.000000E+00	0	7.700370E-10	-3.810000E-06	2.230000E-06	0.00000134	-0.00000138	0.00000341	-5.070000E-06	-2.170000E-06	8.920000E-06	0.00000598	0.00000137
$i = 7$	0	0	0	0	3.200000E-06	2.190000E-06	-8.749650E-07	-3.710000E-06	-8.448220E-07	-1.121000E-05	3.000000E-06	3.950000E-06	3.870000E-06	6.780000E-06
$i = 8$	-7.558600E-09	0	0	0	0	0	0	0	0	2.680000E-06	0	0	0	0
$i = 9$	0	0	0	0	7.104126E-07	0	0	-5.997670E-07	-7.360000E-06	0	4.040000E-06	-4.830000E-06	2.954349E-07	0
$i = 10$	0	-2.707880E-08	7.656057E-09	0	4.224508E-07	5.110000E-06	1.070000E-06	3.980000E-06	-6.814160E-07	2.567850E-07	-8.368350E-07	-5.298020E-07	-5.847870E-07	1.070000E-06
$i = 11$	0	0	0	0	0	0	0	-3.540000E-06	-5.660000E-06	-1.051000E-05	2.960000E-06	3.390000E-06	0	9.850000E-06
$i = 12$	0	0	0	0	5.220000E-06	0	1.549000E-05	8.320000E-06	3.531000E-05	0	1.844000E-05	-1.285000E-05	-2.017000E-05	-3.367000E-05
$i = 13$	-2.213810E-08	0	0	0	5.680000E-06	0	2.326000E-05	2.220000E-06	0	2.721000E-05	1.073000E-05	8.830000E-06	1.347000E-05	1.948000E-05
$i = 14$	0	0.000000E+00	-1.079200E-07	0	2.450000E-06	1.231000E-05	8.462583E-07	-1.941000E-05	0	4.500000E-06	1.920000E-06	7.626011E-07	0	-3.220000E-06
$i = 15$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$i = 16$	0	0	0	0	-4.750000E-06	0	0	5.320000E-06	5.810000E-06	0	3.180000E-06	5.850000E-06	0	-1.305000E-05
$i = 17$	0	0	0	9.476480E-10	5.730000E-06	0	-1.139000E-05	0	0	-4.190000E-06	-1.267000E-05	0	3.480000E-06	2.243000E-05
$i = 18$	0	0	0	0	0	0	-2.300000E-06	0	3.320000E-06	0	-3.240000E-06	-3.040000E-06	7.150000E-06	0
$i = 19$	0	0	0	0	0	-8.410000E-06	3.060000E-06	-2.630000E-06	2.190000E-06	-1.091000E-05	2.950000E-06	-5.520000E-06	4.140000E-06	1.273000E-05
$i = 20$	0	0	0	0	1.930000E-06	0	2.440000E-06	0	4.010000E-06	1.550000E-06	0	-2.130000E-06	-7.620000E-06	-3.480000E-06
$i = 21$	0	0	0	0	8.505382E-07	0	0	-2.530000E-06	-5.950000E-06	-5.050000E-06	-7.586750E-07	1.200000E-06	-6.905030E-07	2.410000E-06
$i = 22$	0	0	0	0	1.230000E-06	1.190000E-06	-5.275770E-07	-9.824470E-07	7.012939E-07	-7.170000E-06	0	8.811924E-07	-2.620000E-06	2.990000E-06
$i = 23$	1.626434E-09	0	0	0	1.230000E-06	-1.400000E-06	-1.070000E-06	-1.410000E-06	2.440000E-06	-7.200000E-06	3.290000E-06	-1.300000E-06	-5.200000E-06	2.640000E-06
$i = 24$	0	0	-1.352130E-08	0	0	7.480000E-06	4.230000E-06	0	5.080000E-06	-7.500000E-06	1.016000E-05	-6.050000E-06	1.250000E-06	-7.260000E-06
$i = 25$	0	0	0	0	0	0	-3.050000E-06	-9.600000E-06	-5.340000E-06	-3.810000E-06	-1.165000E-05	1.098000E-05	1.087000E-05	-1.760000E-06
$i = 26$	0	0	0	0	0	0.000000E+00	0.000000E+00	0	0.000000E+00	0.000000E+00	0.000000E+00	9.673192E-07	0.000000E+00	0.000000E+00
$i = 27$	0	0	0	0	0	3.864000E-05	-1.311000E-05	0.000000E+00	1.775500E-04	-6.272000E-05	1.293400E-04	-2.005000E-05	-1.199700E-04	5.850000E-05
$i = 28$	0	0	0	0	0.000000E+00	-0.00009113	-0.00004841	0.00008794	-4.731000E-05	0.00007405	-6.783000E-05	-1.797300E-04	-2.034200E-04	-2.251000E-05
$i = 29$	0	0	0	0	1.807000E-05	0	0	0	4.284000E-05	0	1.477000E-05	1.089000E-05	1.692000E-05	3.197000E-05

ε_1^C	ε_1^S	ε_1^T	ε_1^Y	$\varepsilon_1^{z_1^2}$	$\varepsilon_1^{z_2^2}$	$\varepsilon_1^{z_3^2}$	$\varepsilon_1^{z_4^2}$	$\varepsilon_1^{z_5^2}$	$\varepsilon_1^{z_6^2}$	$\varepsilon_1^{z_7^2}$	$\varepsilon_1^{z_8^2}$	$\varepsilon_1^{z_9^2}$	$\varepsilon_1^{z_{10}^2}$
0.00067832	0.00155	0.00183	0.00006338	0.29047	0.40179	0.19584	0.32988	0.19674	0.28449	0.23408	0.17331	0.14544	0.14959

Table B.2 Coefficient Matrix of Stepwise – PLS Metamodel (Phase-2) for Stage-1 (Continued).

	$a_i^{z_{11}^2}$	$a_i^{z_{12}^2}$	$a_i^{z_{13}^2}$	$a_i^{z_{14}^2}$	$a_i^{z_{15}^2}$	$a_i^{z_{16}^2}$	$a_i^{z_{17}^2}$	$a_i^{z_{18}^2}$	$a_i^{z_{19}^2}$	$a_i^{z_{20}^2}$	$a_i^{z_{21}^2}$	$a_i^{z_{22}^2}$	$a_i^{z_{23}^2}$
$i = 0$	1.270560E+00	-2.126660E+00	2.153090E+00	2.778510E+00	8.858400E-01	-1.613760E+00	7.906100E-01	5.343000E-02	-2.144700E+00	-1.800250E+00	9.194000E-01	1.721400E-01	-1.212640E+00
$i = 1$	-3.404000E-05	2.730000E-06	-6.730000E-06	-1.704000E-05	1.782000E-05	2.920000E-06	5.920000E-06	1.629000E-05	-2.531000E-05	6.310000E-06	1.602000E-05	-2.535000E-05	0
$i = 2$	2.890000E-06	1.608000E-05	-6.610000E-06	0	6.090000E-06	-9.110000E-06	0	0	1.744000E-05	0	-7.930000E-06	-1.408000E-05	1.311000E-05
$i = 3$	-2.163000E-05	-2.564000E-05	-2.720000E-06	-2.650000E-06	5.800000E-06	1.013000E-05	4.760000E-06	0	1.100000E-05	1.863000E-05	-4.820000E-06	-1.410000E-06	3.470000E-06
$i = 4$	-1.689000E-05	2.209000E-05	2.800000E-06	-2.329000E-05	5.490000E-06	-1.776000E-05	1.160000E-05	0	-3.380000E-06	4.670000E-06	1.309000E-05	5.570000E-06	1.007000E-05
$i = 5$	-1.140000E-06	-4.890000E-06	-8.930000E-06	-2.013000E-05	1.640000E-06	1.053000E-05	-3.210000E-06	0	1.227000E-05	1.009000E-05	-1.224000E-05	0	-6.460000E-06
$i = 6$	-7.723330E-07	0.000000E+00	0.00000126	-7.880000E-06	0.000000E+00	0.0000041	-8.410000E-06	0	-7.100000E-06	-1.720000E-06	-0.00000229	-3.630000E-06	0.00000734
$i = 7$	6.280000E-06	3.130000E-06	-4.570000E-06	4.070000E-06	8.260000E-06	-7.540000E-06	5.150000E-06	-3.800000E-06	9.630000E-06	3.520000E-06	-3.120000E-06	4.100000E-06	0
$i = 8$	0	1.770000E-06	-2.090000E-06	0	0	0	0	-5.200000E-06	0	0	0	0	-3.430000E-06
$i = 9$	-2.790000E-06	3.210000E-06	-2.180000E-06	-3.150000E-06	-1.530000E-06	-1.660000E-06	-1.080000E-06	0	-1.150000E-06	-1.140000E-06	-2.510000E-06	-7.911850E-07	3.790000E-06
$i = 10$	-4.292650E-07	-2.210040E-07	-2.011400E-07	3.770793E-07	-3.735880E-07	9.109346E-07	5.398109E-07	0	-2.912150E-07	0	-1.542040E-07	2.020115E-07	0
$i = 11$	1.155000E-05	-5.080000E-06	-6.520000E-06	-2.440000E-06	-3.390000E-06	-1.160000E-06	0	3.510000E-06	1.040000E-06	1.850000E-06	4.330000E-06	-6.380000E-06	-9.722360E-07
$i = 12$	0	0	0	1.313000E-05	-5.356000E-05	-2.990000E-06	-1.695000E-05	1.007000E-05	5.126000E-05	4.400000E-05	1.309000E-05	-6.500000E-06	0
$i = 13$	2.638000E-05	4.085000E-05	-4.090000E-06	2.650000E-06	6.270000E-06	7.390000E-06	0	1.442000E-05	1.138000E-05	1.300000E-06	6.040000E-06	0	0
$i = 14$	-1.240000E-06	-1.810000E-06	-2.110000E-06	-6.216320E-07	8.715347E-07	2.800000E-06	2.880000E-06	-2.620000E-06	5.268635E-07	-1.710000E-06	-1.660000E-06	8.560453E-07	0
$i = 15$	0	0	-6.051320E-07	0	0	0	0	0	0	0	0	0	0
$i = 16$	-8.780000E-06	3.660000E-06	-1.429000E-05	0	-1.949000E-05	-1.690000E-06	-2.970000E-05	6.560000E-06	-5.510000E-06	-3.349000E-05	-2.125000E-05	1.691000E-05	-2.149000E-05
$i = 17$	-9.370000E-06	2.180000E-05	-1.065000E-05	-4.972000E-05	-8.790000E-06	-8.390000E-06	-4.450000E-06	-7.550000E-06	1.935000E-05	-3.180000E-06	1.847000E-05	6.070000E-06	-1.305000E-05
$i = 18$	-4.440000E-06	-1.830000E-06	0	3.450000E-06	0	7.360000E-06	-1.768000E-05	-1.569000E-05	1.467000E-05	1.213000E-05	0	0	2.511000E-05
$i = 19$	-1.604000E-05	7.790000E-06	-4.810000E-06	8.220000E-06	-1.788000E-05	1.258000E-05	0	-1.071000E-05	0	1.025000E-05	6.540000E-06	1.846000E-05	-2.540000E-06
$i = 20$	-3.010000E-06	2.940000E-06	-3.630000E-06	-4.189880E-07	6.310000E-06	-2.250000E-06	-1.060000E-06	3.720000E-06	-1.130000E-06	2.390000E-06	3.460000E-06	4.250000E-06	6.090000E-06
$i = 21$	-1.060000E-06	2.720000E-06	-2.620000E-06	4.950000E-06	1.230000E-06	-3.28931E-07	-2.410000E-06	0	1.720000E-06	1.740000E-06	-3.580000E-06	8.650000E-06	-6.100000E-06
$i = 22$	-2.810000E-06	1.130000E-06	6.087100E-07	2.360000E-06	1.700000E-06	0	8.081712E-07	-3.470000E-06	4.890000E-06	-5.100000E-06	-1.520000E-06	-1.620000E-06	3.250000E-06
$i = 23$	7.757425E-07	1.350000E-06	3.020000E-06	1.730000E-06	-5.532940E-07	2.020000E-06	4.900000E-06	0	1.130000E-06	0	-4.770000E-06	1.130000E-06	0
$i = 24$	1.923000E-05	-7.820000E-06	3.760000E-06	-6.720000E-06	-1.517000E-05	1.921000E-05	5.170000E-06	8.320000E-06	-8.020000E-06	8.450000E-06	9.310000E-06	-1.342000E-05	1.274000E-05
$i = 25$	-1.395000E-05	1.123000E-05	0	-4.340000E-06	-1.750000E-05	1.585000E-05	6.730000E-06	3.840000E-06	-4.070000E-06	1.319000E-05	6.480000E-06	-2.010000E-06	3.540000E-06
$i = 26$	0.000000E+00	0	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.000000E+00	0
$i = 27$	-3.956000E-05	0.000000E+00	-1.224300E-04	-1.186700E-04	-5.086000E-05	-9.910000E-06	-5.153000E-05	4.123000E-05	1.016300E-04	2.484000E-05	-7.447000E-05	8.207000E-05	0.000000E+00
$i = 28$	1.483600E-04	-1.154300E-04	1.849000E-04	-4.484500E-04	1.871700E-04	1.544500E-04	-1.608500E-04	-9.970000E-05	1.899300E-04	-4.775000E-05	9.511000E-05	-8.723000E-05	-2.166500E-04
$i = 29$	2.462000E-05	5.244000E-05	1.596000E-05	-3.476000E-05	-3.718000E-05	-5.652000E-05	-8.006000E-05	-4.578000E-05	-7.361000E-05	3.192000E-05	-1.675900E-04	-1.319000E-04	-5.238000E-05

$\varepsilon_1^{z_{11}^2}$	$\varepsilon_1^{z_{12}^2}$	$\varepsilon_1^{z_{13}^2}$	$\varepsilon_1^{z_{14}^2}$	$\varepsilon_1^{z_{15}^2}$	$\varepsilon_1^{z_{16}^2}$	$\varepsilon_1^{z_{17}^2}$	$\varepsilon_1^{z_{18}^2}$	$\varepsilon_1^{z_{19}^2}$	$\varepsilon_1^{z_{20}^2}$	$\varepsilon_1^{z_{21}^2}$	$\varepsilon_1^{z_{22}^2}$	$\varepsilon_1^{z_{23}^2}$
0.16815	0.19676	0.23374	0.17207	0.24603	0.13268	0.1906	0.5288	0.1307	0.18865	0.21509	0.16612	0.29936

Table B.3 Coefficient Matrix of Stepwise – PLS Metamodel (Phase-1) for Stage-2.

	b_i^C	b_i^S	b_i^T	b_i^Y	$b_i^{z_1^3}$	$b_i^{z_2^3}$	$b_i^{z_3^3}$	$b_i^{z_4^3}$	$b_i^{z_5^3}$	$b_i^{z_6^3}$	$b_i^{z_7^3}$	$b_i^{z_8^3}$	$b_i^{z_9^3}$
$i = 1$	0.0460916002	-0.0206900310	-0.0370666930	-0.5166210210	0.1003230915	-0.1594744990	0.3618197584	0.1581337374	-0.0573101270	-0.0319661020	0.2131022779	-0.3551134750	-0.0267587580
$i = 2$	0.0336858695	-0.0611961270	-0.4588087970	0.0126373569	0.4185226396	0.2315036566	0.1418218251	-0.2857451020	-0.0339012530	-0.0351194790	-0.0431557070	0.1121575972	-0.1990071030
$i = 3$	0.2185707219	0.0444286454	-0.0266579050	0.0140375519	0.0922896680	-0.0057673300	-0.0944174410	0.2657987950	-0.3003864850	-0.2674876660	-0.2713181520	-0.0854146280	-0.2158926850
$i = 4$	0.0098590053	-0.0563776710	0.1991635585	0.0012807934	0.1999953004	0.1453138122	0.0561712500	-0.1075660600	0.0330359540	-0.1110790490	-0.0775548490	-0.0637993560	0.2054812285
$i = 5$	0.0365056866	0.1328768105	0.0702626646	-0.0761996280	0.1430432660	-0.4699403450	0.0069543740	-0.2794354860	0.0654181841	-0.1964790970	-0.1268221860	0.0061255552	0.2330693039
$i = 6$	0.2075033629	-0.0158906420	-0.0992268370	0.0553016703	-0.0677335320	0.0239324962	0.0057528399	-0.0208749450	0.4126080150	-0.3276004910	-0.1476690660	-0.0621345730	0.0715759948
$i = 7$	0.0710052051	-0.0051017110	0.0127974239	0.1851432033	0.0636267075	0.2413664964	-0.1939532920	-0.0346696360	-0.1766100590	-0.0653042500	0.3033435597	-0.1099543220	0.1618746997
$i = 8$	0.1195665221	-0.0436796870	0.0340021343	0.2052783867	-0.1103300520	-0.1060251570	-0.2349229640	-0.1531608070	-0.1456458380	0.0075519249	-0.0971911520	0.1128899602	-0.0525644560
$i = 9$	0.1050053381	0.1028886125	0.0794946606	-0.0535982070	0.1163031552	-0.1727895940	0.0138766802	0.0394489107	0.1768310417	0.2600193593	-0.1352686510	0.0672245400	-0.3372628180
$i = 10$	0.1313366106	-0.0652847790	-0.0207353830	0.0237213682	-0.0271668560	-0.0856315410	0.0414266387	-0.1804347690	-0.1196320560	0.2534808218	0.0152587260	0.0032921050	0.0648991977
$i = 11$	0.2824372611	-0.0382072530	0.0429097571	-0.1374683980	0.0409356468	-0.1027177950	0.1365705856	0.0774452581	-0.2579853470	-0.0278882560	-0.0096683540	0.3063230697	0.1824341868
$i = 12$	0.3714351236	0.0857676339	0.0513463652	-0.0373404870	-0.0004411230	0.1007721650	0.0050677707	0.0781513705	0.1349501803	0.1590679541	0.1523305843	0.0024326400	-0.1350151290
$i = 13$	0.0348500887	-0.1548534940	0.0042317704	-0.0462314440	-0.1396519580	-0.0963093230	0.0416302546	-0.1238348050	0.0277285634	-0.2663108270	0.2758700774	0.1703754755	-0.2160182990
$i = 14$	0.0207467730	0.0758259163	0.0559072895	0.0150405721	0.1194084040	-0.1354302920	-0.1538588480	-0.0686412280	-0.0353653330	-0.0480053720	0.0967357631	-0.1513731830	-0.0720664890
$i = 15$	0.1175937551	-0.0983173860	-0.0238255960	0.0421028058	-0.1563979820	0.0024933475	0.0589181913	-0.2041504890	-0.0527765400	0.0044347208	-0.1288912050	-0.2102211620	-0.0494211810
$i = 16$	0.0250335303	0.0436521397	-0.1693313680	0.0295725898	0.0733216993	-0.0510970090	-0.0658576760	-0.0294434390	-0.0301016220	0.0088490924	0.0802706272	-0.0354800420	0.0144496056
$i = 17$	0.0319771408	-0.1663012800	-0.1279299050	0.0082531240	0.0498129667	-0.0053193990	0.0067403143	0.0021655885	-0.0115489470	0.0501443339	-0.0794467190	-0.0074781220	0.0219384220
$i = 18$	0.2309976848	0.0379392875	-0.0027126300	0.0035637841	0.0078521529	-0.0472359360	0.0250377169	0.0070121507	-0.0189873100	-0.0081185680	-0.0101149170	-0.0203952800	0.0020236928
$i = 19$	0.0329799918	-0.0031323140	0.0051598711	0.0687487040	0.0100214329	0.0148308959	-0.0113276860	-0.0380225970	-0.0748125210	-0.0633080560	0.0826008051	0.0276566384	0.0667427638
$i = 20$	0.0061434045	0.0634442785	0.0166647089	0.0625774197	-0.0113542400	0.0292566084	-0.0442620840	0.0263121696	-0.0066620030	0.0192685017	-0.0455398740	0.0018414965	0.0417039868
$i = 21$	0.0153616440	0.0237287002	0.0232910580	-0.0151729410	0.0499611753	-0.0644091870	-0.0295198180	-0.0344440670	0.0304725437	0.0093858511	-0.0156115940	0.0126213327	0.0102385240
$i = 22$	0.0457683285	0.0106665874	-0.0198833310	-0.0158302270	-0.0048014680	-0.0016525480	-0.0043132960	0.0041992000	0.0103595574	-0.0543221660	0.0415116380	-0.0192007710	-0.0374837240
$i = 23$	0.0364669287	0.0188337537	-0.0164583870	0.0347828891	-0.0025643580	0.0485754179	-0.0378707050	0.0273894275	-0.0291711300	0.0309481038	0.0038868103	-0.0206721770	-0.0557617110

Table B.3 Coefficient Matrix of Stepwise – PLS Metamodel (Phase-1) for Stage-2 (Continued).

	$b_i^{z_{10}^3}$	$b_i^{z_{11}^3}$	$b_i^{z_{12}^3}$	$b_i^{z_{13}^3}$	$b_i^{z_{14}^3}$
$i = 1$	0.2347636527	-0.1181980650	0.1118189239	0.0801984500	0.0574059797
$i = 2$	0.1354886097	-0.0365298580	0.0060915933	-0.0209641670	-0.1165412430
$i = 3$	0.0080584825	0.2107944341	-0.0861186100	0.0157069304	0.0887228628
$i = 4$	-0.1418602620	-0.0569465080	0.0086224879	-0.0509756150	0.4017700689
$i = 5$	0.0063600126	0.3657871490	0.2786080258	-0.0727924440	-0.0839344420
$i = 6$	0.0373292901	-0.1488618510	-0.1834610240	0.2325639594	-0.0286494700
$i = 7$	-0.0807643970	0.1728249139	0.1611965975	0.5133234472	-0.0768651530
$i = 8$	0.4206363394	-0.2828084510	0.2517426183	0.0329057089	0.1687422757
$i = 9$	-0.2312839070	-0.1273764980	0.1818024382	0.3681615750	0.1015972985
$i = 10$	0.1415387217	0.1682747353	-0.3949844670	0.1648267727	0.1094043886
$i = 11$	-0.1761840770	-0.2089393490	-0.0386728400	0.0320358017	-0.0872451610
$i = 12$	0.0027559844	0.1905273738	0.0349030333	-0.2185787400	-0.0033592090
$i = 13$	-0.0600713800	0.0154195762	-0.0597417250	0.0179982054	0.1861452624
$i = 14$	-0.0532203930	-0.0942266830	-0.1472577460	-0.0958307440	-0.2253092780
$i = 15$	-0.1467224950	-0.0448500780	0.0470919355	-0.0571355690	0.0111975804
$i = 16$	-0.0657709470	-0.0855197420	-0.0059579300	-0.0392601110	0.1299954507
$i = 17$	0.0834210369	-0.0050537640	-0.0047655310	-0.0324970920	-0.0894262830
$i = 18$	0.0371426582	0.0034021870	-0.0596721920	0.1199606590	0.0071306313
$i = 19$	-0.0165193930	0.0484918525	-0.0121653910	-0.0086012100	-0.0568255270
$i = 20$	0.0389622206	-0.0817695810	0.0197895951	-0.0025741410	-0.0392022420
$i = 21$	-0.0323970490	0.0062348528	0.0859138850	0.0180531572	-0.0405869270
$i = 22$	0.0580325297	0.0049211864	0.0374488388	-0.0912480470	-0.0073899890
$i = 23$	-0.0033898510	0.0630211027	0.0455976674	0.0304655351	-0.0034540290

Table B.4 Coefficient Matrix of Stepwise – PLS Metamodel (Phase-2) for Stage-2.

	a_i^C	a_i^S	a_i^T	a_i^Y	$a_i^{z_1^3}$	$a_i^{z_2^3}$	$a_i^{z_3^3}$	$a_i^{z_4^3}$	$a_i^{z_5^3}$	$a_i^{z_6^3}$	$a_i^{z_7^3}$	$a_i^{z_8^3}$	$a_i^{z_9^3}$
$i = 0$	-4.610000E-03	-4.520000E-03	1.608900E-04	-1.080000E-03	2.071800E-01	-8.190100E-01	9.199600E-01	-3.081400E-01	9.831500E-01	-2.646700E-01	-7.882000E-02	-1.176700E-01	-3.429150E+00
$i = 1$	0	0	0	0	0	5.056000E-05	2.336000E-05	0	-9.501000E-05	-6.926000E-05	7.204000E-05	2.712000E-05	2.245000E-05
$i = 2$	0	-6.643340E-08	0	0	-1.405000E-05	0	1.574000E-05	0	0	0	-3.204000E-05	5.290000E-06	1.340000E-05
$i = 3$	0	0	0	3.515541E-08	-8.210000E-06	-4.720000E-06	-4.588000E-05	-2.156000E-05	-4.330000E-06	1.280000E-05	1.931000E-05	1.532000E-05	-4.190000E-06
$i = 4$	0	0	0	3.288039E-08	-1.042000E-05	2.704000E-05	-5.348000E-05	-2.114000E-05	-2.770000E-06	-3.700000E-06	-7.890000E-06	-4.401000E-05	9.370000E-06
$i = 5$	0	4.803761E-08	0	0	4.840000E-06	0	-9.760000E-06	9.140000E-06	-3.050000E-06	-4.440000E-06	1.144000E-05	-7.120000E-06	3.800000E-06
$i = 6$	0	0	0	0	0	0	0	0	0	5.960000E-06	0	-9.090000E-06	6.980000E-06
$i = 7$	0	0	0	0	-3.830000E-06	0	6.280000E-06	0	-4.980000E-06	-6.970000E-06	1.610000E-06	1.213000E-05	1.060000E-05
$i = 8$	0	0	0	0	0	3.210000E-06	7.210000E-06	-1.157000E-05	-4.480000E-06	2.900000E-06	3.200000E-06	-8.600000E-06	1.114000E-05
$i = 9$	0	0	0	0	-5.462120E-07	7.380000E-06	2.640000E-06	5.890000E-06	4.090000E-06	1.680000E-06	-2.190000E-06	3.190000E-06	4.080000E-06
$i = 10$	0	1.485936E-08	0	0	4.600000E-06	-1.640000E-06	-3.160000E-06	2.670000E-06	8.448230E-07	8.342949E-07	1.060000E-06	6.393651E-07	2.440000E-06
$i = 11$	0	0	0	0	0	-2.690000E-06	2.020000E-06	-3.940000E-06	-8.950000E-06	1.320000E-05	-8.400000E-06	0	4.570000E-06
$i = 12$	1.872175E-08	0	0	0	0	-6.920000E-06	0	6.350000E-06	6.050000E-06	1.141000E-05	0	1.017000E-05	0
$i = 13$	2.252684E-07	0	0	0	3.100000E-06	0	0	3.630000E-06	-2.200000E-06	0	0	0	-7.630000E-06
$i = 14$	0	0	-8.984760E-09	0	1.150000E-06	0	-1.130000E-06	0	0	0	0	-2.660000E-06	1.150000E-06
$i = 15$	0	0	0	0	0	8.900000E-06	0	0	-7.510000E-06	0	0	-2.829000E-05	0
$i = 16$	0	0	2.518705E-08	0	0	0	0	0	0	0	0	0	0
$i = 17$	0	0	0	0	-2.640000E-06	0	2.510000E-06	1.970000E-06	-2.790000E-06	1.720000E-06	-1.740000E-06	2.220000E-06	2.020000E-06
$i = 18$	0	0	0	0	-2.100000E-06	0	0	2.590000E-06	-2.760000E-06	-3.130000E-06	1.550000E-06	6.360000E-06	2.450000E-06
$i = 19$	0	0	0	0	-2.100000E-06	1.990000E-06	3.300000E-06	-8.080050E-07	-1.360000E-06	2.910000E-06	-2.600000E-06	-3.710000E-06	4.410000E-06
$i = 20$	0	0	0	0	-9.480430E-07	-9.055790E-07	0	-2.660000E-06	-3.950000E-06	7.837455E-07	5.830000E-06	1.710000E-06	1.630000E-06
$i = 21$	0	0	0	0	0	6.170000E-06	5.610000E-06	0	-2.570000E-06	-1.151000E-05	1.064000E-05	0	0
$i = 22$	0	0	0	0	-2.760000E-06	-6.270000E-06	0	-4.260000E-06	1.105000E-05	-1.320000E-05	7.020000E-06	0	3.210000E-06
$i = 23$	0	0	0	3.910150E-09	0	0	0	0	0	0	-9.090000E-06	-1.576000E-05	1.773000E-05
$i = 24$	0	0	0	0	-6.933300E-04	0	0	-5.120900E-04	-1.010000E-03	0	-5.177900E-04	0	0
$i = 25$	0	0	0	0	0	-1.014000E-02	7.960000E-03	9.640000E-03	-1.507000E-02	-6.950000E-03	-3.718000E-02	0	2.648000E-02
$i = 26$	0	0	0	0	-7.004000E-02	0	1.833000E-01	-1.725000E-01	2.497900E-01	-9.960000E-02	-1.711700E-01	0	0
$i = 27$	0	6.088078E-07	0	0	0	-4.407000E-05	0	-4.345000E-05	1.606600E-04	1.990900E-04	-2.948000E-05	-1.220100E-04	-4.169000E-05
$i = 28$	0	0	0	0	-2.055000E-05	-2.885000E-05	-7.058000E-05	4.096000E-05	4.618000E-05	-5.775000E-05	1.073700E-04	9.205000E-05	-7.188000E-05

ε_2^C	ε_2^S	ε_2^T	ε_2^Y	$\varepsilon_2^{z_1^3}$	$\varepsilon_2^{z_2^3}$	$\varepsilon_2^{z_3^3}$	$\varepsilon_2^{z_4^3}$	$\varepsilon_2^{z_5^3}$	$\varepsilon_2^{z_6^3}$	$\varepsilon_2^{z_7^3}$	$\varepsilon_2^{z_8^3}$	$\varepsilon_2^{z_9^3}$
0.00106	0.00541	0.00262	0.00015285	0.37649	0.31412	0.38059	0.32737	0.21507	0.25988	0.27048	0.23178	0.28993

Table B.4 Coefficient Matrix of Stepwise – PLS Metamodel (Phase-2) for Stage-2 (Continued).

	$a_i^{z_{10}^3}$	$a_i^{z_{11}^3}$	$a_i^{z_{12}^3}$	$a_i^{z_{13}^3}$	$a_i^{z_{14}^3}$
$i = 0$	-3.111660E+00	-1.469700E-01	2.259180E+00	-5.147300E-01	-8.322000E-01
$i = 1$	-6.394000E-05	-7.486000E-05	0	0	-4.983000E-05
$i = 2$	2.041000E-05	-1.111000E-05	-1.597000E-05	0	-4.770000E-06
$i = 3$	3.271000E-05	1.248000E-05	-1.349000E-05	3.060000E-06	2.352000E-05
$i = 4$	1.752000E-05	-1.025000E-05	8.670000E-06	2.340000E-06	-1.000000E-05
$i = 5$	-1.388000E-05	-4.960000E-06	0	-8.980000E-06	-2.304000E-05
$i = 6$	-1.180000E-05	-3.880000E-06	-6.180000E-06	3.170000E-06	6.860000E-06
$i = 7$	3.780000E-06	-2.970000E-06	-1.540000E-06	1.219000E-05	0
$i = 8$	0	8.950000E-06	-9.070000E-06	4.500000E-06	2.310000E-06
$i = 9$	5.600000E-06	5.660000E-06	3.890000E-06	1.220000E-06	5.469912E-07
$i = 10$	1.220000E-06	-1.130000E-06	-2.230000E-06	0	5.679722E-07
$i = 11$	4.550000E-06	2.980000E-06	-2.960000E-06	6.110000E-06	-4.550000E-06
$i = 12$	0	-1.151000E-05	-8.520000E-06	-3.031000E-05	4.877000E-05
$i = 13$	-3.050000E-06	5.720000E-06	-7.900000E-06	1.482000E-05	4.720000E-06
$i = 14$	0	-1.790000E-06	-1.310000E-06	-1.240000E-06	0
$i = 15$	-8.550000E-06	1.378000E-05	1.177000E-05	-4.633000E-05	2.337000E-05
$i = 16$	-2.930000E-06	0	0	0	0
$i = 17$	3.420000E-06	-3.120000E-06	-9.056690E-07	-3.600000E-06	-2.010000E-06
$i = 18$	0	-3.820000E-06	6.480000E-06	2.030000E-06	1.580000E-06
$i = 19$	-1.560000E-06	-2.070000E-06	-1.820000E-06	-3.540000E-06	0
$i = 20$	1.500000E-06	4.040000E-06	1.920000E-06	-1.990000E-06	3.410000E-06
$i = 21$	0	3.300000E-06	-1.536000E-05	-4.010000E-06	-8.240000E-06
$i = 22$	8.070000E-06	5.270000E-06	-1.563000E-05	8.600000E-06	-1.825000E-05
$i = 23$	3.712000E-05	2.380000E-05	-1.802000E-05	-2.262000E-05	2.069000E-05
$i = 24$	0	-2.680900E-04	-1.070000E-03	1.170000E-03	2.940000E-03
$i = 25$	1.314000E-02	-1.473000E-02	7.250000E-03	8.670000E-03	-3.186000E-02
$i = 26$	1.759800E-01	5.214000E-02	-1.344800E-01	9.839000E-02	3.612700E-01
$i = 27$	3.892000E-05	1.293500E-04	-1.572400E-04	9.928000E-05	7.518000E-05
$i = 28$	1.817200E-04	4.109000E-05	-6.108000E-05	-3.290000E-05	1.081600E-04

$\varepsilon_2^{z_{10}^3}$	$\varepsilon_2^{z_{11}^3}$	$\varepsilon_2^{z_{12}^3}$	$\varepsilon_2^{z_{13}^3}$	$\varepsilon_2^{z_{14}^3}$
0.29622	0.21436	0.23764	0.19563	0.28991

Table B.5 Coefficient Matrix of Stepwise – PLS Metamodel (Phase-1) for Stage-3.

	b_i^C	b_i^S	b_i^T	b_i^Y	$b_i^{z_1^4}$	$b_i^{z_2^4}$	$b_i^{z_3^4}$	$b_i^{z_4^4}$	$b_i^{z_5^4}$	$b_i^{z_6^4}$	$b_i^{z_7^4}$	$b_i^{z_8^4}$	$b_i^{z_9^4}$
$i = 1$	0.0154220120	0.5270868764	0.6052128131	-0.1413829990	0.5490727066	0.1195558978	0.0690586168	-0.3478333360	-0.0635235340	-0.1435425590	0.0045163718	0.0713448838	0.0511978958
$i = 2$	0.5337053087	-0.0572521420	-0.0731047070	0.2945804971	0.0773010106	0.4167088229	-0.1801109070	0.2084634496	-0.3387112460	0.1400805608	0.0794127196	-0.0719267930	0.1755193968
$i = 3$	0.0764920137	-0.1351226050	-0.1660924800	-0.5015653020	-0.1266062960	0.0805158301	0.1038907921	0.1164215962	-0.1830062060	-0.0146347130	0.0559203445	0.2696819588	0.1466297536
$i = 4$	0.3140946722	0.0594081021	0.1279164746	-0.1834334980	0.1227956331	0.2077593707	0.1150757843	0.1552431529	0.0614691980	0.1349138573	0.1181093508	-0.2708605050	-0.3358730350
$i = 5$	0.1269106820	-0.0355299800	0.0497008438	-0.0462028260	-0.0522053020	0.2018454159	0.0050073008	-0.2413001550	0.0822360285	0.4937976947	-0.3072604970	0.2348843474	-0.0898830950
$i = 6$	0.1619292729	-0.0476942680	0.0400530465	-0.0592049870	0.0371311597	0.1374804092	-0.2509332730	0.2037867885	-0.0056574420	-0.4309020710	-0.3162004550	0.2385873308	-0.2803267410
$i = 7$	0.0628347120	0.0924234541	0.0438955303	-0.0690011180	0.1273795459	-0.1473194670	-0.0851675740	0.0936663659	-0.0202635610	0.0545106833	-0.3455364870	-0.3221844240	0.2580443107
$i = 8$	0.0139791722	0.0027197304	0.0261891780	-0.1646855850	0.0396515431	0.0885691882	0.3174537994	0.1468992509	0.1329109651	-0.0403543910	-0.0535944930	-0.0694319050	0.0267492715
$i = 9$	0.0412816429	0.0487994745	0.1459665157	0.0446176411	0.0464448909	-0.0170920180	0.0623588778	-0.0017058720	0.0048645532	-0.0694860150	0.2382874830	0.1155858486	0.1826640116
$i = 10$	0.0607568882	0.0406592217	0.0393992332	0.1315682752	0.0700933022	0.0938685515	-0.0614804690	0.1337069383	0.2583086609	0.0049685725	0.0741944456	0.0667516114	-0.0094973110
$i = 11$	0.1746970295	-0.0681587230	-0.0881383360	-0.1158349950	-0.0146994300	0.0223144651	-0.1320364250	0.0428138216	0.0592877324	0.0089312459	-0.0297589490	0.0664690619	0.1984927881
$i = 12$	0.0147530847	-0.2104186170	-0.1400660280	0.0662749423	-0.1654363250	0.1371606134	0.0774464779	-0.0916424160	0.0380088640	-0.0458625180	0.0364760930	-0.0397893680	-0.0120202100
$i = 13$	0.1479517947	0.0037669081	-0.0531964080	0.1291110225	0.0146124395	-0.0569126940	0.1401760405	0.1003927089	-0.1208864690	0.0375673018	-0.0701365860	0.0781599506	0.0214829092
$i = 14$	0.0092969564	0.0343033747	0.0379797755	0.0264705805	0.0361977272	0.0953522748	0.0631345670	-0.0312480080	0.0592457516	0.0222755042	-0.1256241500	-0.0119188970	0.0309237967

Table B.6 Coefficient Matrix of Stepwise – PLS Metamodel (Phase-2) for Stage-3.

	a_i^C	a_i^S	a_i^T	a_i^Y	$a_i^{z_1^4}$	$a_i^{z_2^4}$	$a_i^{z_3^4}$	$a_i^{z_4^4}$	$a_i^{z_5^4}$	$a_i^{z_6^4}$	$a_i^{z_7^4}$	$a_i^{z_8^4}$	$a_i^{z_9^4}$
$i = 0$	-2.590000E-03	-7.800000E-03	-2.090000E-03	-3.429000E-05	-2.099250E+00	-3.820000E-02	1.324120E+00	-1.101130E+00	-1.116060E+00	-4.198300E-01	-2.069330E+00	-1.163230E+00	-1.424000E-02
$i = 1$	0	0	0	0	0	0	1.412000E-05	9.980000E-06	0	0	0	1.002000E-05	-1.275000E-05
$i = 2$	0	0	0	0	0	0	-5.960000E-05	-1.659000E-05	1.652000E-05	6.610000E-06	2.824000E-05	-6.250000E-06	2.350000E-06
$i = 3$	0	0	0	0	0	4.640000E-06	0	0	-7.950000E-06	0	0	1.374000E-05	-2.102000E-05
$i = 4$	0	0	0	0	0	0	4.460000E-06	2.350000E-06	5.020000E-06	2.320000E-06	4.090000E-06	1.630000E-06	0
$i = 5$	0	0	0	0	3.900000E-06	0	0	1.470000E-06	-3.320000E-06	-7.150000E-06	2.540000E-06	-8.210000E-06	-3.370000E-06
$i = 6$	2.544104E-09	-1.455540E-08	0	0	1.180000E-06	7.630000E-06	0	3.200000E-06	1.136000E-05	-1.660000E-06	0	1.040000E-06	6.520000E-06
$i = 7$	0	3.782174E-08	3.550458E-09	0	5.560000E-06	-3.520000E-06	-4.471470E-07	4.150000E-06	3.470034E-07	2.650000E-06	9.363765E-07	2.540000E-06	-7.511410E-07
$i = 8$	0	0	0	0	1.940000E-06	-1.110000E-06	0	2.990000E-06	-2.080000E-06	-5.700000E-06	2.400000E-06	0	-1.880000E-06
$i = 9$	0	0	0	0	0	2.980000E-06	7.970000E-06	0	-8.310000E-06	-6.420000E-06	4.600000E-06	-1.235000E-05	8.080000E-06
$i = 10$	1.023808E-07	0	0	0	3.720000E-06	1.258000E-05	2.850000E-06	8.060000E-06	-2.397000E-05	0	0	0	-5.880000E-06
$i = 11$	0	0	1.656470E-08	0	0	0	2.380000E-06	-2.780000E-06	0	0	3.700000E-06	3.930000E-06	-5.974980E-07
$i = 12$	0	0	0	0	0	-1.730000E-06	1.580000E-06	-1.370000E-06	-1.410000E-06	-1.430000E-06	-2.510000E-06	2.170000E-06	5.160000E-06
$i = 13$	0	0	0	0	0	0	1.305000E-05	-9.210000E-06	0	-5.460000E-06	7.360000E-06	-9.560000E-06	6.500000E-06
$i = 14$	1.220734E-08	0	0	0	0	0	0	0	0	0	0	0	0
$i = 15$	0	0	0	0	8.806692E-07	1.180000E-06	-2.570000E-06	7.482307E-07	0	7.373844E-07	0	0	-5.680000E-06
$i = 16$	0	0	0	0	-9.141550E-07	-9.932150E-07	-2.050000E-06	0	2.060000E-06	2.950000E-06	4.910000E-06	2.300000E-06	0
$i = 17$	0	0	0	0	9.525749E-07	0	-1.740000E-06	-1.740000E-06	-1.180000E-06	0	1.950000E-06	7.932426E-07	1.300000E-06
$i = 18$	0	0	0	0	1.130000E-06	0	-4.270000E-06	-1.470000E-06	-7.021190E-07	1.770000E-06	-1.330000E-06	0	-2.480000E-06
$i = 19$	0	0	0	0	5.630000E-06	-5.570000E-06	0	8.710000E-06	0	0	-1.010000E-05	-2.440000E-06	5.510000E-06
$i = 20$	0	0	0	0	0	-5.980000E-06	0	4.110000E-06	6.430000E-06	2.250000E-06	1.116000E-05	-8.920000E-06	9.040000E-06
$i = 21$	0	0	0	0	9.111247E-07	0	-2.220000E-06	0	0	-1.240000E-06	-1.990000E-06	-8.887940E-07	-1.970000E-06
$i = 22$	0	0	0	0	0	0	3.740000E-03	-6.570000E-03	-4.920000E-03	5.500000E-03	-7.950000E-03	1.443000E-02	0
$i = 23$	0	0	0	0	0	2.486000E-05	2.614000E-05	-4.086000E-05	4.136000E-05	5.259000E-05	1.070500E-04	8.309000E-05	-3.330000E-05
$i = 24$	0	0	0	0	0	5.232000E-05	0	0	0	-6.684000E-05	1.717000E-04	0	-2.067900E-04
$i = 25$	0	0	0	1.018569E-08	-1.639000E-05	-1.759000E-05	-4.140000E-05	-1.597000E-05	1.780000E-05	0	-2.937000E-05	1.620000E-05	1.048900E-04

ε_3^C	ε_3^S	ε_3^T	ε_3^Y	$\varepsilon_3^{z_1^4}$	$\varepsilon_3^{z_2^4}$	$\varepsilon_3^{z_3^4}$	$\varepsilon_3^{z_4^4}$	$\varepsilon_3^{z_5^4}$	$\varepsilon_3^{z_6^4}$	$\varepsilon_3^{z_7^4}$	$\varepsilon_3^{z_8^4}$	$\varepsilon_3^{z_9^4}$
0.00122	0.00287	0.00189	0.0002039	0.32593	0.31621	0.26154	0.24607	0.33266	0.25136	0.28639	0.31278	0.25574

Table B.7 Coefficient Matrix of Stepwise – PLS Metamodel (Phase-1) for Stage-4.

	b_i^C	b_i^S	b_i^T	b_i^Y
$i = 1$	0.3358517266	0.4792883710	0.3166456184	-0.0137679870
$i = 2$	0.5052850070	-0.2860937110	-0.2368713700	-0.0086694440
$i = 3$	0.0030563475	0.0049466003	-0.1364275100	-0.6735887000
$i = 4$	0.1335561790	0.1391761831	0.3219817774	-0.0971187040
$i = 5$	0.2370737859	-0.0226738580	0.0056431146	0.0700737229
$i = 6$	0.0264281999	0.2075999308	-0.1268379610	0.0193701305
$i = 7$	0.0021467305	0.0543956307	0.0892329066	0.1746416600
$i = 8$	0.0373848760	0.0785234119	0.1090542283	-0.0669318760
$i = 9$	0.0930298236	-0.0367671460	-0.0035323440	0.0205036017

Table B.8 Coefficient Matrix of Stepwise – PLS Metamodel (Phase-2) for Stage-4.

	a_i^C	a_i^S	a_i^T	a_i^Y
$i = 0$	-1.640000E-03	-7.783200E-04	-5.220000E-03	-7.447900E-04
$i = 1$	0	-5.018880E-08	-4.381580E-08	0
$i = 2$	0	0	0	1.102282E-08
$i = 3$	0	0	0	2.546440E-08
$i = 4$	4.502947E-09	-1.571670E-09	0	0
$i = 5$	0	3.963724E-09	1.965014E-08	0
$i = 6$	3.844507E-08	0	0	0
$i = 7$	0	0	-1.049900E-08	0

ε_4^C	ε_4^S	ε_4^T	ε_4^Y
0.00141	0.00122	0.00164	0.00018454

APPENDIX C

LIST OF STATE AND DECISION VARIABLES FOR ALL METHODS

Table C.1 List of Decision Variables for All Methods (Stage-1, Stage-2, Stage-3 and Stage-4).

Decision Variables (Stage-1)	Zehua	Low-VIF	High-VIF	Stepwise PLS
sq1_1p1				
sq2_1p1			✓	✓
sq3_1p1	✓	✓	✓	✓
sq4_1p1				
sq5_1p1				
sq1_2p1	✓	✓	✓	✓
sq2_2p1			✓	✓
sq3_2p1	✓	✓	✓	✓
sq4_2p1	✓	✓	✓	✓
sq5_2p1				✓
sq1_3p1	✓	✓	✓	✓
sq2_3p1	✓	✓	✓	✓
sq3_3p1	✓	✓	✓	✓
sq4_3p1	✓	✓	✓	✓
sq5_3p1			✓	✓
sq1_4p1	✓	✓	✓	✓
sq2_4p1	✓	✓	✓	✓
sq3_4p1	✓	✓	✓	✓
sq4_4p1	✓	✓	✓	✓
sq5_4p1	✓	✓	✓	✓
sq1_5p1				
sq2_5p1				
sq3_5p1	✓	✓	✓	✓
sq4_5p1				
sq5_5p1			✓	✓
pt1p1			✓	✓
pt2p1			✓	✓
pt3p1			✓	✓
pt4p1	✓	✓	✓	✓
pt5p1	✓	✓	✓	✓
pt6p1	✓	✓	✓	✓
pt9p1				
pt12p1			✓	✓
pt15p1			✓	
pt21p1				
pt23p1				
pt30p1			✓	✓
pt37p1				
pt63p1			✓	✓
pt64p1			✓	✓

Decision Variables (Stage-2)	Zehua	Low-VIF	High-VIF	Stepwise PLS
sq1_1p2			✓	✓
sq2_1p2			✓	✓
sq3_1p2				
sq4_1p2				
sq5_1p2			✓	✓
sq1_2p2			✓	✓
sq2_2p2			✓	
sq3_2p2	✓	✓	✓	✓
sq4_2p2	✓	✓	✓	✓
sq5_2p2			✓	
sq1_3p2	✓	✓	✓	✓
sq2_3p2			✓	✓
sq3_3p2	✓	✓	✓	✓
sq4_3p2	✓	✓	✓	✓
sq5_3p2				
sq1_4p2	✓	✓	✓	✓
sq2_4p2	✓	✓	✓	✓
sq3_4p2	✓	✓	✓	✓
sq4_4p2				
sq5_4p2			✓	✓
sq1_5p2			✓	✓
sq2_5p2			✓	
sq3_5p2			✓	✓
sq4_5p2				
sq5_5p2				
pt1p2			✓	✓
pt2p2			✓	✓
pt3p2			✓	✓
pt4p2			✓	✓
pt5p2	✓	✓	✓	✓
pt6p2			✓	✓
pt9p2				✓
pt12p2				
pt15p2			✓	
pt21p2			✓	✓
pt23p2			✓	✓
pt30p2				
pt37p2			✓	✓
pt63p2			✓	✓
pt64p2			✓	✓

Decision Variables (Stage-3)	Zehua	Low-VIF	High-VIF	Stepwise PLS
sq1_1p3				
sq2_1p3			✓	✓
sq3_1p3				
sq4_1p3			✓	✓
sq5_1p3			✓	
sq1_2p3				
sq2_2p3			✓	
sq3_2p3	✓	✓	✓	✓
sq4_2p3	✓	✓	✓	✓
sq5_2p3				
sq1_3p3	✓	✓	✓	✓
sq2_3p3			✓	✓
sq3_3p3	✓	✓	✓	✓
sq4_3p3	✓	✓	✓	✓
sq5_3p3			✓	
sq1_4p3	✓	✓	✓	✓
sq2_4p3			✓	✓
sq3_4p3			✓	✓
sq4_4p3			✓	✓
sq5_4p3				
sq1_5p3				
sq2_5p3			✓	
sq3_5p3				
sq4_5p3			✓	✓
sq5_5p3			✓	✓
pt1p3			✓	✓
pt2p3			✓	✓
pt3p3	✓	✓	✓	✓
pt4p3	✓	✓	✓	✓
pt5p3			✓	✓
pt6p3	✓	✓	✓	✓
pt9p3				
pt12p3				
pt15p3			✓	✓
pt21p3				
pt23p3			✓	✓
pt30p3			✓	✓
pt37p3			✓	
pt63p3			✓	✓
pt64p3			✓	✓

Decision Variables (Stage-4)	Zehua	Low-VIF	High-VIF	Stepwise PLS
sq1_1p4			✓	✓
sq2_1p4				
sq3_1p4				
sq4_1p4				
sq5_1p4				
sq1_2p4				
sq2_2p4				
sq3_2p4			✓	✓
sq4_2p4			✓	✓
sq5_2p4				
sq1_3p4	✓	✓	✓	✓
sq2_3p4				
sq3_3p4	✓	✓	✓	✓
sq4_3p4			✓	✓
sq5_3p4				
sq1_4p4	✓	✓	✓	✓
sq2_4p4				
sq3_4p4				
sq4_4p4				
sq5_4p4				
sq1_5p4				
sq2_5p4			✓	
sq3_5p4				
sq4_5p4				
sq5_5p4				
pt1p4			✓	
pt2p4				
pt3p4				
pt4p4				
pt5p4				
pt6p4			✓	
pt9p4				
pt12p4				
pt15p4			✓	
pt21p4				
pt23p4				
pt30p4				
pt37p4				
pt63p4				
pt64p4			✓	

Table C.2 List of State Variables for All Methods (Stage-1).

State Variables (Stage-1)	Zehua	Low-VIF	High-VIF	Stepwise PLS
cyM3p0			✓	Zpls1_1
skM3p0	✓	✓	✓	Zpls1_2
tkM3p0	✓	✓	✓	Zpls1_3
ykM3p0	✓		✓	Zpls1_4
sq1_1p0			✓	Zpls1_5
sq2_1p0				Zpls1_6
sq3_1p0			✓	Zpls1_7
sq4_1p0			✓	Zpls1_8
sq5_1p0				Zpls1_9
sq1_2p0				Zpls1_10
sq2_2p0				Zpls1_11
sq3_2p0	✓	✓	✓	Zpls1_12
sq4_2p0	✓	✓	✓	Zpls1_13
sq5_2p0				Zpls1_14
sq1_3p0	✓	✓	✓	Zpls1_15
sq2_3p0	✓	✓	✓	Zpls1_16
sq3_3p0	✓	✓	✓	Zpls1_17
sq4_3p0	✓	✓	✓	Zpls1_18
sq5_3p0	✓	✓	✓	Zpls1_19
sq1_4p0			✓	Zpls1_20
sq2_4p0			✓	Zpls1_21
sq3_4p0			✓	Zpls1_22
sq4_4p0	✓	✓		Zpls1_23
sq5_4p0			✓	Zpls1_24
sq1_5p0			✓	Zpls1_25
sq2_5p0	✓	✓	✓	
sq3_5p0			✓	
sq4_5p0				
sq5_5p0			✓	
pt1p0			✓	
pt2p0			✓	
pt3p0			✓	
pt4p0			✓	
pt5p0	✓	✓	✓	
pt6p0			✓	
pt9p0			✓	
pt12p0			✓	
pt15p0	✓	✓		
pt21p0				
pt23p0			✓	
pt30p0	✓	✓	✓	
pt37p0				
pt63p0	✓	✓	✓	
pt64p0	✓	✓	✓	

Table C.3 List of State Variables for All Methods (Stage-2).

State Variables (Stage-2)	Zehua	Low-VIF	High-VIF	Stepwise PLS
cyM3p0			✓	Zpls2_1
skM3p0			✓	Zpls2_2
tkM3p0			✓	Zpls2_3
ykM3p0			✓	Zpls2_4
sq1_1p0			✓	Zpls2_5
sq2_1p0				Zpls2_6
sq3_1p0				Zpls2_7
sq4_1p0				Zpls2_8
sq5_1p0				Zpls2_9
sq1_2p0				Zpls2_10
sq2_2p0				Zpls2_11
sq3_2p0	✓	✓	✓	Zpls2_12
sq4_2p0	✓	✓	✓	Zpls2_13
sq5_2p0				Zpls2_14
sq1_3p0	✓	✓	✓	Zpls2_15
sq2_3p0	✓	✓	✓	Zpls2_16
sq3_3p0	✓	✓	✓	Zpls2_17
sq4_3p0	✓	✓	✓	Zpls2_18
sq5_3p0				Zpls2_19
sq1_4p0			✓	Zpls2_20
sq2_4p0			✓	Zpls2_21
sq3_4p0			✓	Zpls2_22
sq4_4p0	✓	✓		Zpls2_23
sq5_4p0			✓	
sq1_5p0			✓	
sq2_5p0				
sq3_5p0			✓	
sq4_5p0				
sq5_5p0				
pt1p0			✓	
pt2p0			✓	
pt3p0			✓	
pt4p0			✓	
pt5p0	✓	✓	✓	
pt6p0			✓	
pt9p0			✓	
pt12p0			✓	
pt15p0	✓	✓		
pt21p0				
pt23p0			✓	
pt30p0			✓	
pt37p0				
pt63p0	✓	✓	✓	
pt64p0			✓	
cyM3p1	✓	✓	✓	
skM3p1	✓	✓	✓	
tkM3p1	✓	✓	✓	
ykM3p1	✓		✓	
sq1_1p1				
sq2_1p1			✓	
sq3_1p1				
sq4_1p1				
sq5_1p1				
sq1_2p1			✓	
sq2_2p1			✓	
sq3_2p1	✓	✓	✓	
sq4_2p1	✓	✓	✓	
sq5_2p1				
sq1_3p1	✓	✓	✓	
sq2_3p1			✓	
sq3_3p1	✓	✓	✓	
sq4_3p1	✓		✓	
sq5_3p1			✓	
sq1_4p1	✓	✓	✓	
sq2_4p1	✓	✓	✓	
sq3_4p1	✓	✓	✓	
sq4_4p1				
sq5_4p1	✓	✓	✓	
sq1_5p1				
sq2_5p1				
sq3_5p1	✓	✓	✓	
sq4_5p1				
sq5_5p1			✓	
pt1p1			✓	
pt2p1			✓	
pt3p1			✓	
pt4p1			✓	
pt5p1			✓	
pt6p1	✓	✓	✓	
pt9p1				
pt12p1				
pt15p1			✓	
pt21p1				
pt23p1				
pt30p1			✓	
pt37p1				
pt63p1			✓	
pt64p1			✓	

Table C.4 List of State Variables for All Methods (Stage-3).

State Variables (Stage-3)	Zehua	Low-VIF	High-VIF	Stepwise PLS
cyM3p0			✓	Zpls3_1
skM3p0			✓	Zpls3_2
tkM3p0			✓	Zpls3_3
ykM3p0			✓	Zpls3_4
sq1_1p0			✓	Zpls3_5
sq2_1p0				Zpls3_6
sq3_1p0				Zpls3_7
sq4_1p0				Zpls3_8
sq5_1p0				Zpls3_9
sq1_2p0				Zpls3_10
sq2_2p0				Zpls3_11
sq3_2p0	✓	✓	✓	Zpls3_12
sq4_2p0			✓	Zpls3_13
sq5_2p0				Zpls3_14
sq1_3p0			✓	
sq2_3p0			✓	
sq3_3p0	✓	✓	✓	
sq4_3p0				
sq5_3p0				
sq1_4p0			✓	
sq2_4p0			✓	
sq3_4p0			✓	
sq4_4p0				
sq5_4p0				
sq1_5p0			✓	
sq2_5p0				
sq3_5p0			✓	
sq4_5p0				
sq5_5p0				
pt1p0			✓	
pt2p0			✓	
pt3p0			✓	
pt4p0			✓	
pt5p0			✓	
pt6p0			✓	
pt9p0			✓	
pt12p0			✓	
pt15p0				
pt21p0				
pt23p0			✓	
pt30p0			✓	
pt37p0				
pt63p0				
pt64p0			✓	

State Variables (Stage-3)	Zehua	Low-VIF	High-VIF	Stepwise PLS
cyM3p1			✓	
skM3p1	✓	✓	✓	
tkM3p1			✓	
ykM3p1	✓		✓	
sq1_1p1				
sq2_1p1			✓	
sq3_1p1				
sq4_1p1				
sq5_1p1				
sq1_2p1			✓	
sq2_2p1			✓	
sq3_2p1	✓	✓	✓	
sq4_2p1				
sq5_2p1				
sq1_3p1	✓		✓	
sq2_3p1			✓	
sq3_3p1	✓	✓	✓	
sq4_3p1				
sq5_3p1			✓	
sq1_4p1	✓	✓	✓	
sq2_4p1	✓	✓	✓	
sq3_4p1	✓	✓	✓	
sq4_4p1				
sq5_4p1				
sq1_5p1				
sq2_5p1				
sq3_5p1			✓	
sq4_5p1				
sq5_5p1			✓	
pt1p1			✓	
pt2p1			✓	
pt3p1			✓	
pt4p1			✓	
pt5p1			✓	
pt6p1	✓	✓	✓	
pt9p1				
pt12p1				
pt15p1			✓	
pt21p1				
pt23p1				
pt30p1			✓	
pt37p1				
pt63p1			✓	
pt64p1			✓	

State Variables (Stage-3)	Zehua	Low-VIF	High-VIF	Stepwise PLS
cyM3p2	✓	✓	✓	
skM3p2	✓	✓	✓	
tkM3p2	✓	✓	✓	
ykM3p2	✓	✓	✓	
sq1_1p2			✓	
sq2_1p2			✓	
sq3_1p2				
sq4_1p2				
sq5_1p2			✓	
sq1_2p2			✓	
sq2_2p2				
sq3_2p2	✓	✓	✓	
sq4_2p2				
sq5_2p2				
sq1_3p2	✓	✓	✓	
sq2_3p2			✓	
sq3_3p2	✓	✓	✓	
sq4_3p2	✓	✓	✓	
sq5_3p2				
sq1_4p2	✓	✓	✓	
sq2_4p2	✓	✓	✓	
sq3_4p2	✓	✓	✓	
sq4_4p2				
sq5_4p2				
sq1_5p2			✓	
sq2_5p2			✓	
sq3_5p2			✓	
sq4_5p2				
sq5_5p2				
pt1p2			✓	
pt2p2			✓	
pt3p2			✓	
pt4p2			✓	
pt5p2	✓	✓	✓	
pt6p2			✓	
pt9p2				
pt12p2				
pt15p2				
pt21p2			✓	
pt23p2			✓	
pt30p2				
pt37p2				
pt63p2			✓	
pt64p2			✓	

Table C.5 List of State Variables for All Methods (Stage-4).

State Variables (Stage-4)	Zehua	Low-VIF	High-VIF	Stepwise PLS
cyM3p0			✓	Zpls4_1
skM3p0			✓	Zpls4_2
tkM3p0			✓	Zpls4_3
ykM3p0			✓	Zpls4_4
sq1_1p0			✓	Zpls4_5
sq2_1p0				Zpls4_6
sq3_1p0				Zpls4_7
sq4_1p0				Zpls4_8
sq5_1p0				Zpls4_9
sq1_2p0				
sq2_2p0				
sq3_2p0			✓	
sq4_2p0				
sq5_2p0				
sq1_3p0				
sq2_3p0			✓	
sq3_3p0				
sq4_3p0				
sq5_3p0				
sq1_4p0			✓	
sq2_4p0			✓	
sq3_4p0			✓	
sq4_4p0				
sq5_4p0				
sq1_5p0				
sq2_5p0				
sq3_5p0			✓	
sq4_5p0				
sq5_5p0				
pt1p0			✓	
pt2p0			✓	
pt3p0			✓	
pt4p0			✓	
pt5p0				
pt6p0			✓	
pt9p0				
pt12p0			✓	
pt15p0				
pt21p0				
pt23p0				
pt30p0				
pt37p0				
pt63p0				
pt64p0			✓	
cyM3p1			✓	
skM3p1			✓	
tkM3p1			✓	
ykM3p1			✓	
sq1_1p1				
sq2_1p1				
sq3_1p1				
sq4_1p1				
sq5_1p1				
sq1_2p1			✓	
sq2_2p1				
sq3_2p1			✓	
sq4_2p1				
sq5_2p1				
sq1_3p1				
sq2_3p1			✓	
sq3_3p1	✓	✓	✓	
sq4_3p1				
sq5_3p1				
sq1_4p1	✓	✓		
sq2_4p1	✓	✓	✓	
sq3_4p1	✓	✓	✓	
sq4_4p1				
sq5_4p1				
sq1_5p1				
sq2_5p1				
sq3_5p1			✓	
sq4_5p1				
sq5_5p1			✓	
pt1p1			✓	
pt2p1			✓	
pt3p1			✓	
pt4p1			✓	
pt5p1			✓	
pt6p1			✓	
pt9p1				
pt12p1				
pt15p1			✓	
pt21p1				
pt23p1				
pt30p1			✓	
pt37p1				
pt63p1			✓	
pt64p1			✓	
cyM3p2			✓	
skM3p2			✓	
tkM3p2			✓	
ykM3p2			✓	
sq1_1p2			✓	
sq2_1p2				
sq3_1p2				
sq4_1p2				
sq5_1p2				
sq1_2p2			✓	
sq2_2p2				
sq3_2p2	✓	✓	✓	
sq4_2p2				
sq5_2p2				
sq1_3p2			✓	
sq2_3p2			✓	
sq3_3p2			✓	
sq4_3p2				
sq5_3p2				
sq1_4p2	✓	✓	✓	
sq2_4p2	✓	✓	✓	
sq3_4p2	✓	✓	✓	
sq4_4p2				
sq5_4p2				
sq1_5p2			✓	
sq2_5p2				
sq3_5p2			✓	
sq4_5p2				
sq5_5p2				
pt1p2			✓	
pt2p2			✓	
pt3p2			✓	
pt4p2			✓	
pt5p2	✓	✓	✓	
pt6p2			✓	
pt9p2				
pt12p2				
pt15p2				
pt21p2				
pt23p2			✓	
pt30p2				
pt37p2				
pt63p2			✓	
pt64p2			✓	
cyM3p3	✓	✓	✓	
skM3p3	✓	✓	✓	
tkM3p3	✓	✓	✓	
ykM3p3			✓	
sq1_1p3				
sq2_1p3			✓	
sq3_1p3				
sq4_1p3			✓	
sq5_1p3				
sq1_2p3				
sq2_2p3			✓	
sq3_2p3	✓	✓	✓	
sq4_2p3	✓	✓	✓	
sq5_2p3				
sq1_3p3			✓	
sq2_3p3			✓	
sq3_3p3	✓	✓	✓	
sq4_3p3			✓	
sq5_3p3			✓	
sq1_4p3	✓	✓	✓	
sq2_4p3			✓	
sq3_4p3			✓	
sq4_4p3			✓	
sq5_4p3				
sq1_5p3				
sq2_5p3				
sq3_5p3				
sq4_5p3			✓	
sq5_5p3				
pt1p3			✓	
pt2p3			✓	
pt3p3	✓	✓	✓	
pt4p3	✓	✓	✓	
pt5p3			✓	
pt6p3	✓	✓	✓	
pt9p3				
pt12p3				
pt15p3			✓	
pt21p3				
pt23p3			✓	
pt30p3				
pt37p3				
pt63p3				
pt64p3			✓	

APPENDIX D

LOWER AND UPPER BOUNDS OF ALL STATE AND DECISION VARIABLES

Table D.1 Lower and Upper Bounds of All Ozone State Variables.

Period	Ozone	Min	Max
p0	**cyAMp0**	0.01871	0.01926
p1	**cyAMp1**	0.05157	0.0528
p2	**cyAMp2**	0.06731	0.07645
p3	**cyAMp3**	0.07289	0.08918
p4	**cyAMp4**	0.08832	0.11926
p0	**skAMp0**	0.01476	0.02182
p1	**skAMp1**	0.03795	0.06288
p2	**skAMp2**	0.09323	0.1107
p3	**skAMp3**	0.10071	0.12355
p4	**skAMp4**	0.11554	0.13068
p0	**tkAMp0**	0.02016	0.02174
p1	**tkAMp1**	0.05853	0.06224
p2	**tkAMp2**	0.07947	0.0939
p3	**tkAMp3**	0.08988	0.11309
p4	**tkAMp4**	0.10079	0.12895
p0	**ykAMp0**	0.03355	0.03374
p1	**ykAMp1**	0.06301	0.06346
p2	**ykAMp2**	0.08365	0.08648
p3	**ykAMp3**	0.08998	0.0915
p4	**ykAMp4**	0.0927	0.09396
p0	**cyM3p0**	0.01979	0.02122
p1	**cyM3p1**	0.05249	0.0552
p2	**cyM3p2**	0.06686	0.08669
p3	**cyM3p3**	0.07	0.09637
p4	**cyM3p4**	0.10035	0.15205
p0	**skM3p0**	0.01933	0.0223
p1	**skM3p1**	0.04355	0.06085
p2	**skM3p2**	0.07658	0.11223
p3	**skM3p3**	0.08524	0.14338
p4	**skM3p4**	0.09986	0.14935
p0	**tkM3p0**	0.0197	0.02611
p1	**tkM3p1**	0.04461	0.06659
p2	**tkM3p2**	0.09015	0.1164
p3	**tkM3p3**	0.09821	0.13573
p4	**tkM3p4**	0.10551	0.14388
p0	**ykM3p0**	0.03625	0.03634
p1	**ykM3p1**	0.0702	0.07148
p2	**ykM3p2**	0.08175	0.08605
p3	**ykM3p3**	0.08233	0.08819
p4	**ykM3p4**	0.0933	0.0967

Table D.2 Lower and Upper Bounds of Initial Emission Variables.

Period	Emission	Min	Max
p0	**sq1_1p0**	9.66507	4832.534
p0	**sq2_1p0**	25.89392	12946.96
p0	**sq3_1p0**	26.91656	13458.29
p0	**sq4_1p0**	38.0638	19031.9
p0	**sq5_1p0**	11.39615	5698.074
p0	**sq1_2p0**	25.31859	12659.3
p0	**sq2_2p0**	32.80566	16402.83
p0	**sq3_2p0**	228.9769	114488.4
p0	**sq4_2p0**	35.87039	17935.21
p0	**sq5_2p0**	20.50761	10253.81
p0	**sq1_3p0**	22.46705	11233.52
p0	**sq2_3p0**	56.58833	28294.17
p0	**sq3_3p0**	436.3238	218161.8
p0	**sq4_3p0**	123.2852	61642.62
p0	**sq5_3p0**	16.72785	8363.926
p0	**sq1_4p0**	31.92705	15963.52
p0	**sq2_4p0**	51.54295	25771.48
p0	**sq3_4p0**	75.43491	37717.45
p0	**sq4_4p0**	93.64388	46821.95
p0	**sq5_4p0**	35.91177	17955.9
p0	**sq1_5p0**	31.42341	15711.7
p0	**sq2_5p0**	25.61034	12805.17
p0	**sq3_5p0**	16.9294	8464.698
p0	**sq4_5p0**	16.88412	8442.062
p0	**sq5_5p0**	30.65759	15328.79
p0	**pt1p0**	265.2148	132607.4
p0	**pt2p0**	269.3769	134688.5
p0	**pt3p0**	302.2846	151142.3
p0	**pt4p0**	312.115	156057.5
p0	**pt5p0**	91.54986	45774.93
p0	**pt6p0**	103.5711	51785.57
p0	**pt9p0**	26.38951	13194.75
p0	**pt12p0**	116.2514	58125.71
p0	**pt15p0**	275.1748	137587.4
p0	**pt21p0**	0	0
p0	**pt23p0**	0.05498	27.492
p0	**pt30p0**	11.06203	5531.013
p0	**pt37p0**	0	0
p0	**pt63p0**	6.29568	3147.84
p0	**pt64p0**	13.43842	6719.208

Table D.3 Lower and Upper Bounds of Emission Variables for Stage-1 and Stage-2.

Period	Emission	Min	Max
p1	**sq1_1p1**	22.116	11057.99
p1	**sq2_1p1**	66.08985	33044.89
p1	**sq3_1p1**	78.03279	39016.42
p1	**sq4_1p1**	50688.54	50688.54
p1	**sq5_1p1**	28.37495	14187.48
p1	**sq1_2p1**	68.43769	34218.83
p1	**sq2_2p1**	96.66035	48330.18
p1	**sq3_2p1**	551.9965	275998.2
p1	**sq4_2p1**	100.5936	50296.8
p1	**sq5_2p1**	54.97054	27485.27
p1	**sq1_3p1**	59.80548	29902.73
p1	**sq2_3p1**	164.2707	82135.38
p1	**sq3_3p1**	1274.602	637300.2
p1	**sq4_3p1**	364.1879	182093.9
p1	**sq5_3p1**	43.77184	21885.93
p1	**sq1_4p1**	92.16656	46083.31
p1	**sq2_4p1**	145.6088	72804.38
p1	**sq3_4p1**	234.3535	117176.8
p1	**sq4_4p1**	274.7352	137367.6
p1	**sq5_4p1**	97.56876	48784.35
p1	**sq1_5p1**	87.54062	43770.31
p1	**sq2_5p1**	67.05792	33528.95
p1	**sq3_5p1**	45.23076	22615.39
p1	**sq4_5p1**	48.82424	24412.1
p1	**sq5_5p1**	89.218	44609
p1	**pt1p1**	265.2148	132607.4
p1	**pt2p1**	269.3769	134688.5
p1	**pt3p1**	302.2846	151142.3
p1	**pt4p1**	312.115	156057.5
p1	**pt5p1**	91.54986	45774.93
p1	**pt6p1**	103.5711	51785.57
p1	**pt9p1**	26.38951	13194.75
p1	**pt12p1**	116.2514	58125.71
p1	**pt15p1**	275.1748	137587.4
p1	**pt21p1**	0.78812	394.062
p1	**pt23p1**	0.05498	27.492
p1	**pt30p1**	11.06203	5531.013
p1	**pt37p1**	0.00222	1.11
p1	**pt63p1**	6.29568	3147.84
p1	**pt64p1**	13.43842	6719.208
p2	**sq1_1p2**	17.15996	8579.976
p2	**sq2_1p2**	50.01805	25009.02
p2	**sq3_1p2**	64.49807	32249.05
p2	**sq4_1p2**	75.94629	37973.15
p2	**sq5_1p2**	22.29067	11145.33
p2	**sq1_2p2**	54.21173	27105.86
p2	**sq2_2p2**	75.59088	37795.45
p2	**sq3_2p2**	446.1924	223096.3
p2	**sq4_2p2**	78.86349	39431.75
p2	**sq5_2p2**	44.29789	22148.96
p2	**sq1_3p2**	46.70567	23352.83
p2	**sq2_3p2**	126.8336	63416.76
p2	**sq3_3p2**	974.8786	487439.6
p2	**sq4_3p2**	284.2981	142148.9
p2	**sq5_3p2**	36.72416	18362.08
p2	**sq1_4p2**	77.53512	38767.54
p2	**sq2_4p2**	112.0928	56046.38
p2	**sq3_4p2**	186.5653	93282.63
p2	**sq4_4p2**	211.7902	105895.1
p2	**sq5_4p2**	75.91461	37957.29
p2	**sq1_5p2**	69.05902	34529.5
p2	**sq2_5p2**	49.9189	24959.43
p2	**sq3_5p2**	35.03601	17518
p2	**sq4_5p2**	38.10293	19051.48
p2	**sq5_5p2**	71.32199	35660.99
p2	**pt1p2**	265.2148	132607.4
p2	**pt2p2**	269.3769	134688.5
p2	**pt3p2**	302.2846	151142.3
p2	**pt4p2**	312.115	156057.5
p2	**pt5p2**	91.54986	45774.93
p2	**pt6p2**	103.5711	51785.57
p2	**pt9p2**	26.38951	13194.75
p2	**pt12p2**	116.2514	58125.71
p2	**pt15p2**	275.1748	137587.4
p2	**pt21p2**	0.78812	394.062
p2	**pt23p2**	0.05498	27.492
p2	**pt30p2**	11.06203	5531.013
p2	**pt37p2**	0.00333	1.665
p2	**pt63p2**	6.29568	3147.84
p2	**pt64p2**	13.43842	6719.208

Table D.4 Lower and Upper Bounds of Emission Variables for Stage-3 and Stage-4.

Period	Emission	Min	Max
p3	**sq1_1p3**	18.11205	9056.023
p3	**sq2_1p3**	51.86191	25930.96
p3	**sq3_1p3**	66.16741	33083.69
p3	**sq4_1p3**	78.46716	39233.59
p3	**sq5_1p3**	23.29167	11645.82
p3	**sq1_2p3**	56.35691	28178.46
p3	**sq2_2p3**	77.86413	38932.05
p3	**sq3_2p3**	454.6599	227330
p3	**sq4_2p3**	81.15749	40578.75
p3	**sq5_2p3**	45.79075	22895.36
p3	**sq1_3p3**	48.4517	24225.86
p3	**sq2_3p3**	130.1247	65062.32
p3	**sq3_3p3**	997.8658	498932.7
p3	**sq4_3p3**	290.9413	145470.8
p3	**sq5_3p3**	38.09953	19049.75
p3	**sq1_4p3**	79.59383	39796.9
p3	**sq2_4p3**	115.0645	57532.23
p3	**sq3_4p3**	190.5626	95281.33
p3	**sq4_4p3**	217.078	108539
p3	**sq5_4p3**	78.37529	39187.65
p3	**sq1_5p3**	71.21631	35608.16
p3	**sq2_5p3**	51.79794	25898.96
p3	**sq3_5p3**	36.14161	18070.8
p3	**sq4_5p3**	39.23457	19617.29
p3	**sq5_5p3**	73.00446	36502.26
p3	**pt1p3**	265.2148	132607.4
p3	**pt2p3**	269.3769	134688.5
p3	**pt3p3**	302.2846	151142.3
p3	**pt4p3**	312.115	156057.5
p3	**pt5p3**	91.54986	45774.93
p3	**pt6p3**	103.5711	51785.57
p3	**pt9p3**	26.38951	13194.75
p3	**pt12p3**	116.2514	58125.71
p3	**pt15p3**	275.1748	137587.4
p3	**pt21p3**	0	0
p3	**pt23p3**	0.05498	27.492
p3	**pt30p3**	11.06203	5531.013
p3	**pt37p3**	0.00333	1.665
p3	**pt63p3**	6.29568	3147.84
p3	**pt64p3**	13.43842	6719.208

Period	Emission	Min	Max
p4	**sq1_1p4**	24.20892	12104.46
p4	**sq2_1p4**	69.3261	34663.04
p4	**sq3_1p4**	77.68313	38841.59
p4	**sq4_1p4**	105.5735	52786.78
p4	**sq5_1p4**	29.98914	14994.56
p4	**sq1_2p4**	71.33415	35667.06
p4	**sq2_2p4**	100.8285	50414.28
p4	**sq3_2p4**	566.3564	283178
p4	**sq4_2p4**	103.7663	51883.16
p4	**sq5_2p4**	56.39738	28198.68
p4	**sq1_3p4**	61.85406	30927.02
p4	**sq2_3p4**	168.876	84438.01
p4	**sq3_3p4**	1314.98	657489.6
p4	**sq4_3p4**	375.0222	187511.1
p4	**sq5_3p4**	45.11403	22557.02
p4	**sq1_4p4**	89.98418	44992.09
p4	**sq2_4p4**	148.7417	74370.84
p4	**sq3_4p4**	239.6858	119842.9
p4	**sq4_4p4**	283.5426	141771.3
p4	**sq5_4p4**	99.92738	49963.7
p4	**sq1_5p4**	88.51586	44257.96
p4	**sq2_5p4**	70.57362	35286.78
p4	**sq3_5p4**	47.27283	23636.42
p4	**sq4_5p4**	50.41827	25209.14
p4	**sq5_5p4**	88.87865	44439.29
p4	**pt1p4**	265.2148	132607.4
p4	**pt2p4**	269.3769	134688.5
p4	**pt3p4**	302.2846	151142.3
p4	**pt4p4**	312.115	156057.5
p4	**pt5p4**	91.54986	45774.93
p4	**pt6p4**	103.5711	51785.57
p4	**pt9p4**	26.38951	13194.75
p4	**pt12p4**	116.2514	58125.71
p4	**pt15p4**	275.1748	137587.4
p4	**pt21p4**	0	0
p4	**pt23p4**	0.05498	27.492
p4	**pt30p4**	11.06203	5531.013
p4	**pt37p4**	0.00333	1.665
p4	**pt63p4**	6.29568	3147.84
p4	**pt64p4**	13.43842	6719.208

APPENDIX E

50 RANDOM INITIAL STATE VARIABLES

Table E.1 50 Random Initial State Variables.

No.	**sq1_1p0**	**sq2_1p0**	**sq3_1p0**	**sq4_1p0**	**sq5_1p0**	**sq1_2p0**	**sq2_2p0**	**sq3_2p0**	**sq4_2p0**	**sq5_2p0**
1	2303.104	1905.028	10533.81	16218.22	2571.76	3343.62	12870.51	12993.28	3761.387	8899.054
2	1298.47	2149.318	11820.63	12490.53	2467.109	1647.891	8697.465	31129.57	15587.39	5006.995
3	2815.874	8060.137	8248.995	746.2565	100.8425	8261.546	2355.258	209.6023	15606.79	8339.509
4	332.9034	9895.315	9372.886	13882.02	458.5998	953.6513	3543.272	34646.42	7949.344	2975.525
5	4406.811	2687.85	6574.846	17670.24	2369.911	12154.88	15796.4	61774.49	6600.32	7499.214
6	1018.746	10015.09	79.81646	15750.04	5638.715	5777.021	15924.8	80608.3	15912.98	4728.248
7	1310.509	11490.44	1991.603	6688.819	1927.762	6439.939	4165.321	114076.5	17786.31	9710.635
8	1626.58	5212.601	7202.364	11351.81	1706.581	11341.13	7520.771	57700.6	17016.3	8888.803
9	4404.433	5424.409	1686.642	15380.88	1288.611	2329.439	10158.8	83027.45	14874.09	4026.118
10	356.7467	9447.687	5070.004	7668.126	3013.478	1659.97	163.9288	56684.29	1930.574	773.5077
11	1068.05	1765.693	13032.77	6891.172	4048.375	356.4133	9396.611	108499	16370.38	2667.021
12	3506.636	9344.151	3966.843	16794.72	103.6649	8519.736	1287.129	72381.04	17323.49	2478.075
13	394.0318	3358.906	1227.905	841.096	2944.135	10536.9	8047.802	33937.82	3551.373	4254.821
14	713.289	7958.497	12657.75	12462.06	4470.831	11730.62	14784.36	87603.29	14833.97	3383.805
15	2763.572	1456.257	5178.053	9750.065	4490.872	9554.054	9490.879	53340	13639.97	6687.081
16	64.61126	8442.08	5397.524	9846.902	278.8801	8228.146	13559.9	50532.14	8987.211	8013.649
17	108.7428	10066.37	9586.215	11854.33	2770.136	10897.54	8872.06	77642.32	11786.87	6775.587
18	1279.297	7997.02	7643.056	4801.306	2444.534	1017.97	3038.379	35665.48	14857.84	8141.991
19	989.7981	517.4843	5588.349	15323.02	2321.802	3269.617	14921.66	3709.056	750.8733	1938.617
20	1968.101	8147.256	8906.452	4921.841	1484.605	7588.351	737.5513	56795.93	2117.099	1186.742
21	1563.083	8143.836	10466.29	18023.19	3426.317	9923.006	5086.173	13809.78	5340.133	4349.663
22	1985.25	10343.65	7069.81	17296.13	5589.621	1398.323	15602.27	44500.58	15437.25	899.3729
23	4366.416	1170.663	4335.411	4852.14	5003.059	6330.91	15287.09	75089.35	14597.39	6920.042
24	4405.439	7097.842	5919.253	3342.709	1394.393	10123.16	15268.74	101851.4	6457.087	713.199
25	227.4708	12587.58	7771.444	8746.619	5110.406	11091.35	9809.535	31451.35	3764.462	7140.44
26	1128.308	7061.337	6100.013	14454.98	2740.597	3924.723	3324.381	76637.07	717.2471	4709.491
27	2975.68	12539.03	4919.77	14797.04	5005.473	10492.35	5237.685	20548.72	6560.157	4150.481
28	4539.396	12141.31	8232.929	14690.49	4923.279	11741.85	9759.789	44394.23	14269.36	5141.856
29	3220.267	11103.82	5902.329	8426.259	1928.202	7230.427	12036.83	16470.62	2660.002	4482.153
30	3794.614	4352.859	2143.931	1223.188	1757.117	6668.777	5237.991	79846.48	5060.096	9927.046
31	2856.662	6759.212	12796.41	17448.44	217.9114	241.3449	9129.294	64414.96	5305.332	4078.492
32	2364.742	803.1501	11026.81	11974.23	4100.702	2274.804	987.8903	71277.13	15400.02	7803.961
33	2100.086	11907.05	5604.685	6661.937	366.1321	10176.79	11267.26	24724.81	15258.02	7491.757
34	3581.546	5421.73	6042.025	1375.42	3787.53	3795.742	5345.386	34395.37	3858.545	4714.349
35	1121.221	4796.074	8561.486	11674.15	5269.293	12596.75	8642.291	30658.15	17127.56	3542.193
36	2118.059	2724.054	4801.768	3133.695	4658.703	1350.697	8538.447	72969.47	908.7851	4052.5
37	4203.899	1418.658	3907.908	3253.278	576.4381	6252.571	5855.161	18490.3	17909.86	1912.983
38	1063.04	11576.94	5764.469	16394.77	5557.903	6320.27	13917.48	1803.445	13437.42	6863.596
39	4430.47	2908.302	5797.66	13361.41	3555.297	4950.619	11790.74	77868.34	16112.31	5995.424
40	1514.197	8032.689	1084.763	3179.366	3525.269	9435.436	2930.258	50137.92	2057.118	3569.298
41	3535.067	5636.342	11782.46	13566.03	5070.017	12122.35	12388.08	11238.12	8681.934	9268.611
42	2096.286	9581.094	10623.01	11869.19	1998.381	8663.857	6326.665	18596.79	9784.592	9672.828
43	3420.887	11444.55	11088.26	3260.785	3679.978	3953.204	8156.651	3409.395	11358.68	8692.264
44	2745.584	10096.45	3032.585	6299.601	3040.181	8061.239	15855.29	41338.12	16216.23	6777.232
45	707.0372	3058.264	5953.159	15862.39	2457.876	11067.37	6225.761	102249.6	15897.81	10139.61
46	3493.346	10050.17	6649.43	5757.188	1621.178	12500.92	8451.116	69649.37	7115.808	3422.907
47	286.6717	10948.87	4602.166	16134.3	2154.283	7061.301	1928.418	82996.87	939.826	3986.964
48	3984.951	10809.39	5060.941	8505.781	1141.015	4354.43	7728.262	71489.98	10945.59	1732.477
49	2408.047	10875.99	9114.138	11819.09	5400.705	12436.69	2196.17	68768.88	14295.24	1158.067
50	1455.595	10003.51	998.5794	14568.48	5328.977	6583.079	15418.21	24752	7249.566	7517.197

Table E.1 50 Random Initial State Variables (Continued).

No.	sq1_3p0	sq2_3p0	sq3_3p0	sq4_3p0	sq5_3p0	sq1_4p0	sq2_4p0	sq3_4p0	sq4_4p0	sq5_4p0
1	5643.982	14054.29	191880.7	28951.16	298.2929	6237.435	16771.14	16434.7	27408.54	8322.58
2	8348.211	12876.66	127797.4	36113.11	5355.412	2609.645	9169.12	25033.01	17399.87	15291.52
3	4673.727	7352.868	45355.94	18779.76	4202.056	15188.89	17818.42	20431.86	15869.49	15349.08
4	5208.221	26491.4	28369.06	52082.42	6509.6	6738.65	15667.06	17379.93	20501.5	482.4838
5	1231.937	3376.223	93416.35	39940.74	4299.435	9495.907	20516.39	35670.85	27685.82	12332.55
6	4122.465	5992.901	190205.6	22434	4443.971	11957.85	12298.5	35580.85	28284.23	17297.99
7	2043.508	9584.958	147028.4	37980.72	2356.824	6673.502	7331.455	10892.53	9681.814	13343.53
8	5461.418	7632.525	7292.63	53074.73	1954.208	2207.672	21491.41	13887.15	25528.89	4972.787
9	5544.363	25491.78	216973.7	48110.29	835.0889	38.31121	9860.45	6279.346	22710.71	9798.807
10	3296.519	631.1727	78332.19	18188.63	4504.379	14190.66	2263.079	33648.61	45477.01	2605.504
11	8617.164	23916.67	73566.27	39498.94	7024.667	7888.44	12456.53	26718.14	17419.15	5968.421
12	7806.413	19857.15	53122.56	2885.165	6304.528	9826.834	24751.67	23439.88	36146.27	2441.568
13	3712.444	2515.445	191929.2	28043.77	2014.329	13174.35	10499.46	18317.99	25882.88	4922.532
14	7703.421	980.9023	5610.182	717.5473	685.3976	4421.116	8451.326	6709.185	17099.31	9449.759
15	796.0234	11232.56	46676.86	9208.104	2475.656	14238.19	4406.93	19209.4	3134.888	11036.66
16	8098.486	1787.68	97590.37	8118.453	8239.519	12347.83	3033.79	10154.83	40711.35	4160.257
17	1471.225	23321.36	106703.3	60213.96	1816.342	7134.176	17050.14	22228.52	7558.667	3182.474
18	4114.919	10988.53	21482.98	16663.06	1440.168	8699.139	24877.92	21135.3	21723.83	6323.913
19	3770.428	8101.693	82053.83	29184.92	4842.631	15289.99	20451.46	782.8976	17972.79	5200.752
20	5853.099	16895	108431.9	41714.92	4258.581	12120.87	25204.04	34844.27	26087.5	9803.999
21	4738.826	21049.1	81256.09	54506	318.2336	14504.04	13178.72	18765.81	20314.87	1645.184
22	7673.62	15091.97	81884.03	60379.14	859.1042	6908.254	10896.02	24932.04	6572.758	6482.867
23	10432.46	25853.16	104925.7	17778.94	6872.775	7969.496	22747.2	28969.34	2706.064	11978.26
24	8734.615	18223.87	217421.6	15486.85	7321.556	12454.69	1123.403	25010.06	37955.05	1931.887
25	9879.181	14164.86	122888.2	35809.01	3465.625	8705.745	24252.14	5918.366	36500.23	3966.295
26	4440.833	14558.16	210086.1	28631.29	4607.571	14339.96	6013.915	10165.52	39760.42	4113.735
27	3108.695	14361.91	95141.03	19841.59	5424.17	1610.298	13616.33	24991.47	43185.06	7817.628
28	8928.812	22660.64	187133	4727.79	7097.427	3219.114	20803.92	22220.46	8331.667	1657.261
29	8059.54	26858.02	170334	36032.33	1587.769	1451.859	11639.65	33325.64	7704.034	3200.363
30	6255.923	27805.4	6408.374	7219.05	8108.355	5620.766	2937.314	17415.6	12114.64	205.4774
31	6750.29	26537.89	68981.68	37482.51	4070.311	4544.541	17849.97	19523.13	12500.88	8522.485
32	2165.589	24779.31	214905.5	58572.47	7283.828	5650.115	2602.688	13943.09	1948.24	11423.3
33	9450.646	8610.203	49870.1	42551.04	7857.61	4382.099	6577.274	6635.13	12279.45	6698.059
34	49.75257	1563.78	17817.45	2364.215	4820.118	6286.588	6024.262	9269.572	37048.52	10840.79
35	5247.653	6462.79	208722.2	15589.11	6005.779	11274.27	9073.133	23269.64	38715.92	854.8479
36	7144.555	19286.55	184517.3	24634.67	8220.16	3957.582	3719.779	14861.98	3450.929	5663.469
37	4526.929	17845.38	71993.84	58848.75	4250.301	7872.901	9388.657	9780.747	8151.469	9170.083
38	8443.704	15815.29	65504.17	15775.73	280.2265	9223.964	12633.15	8317.119	2858.317	2160.182
39	4399.19	11633.94	5230.659	13905.82	8064.162	9612.286	4283.764	16808.79	42939.69	16379.15
40	9542.618	17696.86	142262.3	21248.41	6681.205	7406.113	20242.15	25231.09	22993.36	11925.69
41	2685.252	4399.346	61729.66	17149.56	7539.598	1149.495	19425.38	964.111	15538.69	16892.38
42	7864.82	6823.585	17236.83	6620.14	5286.022	5213.189	8659.732	21346.73	26799.9	16494.46
43	856.1854	20010.94	4594.225	55050.04	4818.291	15836.41	2607.265	15716.31	35939.68	8280.704
44	9826.439	14461.58	202015.7	10953.33	6497.961	559.5501	3939.294	30343.37	24546.57	2724.1
45	10312.35	11525.98	124257	31255.87	7772.29	15176.12	2834.059	1594.781	39449.79	17402.5
46	3517.789	11365.79	152839.8	57003.24	7495.012	8982.481	5880.362	13302.81	23776.58	5765.428
47	6792.6	20116.18	183963.9	12048.88	2215.946	8198.86	14097.41	29567.56	39464.89	12382.59
48	4762.177	5488.892	178474.9	28647.06	691.745	9076.204	9221.186	24361.31	27396.15	119.9348
49	6145.284	8303.971	5895.308	58560.45	3950.521	1736.447	3946.688	8437.975	37737.82	5586.082
50	1475.907	5413.144	205877.7	36342.31	6204.497	14718.91	15029.28	37592.83	9216.563	16036.86

Table E.1 50 Random Initial State Variables (Continued).

No.	sq1_5p0	sq2_5p0	sq3_5p0	sq4_5p0	sq5_5p0	pt1p0	pt2p0	pt3p0	pt4p0	pt5p0
1	10753.93	9680.199	4299.878	6965.297	10788.31	67974.19	108928.2	93771.43	48573.9	8694.366
2	7714.591	10367.28	5879.09	2509.112	4036.628	24561.62	9470.657	114876	103190	24074.42
3	4738.78	2983.286	7036.06	7619.274	14039.74	122372.9	85458.26	72085.32	4589.293	22209.9
4	4608.514	836.717	3786.921	4797.194	244.0879	9923.896	132308.7	28650.01	50897.2	25440.38
5	6887.047	8117.688	7689.992	4771.308	8996.192	40649.36	110762.7	24891.88	122867.5	25040.25
6	8204.988	5536.173	2686.445	6022.832	10578.33	108951.6	107877.5	99568.15	144907.3	29719.88
7	15365.79	4601.474	6803.35	3298.36	7291.144	91962.46	13674.87	139276	124533.5	13898.85
8	12420.68	2069.296	168.2014	4680.113	3608.229	108420.2	12833.53	141160.3	114433.8	16799.52
9	1018.63	2798.974	8092.166	6697.848	11793.1	127067.4	31066.9	116919.6	78934.69	18183.54
10	278.6896	666.024	3159.134	1732.392	5077.38	119649.3	120561.3	144217.2	150390.4	4627.178
11	9677.667	3137.904	4267.715	7700.099	13125.33	10123.59	67842.1	58838.63	83935.52	7607.376
12	10434.54	11273.78	2855.966	3406.228	8139.563	107429.9	27466.99	115702.5	81647.67	18972.57
13	10307.78	2415.886	6432.922	3055.273	7826.033	47440.17	33285.74	22895.05	28802.42	28890
14	2833.908	6813.721	2076.051	3816.308	612.6833	105257	108994	27214.31	77566.34	11000.5
15	9468.586	3343.329	7785.389	2698.669	6524.525	19463.44	86867.75	115080.7	108184.3	19486.65
16	2971.733	8401.855	6009.665	5742.044	8599.294	116034.1	39779.23	109840.4	51103.8	24892.4
17	929.2167	7620.534	6558.336	4526.513	4810.063	14809.47	67521.32	18722.38	89656.84	14029.15
18	5803.819	12753.25	499.0008	222.7946	8321.058	39594.49	77899.46	70385.27	88076.55	7029.85
19	2850.917	12787.01	7495.597	8007.464	10628.86	778.2013	3227.617	93871.33	94884.94	29975.2
20	12893.74	3824.713	4227.454	7307.604	14837.24	58139.96	23405	50832.54	31731.27	8577.711
21	3821.522	2472.805	7976.372	6539.761	10065.3	14525.1	93527.55	126943	127402.9	10949.55
22	10670.99	11675.15	4506.814	1405.477	13170.22	4923.766	9931.233	45698.73	71058.63	25014.85
23	4174.235	9984.541	4376.33	7045.066	12009.21	118674.5	80350.52	123032.2	148762.7	8384.286
24	133.5584	7684.188	3636.506	3177.456	13227.17	131657	111518.2	85843.7	97425.94	3162.899
25	3465.76	4601.685	3970.707	908.7155	11576.08	128985.1	58786.63	127650.9	32288.66	8341.041
26	13463.62	10170.47	1804.897	4291.511	7596.712	38040.92	11785.02	10682.43	144460	9823.539
27	14370.41	5176.695	6806.425	1388.253	13108.36	96527.23	21502.97	44970.17	59225.08	5344.732
28	7391.234	5766.42	1815.373	5211.375	10491.55	85435.88	114707.4	46873.13	107262.6	23253.19
29	14520.21	12030.34	5359.209	967.008	6459.779	109865.4	5834.848	665.2215	125688.8	3201.836
30	12314.21	4632.302	2136.111	6646.701	894.4529	23771.03	115159.7	92355.46	89602.9	23053.15
31	14680.19	12611.84	6315.725	4707.761	5453.126	98046.53	119735	151037.8	68243.14	7844.594
32	2175.716	900.527	1266.145	5091.403	12455.21	73433.79	55717.06	131082.6	154646.4	41994.13
33	8190.327	6533.744	235.8889	6687.887	4249.762	119182.7	30940.23	51377.72	132157	42204.9
34	14013.21	11292.49	3605.779	308.1139	9028.849	108770.1	1530.732	114324.3	85577.83	2827.223
35	5407.587	11443.97	2265.602	7558.152	10342.2	112594.4	23136.78	49533.55	38733.41	17131.76
36	9711.802	599.0831	1461.133	3918.702	7593.668	1088.573	119778	100326.2	52726.18	31157.63
37	7896.096	1112.736	8357.303	6139.975	14207.2	126737.4	108731.8	58627.88	20100.28	5602.257
38	12325.82	8016.56	7662.091	2441.2	10611.29	32840.73	68367.18	60879.26	76767.82	2171.29
39	7286.205	9064.668	6310.934	6886.687	5066.295	27287.96	15718.78	106368.5	48657.71	14289.02
40	4179.078	6944.877	8125.675	4190.094	10665.14	15781.78	16210.9	67497.85	114749.5	1105.943
41	6354.809	6481.395	2926.645	2639.645	2271.763	128654.7	116651.9	111407	43395.62	10883.82
42	9754.228	12068.53	5405.459	7829.975	5296.603	72808.18	14424.7	80153.69	148657.7	1483.857
43	524.8434	11157.74	3337.603	954.9522	5772.279	47739.18	18411.83	11555.48	50844.23	28639.31
44	7108.869	4001.925	2274.558	2752.83	1490.238	100464.2	40691.36	133321.6	64940.14	26629.31
45	7826.865	12122.21	2578.023	3307.331	14029.36	1768.579	86956.53	150624.6	51046.91	23908.82
46	14642.79	748.6616	7725.88	3732.756	3442.065	82921.61	92966.4	18123.23	80799.81	3702.155
47	12785.02	10981.73	8116.531	7246.074	12197.04	1549.977	104345.4	108307.7	152106	11706.52
48	4382.82	3914.153	3492.514	561.439	11674.78	19604.07	70424.54	126541	121226.4	23469.49
49	8577.911	1996.311	5314.238	3946.156	6263.416	31301.1	113281.7	79425.94	91872.12	42990.47
50	3441.339	4167.098	1731.707	1996.16	6838.047	75346.64	45994.41	124794.8	125643.3	9783.211

Table E.1 50 Random Initial State Variables (Continued).

No.	pt6p0	pt9p0	pt12p0	pt15p0	pt21p0	pt23p0	pt30p0	pt37p0	pt63p0	pt64p0
1	2321.697	11175.83	22379.47	14527.56	0	11.80048	1592.017	0	2672.793	6340.916
2	24246.88	5190.169	434.6988	53184.51	0	15.93264	4884.721	0	2646.28	1650.671
3	4117.402	5614.011	28811.77	69196.81	0	25.61931	4734.274	0	1593.405	1021.219
4	30518.92	1864.429	1859.116	136303.4	0	10.76404	5253.12	0	1173.358	4087.721
5	11252.78	9446.253	17327.75	94078.56	0	18.26366	5023.193	0	410.0982	29.89597
6	28522.15	5613.464	12267.98	51042.78	0	1.617375	3441.224	0	1579.58	1778.432
7	17457.03	2205.44	24204.87	108673.1	0	13.03407	3215.247	0	2089.985	6367.115
8	36827.79	3728.106	50725.11	34731.76	0	21.3906	4172.067	0	3147.212	1836.677
9	28336.44	7641.663	21138.28	37702.2	0	2.72095	690.3987	0	360.6066	4350.561
10	25273.69	9325.438	20793.16	38720.74	0	21.86879	4820.461	0	2530.859	1233.321
11	20099.29	10527.05	32399.05	100489.6	0	27.19422	2494.688	0	72.28366	5318.197
12	19527.3	1584.341	4502.518	43474.36	0	7.038821	1603.122	0	1078.267	1533.957
13	6118.014	10640.45	12773.1	98282.6	0	0.340886	946.1628	0	62.02184	807.29
14	35646.08	5117.973	32020.55	129476.3	0	26.47956	5368.18	0	680.3802	2354.739
15	4857.957	8183.181	53176.8	50493.28	0	24.26207	5404.345	0	3049.169	622.4321
16	32184.69	7726.049	16388.44	40590.21	0	18.65489	3693.222	0	2593.685	4663.597
17	38141.31	9715.492	56766.13	129827.5	0	7.743101	5340.098	0	703.138	5565.534
18	13311.34	5537.844	33230.11	42742.21	0	21.37954	1132.537	0	2217.719	6290.915
19	48431.09	2544.738	47627.35	7767.482	0	5.98791	4183.525	0	1435.886	868.5813
20	33540.51	12924.58	46300.12	56401.95	0	16.41565	2990.666	0	2154.929	5043.223
21	20455.04	7040.994	45191.81	28831.96	0	22.80377	1519.368	0	2168.647	2494.518
22	34714.58	1476.608	31651.52	80965.65	0	9.924166	2299.975	0	2469.417	1217.274
23	9312.862	13057.16	25144.19	127262	0	10.39249	4865.112	0	1790.02	1358.529
24	28957.64	7249.909	42757.51	135442	0	8.845321	4195.519	0	2137.484	6037.467
25	30437.28	2576.659	7597.993	97337.67	0	1.231549	20.95208	0	1719.435	1696.593
26	12546.74	9418.413	49886.9	27472.7	0	16.89032	133.1022	0	1999.088	1771.181
27	38558.26	4065.189	19194.85	113041.4	0	16.00493	5104.93	0	209.8166	5775.544
28	19829.67	12142.94	31889.24	66129.04	0	17.71054	3096.172	0	1413.585	3716.636
29	10611.77	3573.316	14035.27	8263.63	0	9.124784	4847.861	0	2783.679	1233.325
30	26555.72	11893.47	23388.6	136078.5	0	25.59504	3620.563	0	1405.735	898.6151
31	10787.34	2788.457	7974.33	123339.2	0	27.48705	679.916	0	1862.449	5200.296
32	14877.32	8235.126	37052.38	30284.44	0	24.25995	4038.388	0	2096.853	5634.473
33	28355.74	13128.76	31375.98	9326.281	0	16.68041	3866.093	0	1918.274	334.8915
34	31724.93	4708.299	3835.367	51118.61	0	0.142526	5484.474	0	2050.426	2743.361
35	16900.45	5854.366	35554.5	106040.3	0	19.11486	1750.656	0	2114.979	3296.39
36	34117.63	3839.634	56477.07	47610.89	0	24.04839	3750.102	0	196.5228	340.3505
37	31401.61	2565.405	47700.59	132668.8	0	12.46075	5013.052	0	3090.708	1442.016
38	13038.68	5142.689	48440.2	45150.36	0	10.65963	2926.758	0	939.806	3923.917
39	25360.52	2130.384	21095.32	109093.5	0	11.93237	2051.534	0	1740.617	1364.339
40	32314.99	7075.293	33199.17	86884.36	0	15.06274	2428.773	0	2646.359	6464.854
41	19647.85	3547.114	17724.13	78201.46	0	8.170834	249.8784	0	392.4326	2293.215
42	15518.93	5657.801	54984.14	118672.1	0	12.98342	582.0042	0	2112.765	3159.412
43	12503.63	4324.469	15566.61	133950.7	0	11.2025	0.768605	0	2513.773	354.2542
44	14025.68	10979.53	51425.11	57178	0	24.95184	5440.096	0	20.25831	5570.335
45	8832.287	9367.267	47156.26	28121.44	0	18.76357	928.5287	0	1281.763	109.4371
46	44263.96	2227.692	3024.46	32570.28	0	22.66903	3605.315	0	2748.479	500.4277
47	47465.65	7941.049	49019.94	54511.63	0	20.86106	2594.611	0	3069.692	2092.36
48	50094.26	9676.154	2530.212	5145.713	0	13.0754	1843.223	0	3027.909	6323.843
49	9279.933	8079.044	31215.92	39096.73	0	17.04868	2659.494	0	865.7515	5914.812
50	26317.49	9382.636	33608.3	16335.12	0	5.595035	3958.344	0	2412.214	6707.238

Table E.1 50 Random Initial State Variables (Continued).

No.	cyM3p0	skM3p0	tkM3p0	ykM3p0
1	0.020669	0.019924	0.02196	0.036292
2	0.019883	0.020692	0.021377	0.03627
3	0.019883	0.021818	0.022158	0.036299
4	0.02035	0.021946	0.020196	0.036295
5	0.020447	0.021046	0.021066	0.036326
6	0.01987	0.019763	0.022692	0.036303
7	0.019794	0.020205	0.02132	0.03632
8	0.019825	0.022146	0.020084	0.036293
9	0.019912	0.019417	0.020923	0.036292
10	0.020947	0.021252	0.022279	0.03631
11	0.019851	0.02115	0.021039	0.036268
12	0.019813	0.021522	0.023702	0.036275
13	0.020701	0.01987	0.022044	0.036307
14	0.019914	0.022075	0.023503	0.036276
15	0.019963	0.02166	0.022891	0.036329
16	0.020274	0.021024	0.023505	0.036272
17	0.020073	0.020831	0.019936	0.036324
18	0.019913	0.022029	0.022217	0.036303
19	0.021124	0.021346	0.021656	0.036306
20	0.020918	0.020871	0.021004	0.03629
21	0.020538	0.02133	0.020197	0.036299
22	0.01989	0.021239	0.019861	0.036276
23	0.019924	0.020859	0.022432	0.036254
24	0.020457	0.019356	0.023773	0.036267
25	0.020668	0.020755	0.021382	0.036258
26	0.021132	0.019525	0.022147	0.036301
27	0.020449	0.021136	0.022228	0.036311
28	0.019937	0.019902	0.025004	0.036266
29	0.020835	0.02019	0.021494	0.036273
30	0.020558	0.022091	0.022739	0.036287
31	0.02054	0.021348	0.021143	0.036283
32	0.019891	0.019476	0.020315	0.036319
33	0.019897	0.021699	0.020801	0.036262
34	0.020656	0.022081	0.023424	0.036335
35	0.019821	0.019663	0.023679	0.036295
36	0.021103	0.01986	0.022379	0.03628
37	0.019789	0.021434	0.019923	0.0363
38	0.019971	0.021559	0.022385	0.03627
39	0.019862	0.02211	0.022333	0.036301
40	0.020928	0.02046	0.022375	0.036261
41	0.020296	0.021584	0.022295	0.036315
42	0.020216	0.02213	0.022913	0.036274
43	0.020103	0.02233	0.019963	0.036329
44	0.019858	0.019721	0.024165	0.036259
45	0.019871	0.020531	0.021648	0.036255
46	0.02041	0.02027	0.020242	0.036308
47	0.021099	0.019838	0.023862	0.036283
48	0.020133	0.019939	0.021941	0.036298
49	0.019936	0.022131	0.019765	0.036288
50	0.0204	0.019716	0.021571	0.036324

APPENDIX F

SOLUTION OF 50 HYPOTHETICAL SCENARIOS FOR LOW-VIF MODEL

Table F.1 Solution of 50 Hypothetical Scenarios for Low-VIF Model (Stage-1).

Scenario No.	Emission Reduction (gm-mol)									
	sq1_2p1	sq1_3p1	sq1_4p1	sq2_3p1	sq3_1p1	sq3_3p1	sq4_2p1	sq4_3p1	sq4_4p1	pt4p1
1	16224.96	0	45991.14	69954.95	20438.63	613487.5	26649.46	95389.34	0	91071.41
2	34150.39	0	45991.14	23428.79	12794.11	0	732.925	28430.87	67762.48	26800.85
3	12571.69	0	6698.946	23636.43	36326.04	45988.22	10866.42	63696.26	68102.32	21515.8
4	22485.12	24961.81	0	44916.06	26880.05	517724.2	50196.21	111085.3	35197.29	62372.13
5	23041.8	22500.85	5246.769	44879.84	27507.12	501264.6	49930.39	110706.5	35178.47	62186.57
6	32930.56	15013.98	38468.04	5848.532	0	0	0	27169.14	23247.54	51405.18
7	30988.54	0	42465.36	17445.72	12320.88	6095.139	696.8622	24713.06	54169.95	62325.15
8	12571.69	0	6698.946	23636.43	36326.04	45988.22	10866.42	63696.26	68102.32	21515.8
9	34150.39	0	45991.14	22095.57	9386.804	0	0	26100.06	65580.94	42958.42
10	908.7837	27281.25	44127.26	13246.3	1551.059	568271.7	22231.03	159363.3	50012.25	91861.22
11	34150.39	0	45991.14	23043.41	0	0	0	0	67128.8	50942.47
12	34150.39	0	45991.14	22994.79	656.4513	0	0	16835.31	67046.24	44209.22
13	23125.46	13581.91	4118.88	44834.25	28144.26	493733	50051.6	109864.9	35154.84	61910.82
14	12571.69	0	6698.946	23636.43	36326.04	45988.22	10866.42	63696.26	68102.32	21515.8
15	12571.69	0	6698.946	23636.43	36326.04	45988.22	10866.42	63696.26	68102.32	21515.8
16	34150.39	0	0	0	0	0	0	0	0	0
17	34150.39	0	45991.14	23394.62	1023.362	0	0	22843.86	67706.57	29495.96
18	13264.52	0	11368.98	23634.13	36091.36	44001.12	9385.634	63290.74	68098.61	21568.39
19	34150.39	29842.92	45991.14	81971.11	38938.39	636025.6	50196.21	181729.7	137092.9	155745.4
20	34150.39	29842.92	45991.14	81966.59	37346.32	635917.9	46830.24	177884.1	137088.3	155745.4
21	21694.12	22383.15	24072.31	44955.81	27340.17	524043	46588.27	111606.3	35217.89	62310.64
22	27305.09	0	36229.96	23520.86	21100.78	14115.56	2279.753	43908.48	67913.44	25473.89
23	34150.39	0	45991.14	5988.491	31306.54	9994.779	16.14527	0	18230.47	28561.02
24	26256.01	26555.75	45991.14	75195.76	1663.933	636025.6	44756.91	76283.32	18391.74	122066.1
25	34150.39	29842.92	45991.14	81966.92	37296.62	636025.6	47096.57	176866.2	137088.6	155745.4
26	34150.39	29842.92	45991.14	81967.25	37378.78	636025.6	47307.56	176412.6	137089	155745.4
27	124.2144	0	45831.74	13118.25	30.78396	556235.6	2062.923	148127	49596.3	103856.9
28	34150.39	0	45991.14	23428.62	4634.448	0	0	26799.12	67761.93	28681.96
29	34150.39	1353.338	45991.14	34528.73	0	563124.2	0	50420.89	20797.45	129910.2
30	0	24988.61	0	13532.46	4367.537	567531.8	43383.45	162576.5	50943.19	82011.49
31	34150.39	29842.92	13979.14	25150.59	7292.442	566054.5	2525.251	170402.6	70491.42	26940.67
32	34150.39	0	45991.14	23244.07	0	0	0	40.42485	67458.07	35172.86
33	13312.56	0	11256.31	23634.04	36037.05	44148.33	8790.824	63262.7	68098.48	21580.88
34	24605.94	0	35376.36	12869.63	28828.96	576128.9	6726.895	126054.9	48771.82	72923.64
35	34150.39	0	45991.14	23052.77	12217.45	0	0	21017.1	67144.05	33859.33
36	34150.39	29842.92	45991.14	81675.67	8778.734	636025.6	0	69779.84	136797.4	155311.2
37	34150.39	0	45991.14	23181.97	12592.55	0	0	28026.25	67356.42	38891.56
38	16464.9	0	30288.12	23623.86	34695.16	36291.7	0	61417.54	68081.86	21883.79
39	34150.39	0	38279.56	15932.29	0	0	12613.93	0	21630.04	62500.87
40	3771.155	0	17888.2	12836.94	1341.463	566068.5	40410.11	135623	48675.38	93816.46
41	34150.39	29842.92	0	0	0	18802.27	0	0	0	155745.4
42	18158.02	0	45991.14	23618.6	34544.44	27554.31	134.5439	60426.95	68073.34	21915
43	34150.39	0	0	0	0	39.51261	50196.21	0	0	155745.4
44	34150.39	0	45991.14	23428.38	13039.72	0	0	28348.2	67762.89	26751.06
45	30183.99	0	41018.43	23397.82	16006.84	7510.583	1348.306	28186.86	67712.06	27463.78
46	34150.39	0	45991.14	0	0	74640.6	0	0	0	155745.4
47	34150.39	29842.92	45991.14	81922.4	19227.88	636025.6	0	139299.6	137044.2	155745.4
48	34150.39	0	45991.14	22463.94	0	0	0	0	66155.96	43682.05
49	12571.69	0	6698.946	23636.43	36326.04	45988.22	10866.42	63696.26	68102.32	21515.8
50	34150.39	0	8297.991	0	0	65.00462	40490.94	0	0	118588.4

Table F.1 Solution of 50 Hypothetical Scenarios for Low-VIF Model (Stage-1) (Continued).

Scenario No.	Emission Reduction (gm-mol)						
	pt5p1	sq2_4p1	sq3_4p1	sq3_2p1	sq3_5p1	sq5_4p1	pt6p1
1	0	0	6617.911	71.20754	22570.16	27217.08	39665.83
2	12543.52	0	7132.786	49088.49	11852.79	30405.72	31945.22
3	12741.22	66614.84	7146.73	55653.66	19097.95	23651.24	32572.81
4	24618.76	55834.7	95846.87	135209.9	0	39837.54	20149.3
5	24582.56	57896.37	95810.67	130982.7	2175.555	29927.78	20173.28
6	3943.876	0	6609.826	90733.86	22570.16	48686.78	5602.318
7	9177.69	8840.272	6416.836	71230.44	1584.502	40203.43	23340.79
8	12741.22	66614.84	7146.73	55653.66	19097.95	23651.24	32572.81
9	11273.36	0	7043.38	19043.05	0	33065.15	28067.73
10	28531.06	69551.19	108594.4	74413.53	3802.145	0	23840.42
11	12177.87	0	7106.773	105510.8	0	0	31598.93
12	12132.97	0	7103.492	137147.9	22570.16	11987.05	31516.34
13	24536.92	56187.29	95765.08	146049.1	0	39016.65	20133.3
14	12741.22	66614.84	7146.73	55653.66	19097.95	23651.24	32572.81
15	12741.22	66614.84	7146.73	55653.66	19097.95	23651.24	32572.81
16	0	0	0	16172.39	22570.16	48686.78	0
17	12510.93	0	7130.443	61584.03	5089.752	34029.18	31806.18
18	12739.07	65274.51	7146.496	56170.88	22570.16	24938.75	32566.13
19	45683.38	72658.77	116942.4	275446.2	22570.16	48686.78	51682
20	45678.85	72658.77	116937.9	265679.2	22570.16	48686.78	51677.44
21	24658.5	51644.08	95886.71	129173.8	683.0074	34515.76	20223.92
22	12631.04	20952.37	7138.997	83616.41	3846.72	29044.3	32211.97
23	1725.578	0	17152.93	26805.22	22570.16	36097.35	0
24	41385.76	19221.67	23723.5	258360.3	8502.143	48686.78	12709.27
25	45679.17	72658.77	116938.2	266060.1	22570.16	48686.78	51673.61
26	45679.49	72658.77	116938.6	266218.5	22570.16	48686.78	51674.23
27	28038.2	1351.832	108101.6	69843.55	22570.16	0	22983.26
28	12543.48	0	7132.786	61940.9	4177.809	34644.06	32232.32
29	40697.71	0	24953.03	0	22570.16	0	38675.59
30	29636.52	69747.11	109700	170208.4	22570.16	48686.78	25483.47
31	13517.98	0	9739.618	117463.2	22526.76	31790.86	32705.59
32	12368.57	0	7120.248	67149.81	0	15382.53	31928.24
33	12738.98	65359.7	7146.496	57226.57	20551.96	13033.96	32565.77
34	27038.29	837.6144	107101.7	212619.6	0	16871.73	22534.65
35	12186.8	0	7107.476	64712.75	1728.901	32574.48	30725.26
36	45387.9	72658.77	116646.9	271756.1	22570.16	12279.17	51091.02
37	12309.43	0	7116.147	106010.1	0	48686.78	31123.59
38	12729.23	65213.87	7145.793	59545.23	15188.27	21546	32552.31
39	0	0	18688.76	45976.33	22570.16	48686.78	0
40	26936.17	72658.77	106999.6	177945.1	2978.175	8739.326	22888.65
41	0	0	0	0	0	0	0
42	12724.24	59394.54	7145.441	63437.63	21378.74	36063.49	32519.78
43	0	0	0	0	22570.16	48686.78	0
44	12542.65	0	7132.786	64347.6	0	27458.61	31960.4
45	12513.95	11577.93	7130.677	80020.99	2790.92	33603.25	31803.64
46	0	72658.77	0	0	0	48686.78	0
47	45634.72	72658.77	116893.8	235550.1	22570.16	37336.08	51633.32
48	11637.96	0	7067.167	87347.36	2628.067	14420.46	30624.74
49	12741.22	66614.84	7146.73	55653.66	19097.95	23651.24	32572.81
50	0	59861.14	0	35270.36	22570.16	39273.35	0

Table F.2 Solution of 50 Hypothetical Scenarios for Low-VIF Model (Stage-2).

Scenario No.	Emission Reduction (gm-mol)								
	sq1_3p2	sq1_4p2	sq3_2p2	sq3_3p2	sq4_2p2	sq4_3p2	sq2_4p2	sq3_4p2	pt5p2
1	451.6904	0	222650.1	324116.1	0	127948.1	29122.88	43136.5	5919.889
2	11788.11	38690	204039	483529.8	38962.87	120729.6	47787.44	46052.52	6165.654
3	11792.97	17657.49	183311.5	463418.1	23749.66	109304.3	31992.56	46057.37	6166.524
4	5640.689	27174.07	222650.1	162605.5	39352.89	130921.6	37688.67	68398.37	17113.14
5	20966.45	1637.347	152317.2	400913.7	38018.28	86658.38	14058.11	36486.1	24395.15
6	23306.12	38690	222650.1	486464.7	39352.89	141864.6	55934.29	93096.06	45683.38
7	11788.56	35804.96	201944.1	477032.3	39352.89	121713.1	45987.57	46052.98	6155.95
8	11798.29	5612.92	174609.2	450126.1	2755.924	100458.3	19758.48	46062.68	6167.439
9	23306.12	38690	222650.1	486464.7	39352.89	141864.6	55934.29	93096.06	45683.38
10	20966.45	1637.347	152317.2	400913.7	38018.28	86658.38	14058.11	36486.1	24395.15
11	11792.97	21007.2	188492.3	468507.9	22680.71	111052.1	34383.56	46057.37	6161.168
12	11792.97	19572.8	186997.5	468092.6	22654.57	111058.4	34383.56	46057.37	6161.168
13	20966.45	1637.347	152317.2	400913.7	38018.28	86658.38	14058.11	36486.1	24395.15
14	11792.97	16750.41	182363.8	463319.1	24262.87	109304.3	31992.56	46057.37	6161.168
15	11792.97	17466.13	182932.9	463031.1	23432.28	109304.3	31992.56	46057.37	6166.524
16	23306.12	38690	222650.1	486464.7	39352.89	141864.6	55934.29	93096.06	45683.38
17	11792.97	22195.42	189180.1	467566.2	21204.54	111040.3	34383.56	46057.37	6161.168
18	11792.97	17271.13	182967.3	463412.7	24299.78	109378.9	32095.86	46057.37	6166.524
19	18191.9	38690	59014.99	147769.8	39352.89	141864.6	55934.29	25530.99	41894.04
20	20966.45	1637.347	152317.2	400913.7	38018.28	86658.38	14058.11	36486.1	24395.15
21	14873.58	23270.33	108719.3	383064.2	21932.25	127958	55934.29	23637.73	35254.02
22	11792.97	20097.09	186754.4	463467.3	22034.11	110502.7	33649.69	46057.37	6166.524
23	23306.12	38690	222650.1	486464.7	39352.89	141864.6	55934.29	93096.06	45683.38
24	294.3858	0	222650.1	394296.2	62.2233	15132.03	3937.258	10905.77	1820.332
25	20966.45	1637.347	152317.2	400913.7	38018.28	86658.38	14058.11	36486.1	24395.15
26	77.60145	0	222650.1	400287.8	0	7864.53	718.9069	11389.25	5697.651
27	20966.45	1637.347	152317.2	400913.7	38018.28	86658.38	14058.11	36486.1	24395.15
28	8482.192	38690	222650.1	463602.3	39352.89	139548.1	55934.29	32537.73	22478.24
29	20966.45	1637.347	152317.2	400913.7	38018.28	86658.38	14058.11	36486.1	24395.15
30	5639.732	35325.87	173786.7	158399.3	39352.89	125720.5	20443.65	68396.41	17111.4
31	5398.38	0	109623.9	424759.3	0	54381.19	25581.64	29548.21	15559.86
32	23306.12	38690	222650.1	486464.7	39352.89	141864.6	55934.29	93096.06	45683.38
33	11792.97	18002.37	183827.3	463684.7	21865.69	109373.5	32088.23	46057.37	6166.524
34	23210.28	0	162531.5	154704.1	20078.65	141853.4	55923.13	93000.26	45491.72
35	23306.12	38690	222650.1	486464.7	39352.89	141864.6	55934.29	93096.06	45683.38
36	20966.45	1637.347	152317.2	400913.7	38018.28	86658.38	14058.11	36486.1	24395.15
37	11792.97	20107.72	186853.4	467043.2	21982.14	111098.9	34383.56	46057.37	6161.168
38	8492.046	38690	222650.1	438595.2	39352.89	130109.3	55934.29	32547.06	22499.93
39	23306.12	38690	222650.1	486464.7	39352.89	141864.6	55934.29	93096.06	45683.38
40	20966.45	1637.347	152317.2	400913.7	38018.28	86658.38	14058.11	36486.1	24395.15
41	23306.12	38690	222650.1	486464.7	39352.89	141864.6	55934.29	93096.06	45683.38
42	11792.97	17987.21	183842.5	463064.2	24877.14	109997.4	32950.96	46057.37	6166.524
43	11793.69	19012.61	185141.1	464620.1	16965.04	141864.6	32417.06	46058.11	6166.615
44	23306.12	38690	222650.1	486464.7	39352.89	141864.6	55934.29	93096.06	45683.38
45	11789.23	33666.78	200353.6	475966.7	39352.89	118007.3	44012.33	46053.63	6156.774
46	23306.12	38690	222650.1	486464.7	39352.89	141864.6	55934.29	93096.06	45683.38
47	20966.45	1637.347	152317.2	400913.7	38018.28	86658.38	14058.11	36486.1	24395.15
48	11788.02	38690	207468.2	485213.5	39260.46	121143.4	47993.41	46052.42	6155.355
49	11792.97	17166.07	183121.2	464014.2	21786.71	109304.3	31992.56	46057.37	6166.524
50	23306.12	38690	222650.1	486464.7	39352.89	141864.6	55934.29	93096.06	45683.38

Table F.3 Solution of 50 Hypothetical Scenarios for Low-VIF Model (Stage-3).

Scenario No.	Emission Reduction (gm-mol)								
	sq1_3p3	sq3_2p3	sq3_3p3	sq4_2p3	sq4_3p3	sq1_4p3	pt3p3	pt4p3	pt6p3
1	12063.85	209497.1	403360.6	40497.59	79937.22	19833.78	75395.22	77847.88	51682
2	0	201821.3	497934.8	40497.59	145179.9	2842.931	10797	15323.29	51682
3	2.882877	210800.6	497934.8	40497.59	145179.9	3.422533	0	2302.941	51682
4	12052.24	128651	497934.8	40497.59	145179.9	19822.2	75383.58	77836.18	51682
5	12070.17	201521	342956.9	40497.59	78368.47	19840.11	75401.42	77854.12	51682
6	12042.7	161654.4	497934.8	40497.59	145179.9	19812.65	75374.06	77826.66	51682
7	12043.18	186033.9	497934.8	40497.59	145179.9	19813.13	75374.51	77827.12	51682
8	0	226875.3	497934.8	40497.59	145179.9	0	0	0	51682
9	3421.418	196184.4	497934.8	40497.59	145179.9	2960.491	21345.83	26245.91	51682
10	12067.29	214732.1	352667.6	40497.59	79087.82	19837.24	75398.55	77851.31	48254.26
11	912.4186	209042.7	497934.8	40497.59	145179.9	1498.871	5692.472	10591	51682
12	11505.22	210665.8	497934.8	40497.59	145179.9	0	46984.85	49414.2	51682
13	12070.15	196303.5	352067.4	40497.59	78258.93	19840.11	75401.42	77854.12	51682
14	12043.26	226875.3	497934.8	40497.59	145179.9	19813.21	75374.51	77827.28	51682
15	10.65938	212955.5	497934.8	40497.59	145179.9	219.6789	0	2141.109	51682
16	12043.14	170185.8	497934.8	40497.59	145179.9	19813.09	75374.36	77827.12	51682
17	1322.538	210545.8	497934.8	40497.59	145179.9	2172.592	8251.16	12590.25	51682
18	0	212992.5	497934.8	40497.59	145179.9	0	0	0	51682
19	24177.41	226875.3	497934.8	40497.59	145179.9	39717.31	150840	155745.4	51682
20	12084.73	128724.2	274823.6	40497.59	74108.35	19854.67	75416.08	77868.79	28292.89
21	12067.31	226875.3	353855	40497.59	80001.52	19837.28	75398.55	77851.31	51682
22	0	193688.1	497934.8	40497.59	145179.9	0	0	4730.103	51682
23	12043.01	165437.1	497934.8	40497.59	143478.6	19812.97	75374.36	77826.97	51682
24	12056.85	119604.9	420360.8	40497.59	78022.54	19826.78	75388.12	77840.86	51682
25	12084.63	128378	276235.1	40497.59	74114.61	19854.59	75415.93	77868.64	28819.08
26	12060.19	119689.5	365907.8	40497.59	77135.89	19830.12	75391.44	77844.13	51682
27	12066.61	223068.2	357524.2	40497.59	79361.45	19836.57	75397.94	77850.53	51682
28	0	206603.4	497934.8	40497.59	145179.9	55.59627	0	2167.171	51682
29	100.1013	209795.8	497934.8	40497.59	145179.9	0	0	1184.32	203.1548
30	24177.41	226875.3	497934.8	40497.59	145179.9	39717.31	150840	155745.4	51682
31	12044.44	226875.3	430352.4	40497.59	85970.04	19814.4	75375.72	77828.37	28336.7
32	12044.37	162781.9	497934.8	40497.59	145179.9	19814.32	75375.72	77828.37	51682
33	163.3792	212458.3	497934.8	40497.59	145179.9	656.9672	2127.63	4257.561	51682
34	12034.85	202178.9	497934.8	11856.87	145179.9	19804.81	75366.2	77818.85	51682
35	12044.3	158429	497934.8	40497.59	145179.9	19814.24	75375.57	77828.22	51682
36	12067.97	150639.8	357627.5	40497.59	78878.2	19837.92	75399.3	77851.94	46067.67
37	94.96537	210029.5	497934.8	40497.59	145179.9	0	0	2092.731	51682
38	4.869398	207004	497934.8	40497.59	145179.9	73.78345	0	2186.522	51682
39	12048.95	167390.8	497934.8	40497.59	145179.9	19818.9	75380.26	77832.9	51682
40	12072.06	180618.7	330269.5	40497.59	77448.36	19842.02	75403.38	77855.99	51682
41	12042.84	171174.5	497934.8	40497.59	145179.9	19812.77	75374.21	77826.81	51682
42	2226.575	202817	497934.8	40497.59	145179.9	3657.693	13891.34	16968.76	51682
43	0	214716.1	497934.8	40497.59	145179.9	0	76760.19	81665.67	51682
44	12044.35	162608.2	497934.8	40497.59	145179.9	19814.28	75375.57	77828.37	51682
45	12043.3	187344.5	497934.8	40497.59	145179.9	19813.24	75374.67	77827.28	51682
46	12042.19	167903.4	497934.8	40497.59	128592.3	19812.13	75373.46	77826.19	51682
47	12070.7	160715.3	345792.8	40497.59	78459.82	19840.66	75402.02	77854.75	43976.25
48	0	207692.1	497934.8	40497.59	145179.9	0	0	2735.376	51682
49	12043.35	226875.3	497934.8	40497.59	145179.9	19813.32	75374.67	77827.28	51682
50	12044.15	158841.2	497934.8	40497.59	145179.9	19814.12	75375.42	77828.22	51682

Table F.4 Solution of 50 Hypothetical Scenarios for Low-VIF Model (Stage-4).

Scenario No.	Emission Reduction (gm-mol)		
	sq1_3p4	sq1_4p4	sq3_3p4
1	0	4.31924064	656174.6208
2	0	0	563811.7968
3	0	0	477418.9783
4	0	0	225499.8656
5	0	0	528514.4676
6	0	0	406142.5032
7	0	0	558761.6192
8	0	0	506741.042
9	0	0	409621.9382
10	0	0	454525.1904
11	0	0	592445.4689
12	0	0	589422.3317
13	0	0	535253.0785
14	0	0	472927.6669
15	0	0	477962.7222
16	0	0	407498.9043
17	0	0	598128.809
18	0	0	476201.3076
19	0	0	224407.1179
20	0	0	515910.392
21	0	0	460015.2286
22	0	0	558242.2024
23	0.95873762	0	369776.7535
24	0	0	656174.6208
25	0	0	516183.9076
26	0	0	525436.7588
27	0	0	566178.1018
28	0	0	605228.3817
29	0	0	558265.2145
30	0	0	209183.6037
31	0	1.3497627	651277.6383
32	0	0	404707.2034
33	0	0	480451.9778
34	0	0	160234.8179
35	0	0	403468.493
36	0	0	417290.2394
37	0	0	592693.3424
38	0	0	481041.746
39	0	0	353008.1387
40	0	0	490385.9882
41	0.86595656	0	398313.1171
42	0	0	485293.7312
43	0	2.74451749	608323.1852
44	0	0	402628.8788
45	0	0	552696.9351
46	0	0	282958.5392
47	0	0	433991.1327
48	0	0	572085.6459
49	0	0	472816.5511
50	0	0	325616.4645

APPENDIX G

SOLUTION OF 50 HYPOTHETICAL SCENARIOS FOR HIGH-VIF MODEL

Table G.1 Solution of 50 Hypothetical Scenarios for High-VIF Model (Stage-1).

Scenario No.	Emission Reduction (gm-mol)									
	sq1_2p1	sq1_3p1	sq1_4p1	sq2_3p1	sq3_1p1	sq3_3p1	sq3_4p1	sq4_2p1	sq4_3p1	sq4_4p1
1	34150.4	29842.9	45991.1	81953.0	38938.4	636025.6	116942.4	50196.2	181727.2	137092.6
2	34150.4	0.0	10844.6	0.0	38938.4	636025.6	3032.4	50196.2	13412.3	0.0
3	34150.4	29842.9	5782.3	0.0	38938.4	636025.6	39896.2	50196.2	7245.3	578.7
4	31606.8	0.0	41189.8	0.0	12132.8	532047.5	41225.5	50196.2	12513.7	99587.3
5	34150.4	29842.9	7200.5	1775.6	38938.4	633528.0	67368.0	50196.2	33223.2	57261.5
6	34150.4	0.0	4441.8	29627.8	38938.4	636025.6	98713.5	50196.2	15890.4	4461.3
7	34150.4	29842.9	45991.1	81952.8	38938.4	636025.6	116942.4	50196.2	181724.4	137092.5
8	0.0	0.0	0.0	0.0	38938.4	636025.6	22340.5	50196.2	13819.7	0.0
9	34150.4	29842.9	26863.3	0.0	38938.4	636025.6	38112.3	50196.2	43967.8	5728.4
10	34147.5	29842.9	5016.0	0.0	38938.4	636019.2	10010.9	50196.2	15148.0	0.0
11	34150.4	0.0	10028.4	0.0	38938.4	636025.6	116942.4	50196.2	15710.2	0.0
12	34150.4	29842.9	45991.1	0.0	38938.4	636025.6	0.0	50196.2	68265.4	0.0
13	34150.4	29842.9	45991.1	81463.6	38938.4	636025.6	116941.5	50196.2	179997.3	137079.5
14	34150.4	0.0	0.0	59225.2	38938.4	636025.6	116942.4	50196.2	26217.3	0.0
15	34150.4	29842.9	10562.6	0.0	38938.4	635912.8	106161.2	50196.2	8430.8	0.0
16	34150.4	29842.9	44417.5	0.0	38938.4	636025.6	28769.1	50196.2	14785.8	0.0
17	33405.9	29842.9	20719.9	0.0	38938.4	636025.6	23495.7	50196.2	23721.2	22151.5
18	34150.4	29842.9	45991.1	81953.5	38938.4	636025.6	116942.4	50196.2	181729.7	137092.6
19	34150.4	29842.9	45991.1	0.0	38938.4	636025.6	116942.4	50196.2	22092.9	0.0
20	33640.4	0.0	33262.1	0.0	38938.4	636025.6	52279.1	50196.2	17409.1	69349.6
21	34150.4	29842.9	5175.9	0.0	38938.4	636025.6	18793.9	50196.2	13560.2	0.0
22	34150.4	0.0	0.0	0.0	38938.4	636025.6	0.0	50196.2	16028.6	0.0
23	34150.4	29842.9	6044.2	0.0	38938.4	636025.6	36850.0	50196.2	13653.8	9223.3
24	34150.4	0.0	10983.0	33087.1	38938.4	636025.6	68615.9	50196.2	34357.7	20507.3
25	34150.4	29842.9	45991.1	0.0	38938.4	636025.6	6717.7	50196.2	14980.3	0.0
26	34150.4	29842.9	8079.6	0.0	38938.4	636025.6	103584.6	50196.2	12371.5	28130.3
27	34150.4	29842.9	37762.7	0.0	38938.4	636025.6	51516.9	50196.2	49415.9	12068.4
28	34150.4	29842.9	45991.1	0.0	38938.4	636025.6	0.0	50196.2	54210.8	0.0
29	34150.4	29842.9	1186.9	0.0	38938.4	636025.6	82495.0	50196.2	14508.0	0.0
30	34150.4	29842.9	45991.1	0.0	38938.4	636025.6	86235.9	50196.2	22592.8	0.0
31	34150.4	0.0	37432.7	40872.7	38938.4	636025.6	5124.5	50196.2	34626.1	3100.7
32	34150.4	0.0	13814.1	38868.4	34041.0	636025.6	47073.0	50196.2	22839.1	87761.7
33	34150.4	0.0	8948.3	0.0	38938.4	636025.6	72077.7	50196.2	44079.7	20936.2
34	34150.4	29842.9	14693.6	0.0	26776.9	453681.3	30244.0	50196.2	65434.7	20765.0
35	34095.4	29842.9	6472.2	0.0	38938.4	634750.4	38677.0	50196.2	30522.8	75.6
36	34150.4	29842.9	45991.1	81950.7	38938.4	636025.6	116942.4	50196.2	181711.0	137092.5
37	0.0	0.0	43513.2	0.0	38938.4	636025.6	30978.0	50196.2	20443.5	3577.2
38	0.0	0.0	3213.6	12257.8	38938.4	636025.6	25757.2	50196.2	181729.7	6308.6
39	26794.5	29842.9	45991.1	0.0	38938.4	635194.6	60236.4	50196.2	14810.1	0.0
40	34150.4	0.0	35602.5	8176.2	38938.4	636025.6	91830.4	50196.2	95972.8	21699.3
41	34150.4	29842.9	3636.8	0.0	38938.4	636025.6	4960.3	50196.2	20102.1	0.0
42	0.0	0.0	25648.4	0.0	17135.2	527582.0	41285.7	50196.2	59311.6	93486.2
43	34150.4	29842.9	9050.7	0.0	38938.4	636025.6	43501.3	50189.9	24185.3	2.1
44	34150.4	29842.9	3722.7	0.0	38938.4	636025.6	60727.6	50196.2	16056.9	21632.1
45	34150.4	29842.9	45991.1	81953.6	38938.4	636025.6	116942.4	50196.2	181729.7	137092.5
46	34150.4	29842.9	0.0	0.0	38938.4	636025.6	0.0	50196.2	42444.1	0.0
47	34150.4	29842.9	45991.1	0.0	38938.4	636025.6	107283.8	50196.2	4280.1	0.0
48	34150.4	29842.9	45991.1	81953.7	38938.4	636025.6	116942.4	50196.2	181729.7	137092.5
49	30929.5	29842.9	3776.0	0.0	38938.4	636025.6	32183.0	50196.2	46462.4	8997.7
50	34150.4	29842.9	45991.1	81953.0	38938.4	636025.6	116942.4	50196.2	181729.7	137092.5

Table G.1 Solution of 50 Hypothetical Scenarios for High-VIF Model (Stage-1) (Continued).

Scenario No.	Emission Reduction (gm-mol)									
	sq5_3p1	pt1p1	pt4p1	pt5p1	pt12p1	sq2_1p1	sq2_2p1	sq2_4p1	sq3_2p1	sq3_5p1
1	21842.2	132342.2	155745.2	45683.4	58009.5	32978.8	48233.5	72658.8	275445.7	21253.5
2	0.0	24000.5	0.0	45683.4	17743.7	3918.6	11836.7	64408.4	78525.4	18707.5
3	14607.7	71502.7	0.0	45683.4	23618.7	16525.3	31050.4	20944.7	81373.9	19043.3
4	19109.8	73762.7	29660.8	45683.4	56844.1	4199.9	12789.0	66196.1	23778.6	19062.1
5	21842.2	99469.7	6741.4	45683.4	58009.5	4177.4	12712.9	66055.9	110262.4	18423.4
6	0.0	132342.2	21541.2	45683.4	39385.0	813.9	7820.8	22493.0	42688.9	17323.5
7	21842.2	132342.2	155745.2	45683.4	58009.5	32978.8	48233.5	72658.8	275445.7	21221.3
8	0.0	130563.8	0.0	45683.4	18853.4	16646.9	33504.3	19317.8	10412.3	16288.9
9	13721.0	65500.0	2246.4	45683.4	27725.7	14364.6	26989.3	18426.6	71345.5	17261.1
10	21764.1	6574.1	1887.5	45683.4	56882.4	22471.7	4778.7	42665.3	79733.7	18883.3
11	0.0	132342.2	0.0	45683.4	1992.9	6246.2	5185.6	7403.8	85429.4	18336.5
12	21842.2	0.0	0.0	45683.4	58009.5	2602.9	9219.1	4608.9	227739.9	18048.3
13	21842.2	132341.3	155740.2	45683.4	58009.5	32978.8	48233.5	72658.8	275426.3	19374.8
14	0.0	26017.2	0.0	45683.4	0.0	740.6	5335.0	15607.4	0.0	22570.2
15	20761.6	76431.5	80263.6	45683.4	29015.0	29493.5	4886.6	49687.0	43000.2	18529.6
16	21842.2	20115.1	0.0	45683.4	57546.7	23934.9	3180.1	44128.4	13244.3	19699.4
17	15525.5	55326.6	6197.5	45683.4	25565.1	16444.8	30961.2	20895.4	58835.1	18893.6
18	21842.2	132342.2	155745.2	45683.4	58009.5	32978.8	48233.5	72658.8	275445.7	21282.5
19	21842.2	132342.2	0.0	45683.4	58009.5	924.7	2563.3	13516.7	35958.1	18571.4
20	13674.6	84624.9	18516.4	45683.4	55093.5	4188.0	12749.0	66122.5	77785.1	18170.4
21	21842.2	0.0	63226.9	45683.4	29379.7	29424.9	2968.8	49618.4	43102.4	18869.0
22	0.0	0.0	0.0	45683.4	0.0	1784.7	4641.6	41355.3	108352.5	18657.8
23	21842.2	40055.9	1987.9	45683.4	55108.6	12201.1	36116.5	3152.5	79559.0	19988.1
24	0.0	132342.2	25459.4	45683.4	41139.5	815.0	7859.6	22593.7	61554.2	19448.5
25	21842.2	7602.4	0.0	45683.4	58009.5	2640.1	12156.5	1097.8	80727.8	18770.4
26	21842.2	81159.3	0.0	45683.4	45337.1	24977.5	27055.9	3669.5	55676.0	19157.8
27	14028.0	82936.4	623.6	45683.4	23407.3	16537.3	31074.8	20952.1	77068.1	19205.9
28	21842.2	0.0	0.0	45683.4	58009.5	15624.7	9610.7	30475.0	0.0	18315.3
29	13018.6	53098.1	134328.8	45683.4	17840.2	29819.7	3169.0	50013.2	157930.0	21117.7
30	21842.2	56827.2	53113.9	45683.4	31423.4	29355.4	3675.2	49548.9	0.0	12582.1
31	0.0	116461.9	0.0	45683.4	11269.8	29021.5	5787.7	18259.4	85010.2	19210.2
32	16688.8	79509.8	24417.5	45683.4	56108.3	4195.0	12772.6	66165.9	45684.1	19041.4
33	4541.8	104096.1	0.0	45683.4	52491.9	3948.4	11938.5	64616.4	62657.4	18230.2
34	7964.4	62034.9	10769.2	45683.4	21652.0	16592.8	31106.1	20986.2	111403.6	17159.8
35	21787.5	63844.9	13.9	45683.4	18358.2	7093.0	21430.8	15118.2	73186.2	19337.7
36	21842.2	132342.2	155745.2	45683.4	58009.5	32978.8	48233.5	72658.8	275445.4	21057.5
37	0.0	68865.7	0.0	45683.4	37652.9	20328.7	38724.4	19556.3	57606.1	18755.8
38	201.4	36669.5	88.3	45683.4	31754.9	12048.5	33520.4	19508.5	68254.1	19791.2
39	20328.8	54157.0	33548.8	45683.4	47087.6	25515.1	20398.5	45708.6	89594.0	20134.2
40	2991.7	123846.6	0.0	45683.4	40218.9	2446.6	7744.2	30123.0	93835.5	17497.6
41	21842.2	18461.7	0.0	45683.4	58009.5	4030.9	12217.2	65127.3	82741.5	18790.9
42	19482.7	11908.4	28203.8	45683.4	51675.4	21008.0	37800.1	67477.4	55977.7	19151.1
43	16363.9	14865.4	44860.4	45683.4	31152.8	29307.4	3175.7	49500.9	3780.6	18927.1
44	21842.2	132342.2	29878.3	45683.4	21795.2	28889.0	28805.9	48356.5	85053.0	18774.8
45	21842.2	132342.2	155745.2	45683.4	58009.5	32978.8	48233.5	72658.8	275445.7	21282.6
46	21842.2	0.0	0.0	45683.4	58009.5	0.0	0.0	2590.3	275446.2	18971.3
47	21842.2	77506.4	113654.2	45683.4	23087.8	29699.3	4339.9	49892.8	69460.2	19244.7
48	21842.2	132342.2	155745.2	45683.4	58009.5	32978.8	48233.5	72658.8	275445.7	21282.8
49	10017.1	63932.5	6982.3	45683.4	22245.9	16573.2	31079.5	20974.1	100484.9	3820.1
50	21842.2	132342.2	155745.2	45683.4	58009.5	32978.8	48233.5	72658.8	275445.7	21281.6

Table G.1 Solution of 50 Hypothetical Scenarios for High-VIF Model (Stage-1) (Continued).

Scenario No.	Emission Reduction (gm-mol)								
	sq5_4p1	sq5_5p1	pt2p1	pt3p1	pt6p1	pt15p1	pt30p1	pt63p1	pt64p1
1	48686.8	40472.2	134419.1	150840.0	51682.0	137312.2	5520.0	3141.5	6705.8
2	14826.7	42486.7	15785.9	112896.2	44519.4	5800.8	1983.9	3141.5	6705.8
3	10391.1	17813.0	134089.4	21159.0	40265.1	126546.8	3022.6	3141.5	6705.8
4	16112.1	32347.5	16040.5	114683.9	46307.0	5837.3	3771.5	3141.5	6705.8
5	16009.5	33383.9	16020.4	114543.8	46166.9	5834.4	3631.4	3141.5	6705.8
6	11164.7	36763.0	69201.2	98170.9	40775.7	60065.3	428.6	3141.5	6705.8
7	48686.8	40363.3	134419.1	150840.0	51682.0	137312.2	5520.0	3141.5	6705.8
8	32922.8	0.0	63592.2	82313.9	37348.3	32085.0	226.0	3141.5	6705.8
9	9028.2	16846.0	129980.3	20369.4	36156.1	122454.2	2642.0	3141.5	6705.8
10	4551.6	39641.9	46828.8	19917.8	27622.2	35816.8	1119.2	0.0	6705.8
11	11192.6	8803.6	40289.8	20311.4	18955.8	41485.1	20.2	3141.5	6705.8
12	2659.1	42615.6	8438.4	1581.3	9116.5	8576.1	168.9	3141.5	6705.8
13	48686.7	31612.2	134419.1	150840.0	51681.9	137312.2	5519.9	3141.5	6705.8
14	6776.0	0.0	58656.0	87629.6	30230.4	50055.9	0.0	3141.5	6705.8
15	5422.9	34783.9	52981.9	18237.4	34643.8	41064.3	4868.5	0.0	6705.8
16	4820.4	39301.9	48355.2	10894.8	29086.0	39424.4	1650.4	0.0	6705.8
17	10359.6	22451.8	134008.9	21139.8	40184.6	126487.9	2942.1	3141.5	6705.8
18	48686.8	40556.8	134419.1	150840.0	51682.0	137312.2	5520.0	3141.5	6705.8
19	3023.3	43948.7	5314.5	33442.7	6494.5	3946.4	1030.9	3141.5	6705.8
20	16058.2	31449.8	16030.0	114610.3	46233.5	5835.8	3698.0	3141.5	6705.8
21	5414.1	290.3	52921.3	9059.3	34575.8	43512.0	4799.9	0.0	6705.8
22	5163.1	40385.3	12897.6	89843.1	21467.4	5356.7	1307.6	3141.5	6705.8
23	30408.3	30638.4	81609.8	63495.8	7734.2	58895.9	562.9	3141.5	6705.8
24	11230.5	28931.7	69348.8	98319.6	40923.2	60203.3	439.2	3141.5	6705.8
25	3892.7	41962.3	7626.6	6810.8	6422.8	5964.6	3420.2	3141.5	6705.8
26	47106.5	16434.6	101697.5	65680.1	12770.6	81741.4	4237.7	3141.5	6705.8
27	10395.8	15965.7	134101.5	21166.9	40277.2	126527.7	3034.6	3141.5	6705.8
28	3420.5	44519.8	37411.6	65351.2	15740.2	22188.0	937.4	0.0	6705.8
29	5464.8	32128.4	53271.6	10020.6	34974.2	43541.7	5194.6	0.0	6705.8
30	5405.4	0.0	52860.0	12595.0	34502.2	42527.6	4730.4	0.0	6705.8
31	30996.4	37208.5	61681.9	61568.7	44975.1	2590.1	190.4	3141.5	6705.8
32	16090.0	34600.8	16036.1	114653.7	46276.9	5836.6	3741.4	3141.5	6705.8
33	14965.3	35773.4	15814.9	113104.2	44727.3	5805.1	3443.2	3141.5	6705.8
34	10417.5	16145.4	134157.0	21166.7	40332.7	126643.8	3090.1	3141.5	6705.8
35	6727.8	14379.9	124248.1	19373.7	30423.8	116259.8	893.8	3141.5	6705.8
36	48686.8	39851.2	134419.1	150840.0	51682.0	137312.2	5520.0	3141.5	6705.8
37	33351.3	42550.5	64017.8	26260.5	48519.5	71420.5	234.8	3141.5	6705.8
38	33266.6	42963.2	63933.5	36930.7	24702.5	5817.5	232.9	3141.5	6705.8
39	4915.0	39276.5	49456.3	74501.5	30667.6	24166.7	3059.5	0.0	6705.8
40	10021.4	38005.8	6808.0	48367.3	22685.9	4250.6	3768.4	3141.5	6705.8
41	15340.6	42472.9	15888.1	113615.2	45238.3	5815.5	2702.8	3141.5	6705.8
42	41253.9	36042.3	18032.6	117612.1	21533.2	76853.7	3616.2	3141.5	6705.8
43	5399.1	24586.5	52816.9	10117.0	34457.9	43149.7	4682.3	0.0	6705.8
44	28751.6	18427.0	118029.8	18756.6	8714.1	38572.1	4975.5	3141.5	6705.8
45	48686.8	40553.9	134419.1	150840.0	51682.0	137312.2	5520.0	3141.5	6705.8
46	9325.0	44519.8	63916.2	46831.0	2663.2	9958.3	0.0	3141.5	6705.8
47	5449.3	0.0	53164.8	15744.3	34849.2	41917.9	5074.3	0.0	6705.8
48	48686.8	40551.2	134419.1	150840.0	51682.0	137312.2	5520.0	3141.5	6705.8
49	10409.8	16308.2	134137.4	21159.9	40313.1	126641.8	3070.5	3141.5	6705.8
50	48686.8	40567.4	134419.1	150840.0	51682.0	137312.2	5520.0	3141.5	6705.8

Table G.2 Solution of 50 Hypothetical Scenarios for High-VIF Model (Stage-2).

Scenario No.	Emission Reduction (gm-mol)									
	sq1_3p2	**sq1_4p2**	**sq2_2p2**	**sq2_3p2**	**sq3_2p2**	**sq3_3p2**	**sq4_2p2**	**sq4_3p2**	**sq5_2p2**	**sq5_4p2**
1	17706.1	15558.5	20489.8	11515.2	84560.2	296448.6	5068.9	118453.0	8811.4	37881.4
2	4.2	11.9	12.1	21.4	0.0	486464.7	39352.9	141864.6	9.6	37881.4
3	475.1	6253.6	30306.5	28197.4	0.0	478046.6	39352.9	141864.6	3423.7	37881.4
4	9603.8	17292.6	16761.4	29545.9	6923.3	486464.7	31594.4	141864.6	8953.0	37881.4
5	20517.8	20146.4	6251.4	19570.8	46294.0	471647.5	10192.1	141864.6	11396.9	37881.4
6	18080.0	15909.8	20474.6	11508.8	71112.4	486464.7	7350.3	141864.6	8791.9	37881.4
7	17695.3	15548.5	20489.1	11515.1	86794.1	314710.5	5279.0	120819.6	8810.9	37881.4
8	49.1	38.3	38.4	45.2	0.0	486464.7	39352.9	141864.6	16.2	37881.4
9	14143.1	29740.3	15996.3	4219.2	131816.7	486464.7	39352.9	138776.3	6059.7	37881.4
10	5533.4	34048.5	948.7	10563.2	81537.2	486464.7	25824.3	141149.2	8287.3	37881.4
11	1.5	0.0	0.0	0.0	222650.1	486464.7	1.9	141864.6	0.0	37881.4
12	17673.3	15528.7	20466.0	11508.2	30781.3	425971.5	24060.1	141864.6	8790.3	37881.4
13	17694.5	15547.7	20488.9	11515.0	87632.4	308468.4	5328.1	122373.1	8810.7	37881.4
14	19686.7	34941.1	16029.7	4202.2	78823.7	486464.7	39352.9	119336.6	6003.7	37881.4
15	23306.1	17282.9	5594.3	18187.3	222650.1	486464.7	3778.7	118568.7	10780.3	37881.4
16	0.0	0.0	0.0	0.0	0.0	486464.7	39352.9	141864.6	0.0	37881.4
17	0.0	0.0	4.0	6.7	0.0	486464.7	39352.9	141864.6	0.0	37881.4
18	17666.9	15521.9	20486.0	11514.3	82139.8	343522.1	6140.7	132104.4	8808.5	37881.4
19	11621.6	19314.5	18844.4	31629.6	162120.7	469549.1	19233.5	141291.3	11037.1	37881.4
20	1.8	8.9	16.8	9.2	0.0	486464.7	39352.9	141864.6	0.3	37881.4
21	0.0	0.0	0.0	0.0	0.0	486464.7	39352.9	141864.6	0.0	37881.4
22	17969.0	15805.3	20488.8	11513.6	75023.9	486464.7	5813.5	127280.7	8806.4	37881.4
23	252.5	0.0	0.0	0.0	0.0	486464.7	39352.9	141864.6	0.0	37881.4
24	23306.1	38690.0	5820.5	18062.1	222000.5	486464.7	4844.5	110317.4	10357.3	37881.4
25	17674.0	15529.3	20467.9	11508.7	44100.6	486464.7	14767.5	141864.6	8792.1	37881.4
26	17443.8	15324.2	20212.3	11432.1	2832.7	486464.7	39352.9	141864.6	8565.0	37881.4
27	475.2	6258.0	30324.6	28214.8	9063.3	443916.6	39352.9	140939.5	3427.8	37881.4
28	14021.1	29626.0	15999.1	4219.8	30256.5	486464.7	39352.9	117194.9	6063.1	37881.4
29	0.0	4.0	6.7	14.5	0.0	486464.7	39352.9	141864.6	3.0	37881.4
30	11617.2	19310.4	18843.4	31628.6	77541.8	486464.7	19333.9	141864.6	11036.1	37881.4
31	11655.5	19345.6	18832.2	31617.0	31988.7	486464.7	20817.4	131318.0	11024.1	37881.4
32	23306.1	38690.0	5791.8	18079.0	222650.1	486464.7	5248.3	103555.6	10412.8	37881.4
33	0.6	0.0	2.8	0.0	0.0	486464.7	39352.9	141864.6	0.0	37881.4
34	166.9	2144.3	10457.2	9713.5	0.0	486464.7	39352.9	141864.6	1128.5	37881.4
35	17684.0	15538.1	20484.0	11513.6	96301.1	486464.7	6512.8	141734.0	8806.5	37881.4
36	17704.2	15556.8	20489.7	11515.2	85950.7	298426.1	5105.9	119199.0	8811.3	37881.4
37	0.0	0.0	0.0	0.0	0.0	486464.7	39352.9	141864.6	0.0	37881.4
38	17882.8	15724.3	20490.7	11514.6	76207.2	306658.5	5109.4	118813.7	8809.5	37881.4
39	5749.9	34249.4	949.8	10561.4	7239.0	486464.7	27733.8	141864.6	8281.5	37881.4
40	23.4	15.0	12.2	24.6	0.0	422954.3	39352.9	141864.6	21.7	37881.4
41	11628.2	19321.0	18849.1	31634.2	103185.6	486464.7	19239.5	138641.4	11041.7	37881.4
42	0.0	0.0	0.0	0.0	0.0	486464.7	39352.9	141864.6	0.0	37881.4
43	474.8	6234.0	30226.9	28120.4	0.0	477398.8	39352.9	141864.6	3405.5	37881.4
44	0.0	0.0	0.0	1316.0	0.0	486464.7	39352.9	141864.6	0.0	37881.4
45	17695.2	15548.3	20489.1	11515.1	85110.8	311007.4	5285.7	121041.9	8810.9	37881.4
46	54.5	35.4	0.0	236.2	0.0	486464.7	39352.9	141864.6	58.2	37881.4
47	0.0	0.0	0.0	0.0	0.0	486464.7	39352.9	141864.6	0.0	37881.4
48	17679.8	15534.0	20486.9	11514.5	96436.3	364408.9	5779.4	129716.3	8809.2	37881.4
49	0.0	0.0	0.0	0.0	0.0	486464.7	39352.9	141864.6	0.0	37881.4
50	17706.1	15558.6	20489.8	11515.2	85304.7	302605.4	5072.3	118420.3	8811.4	37881.4

Table G.2 Solution of 50 Hypothetical Scenarios for High-VIF Model (Stage-2) (Continued).

Scenario No.	Emission Reduction (gm-mol)									
	pt1p2	**pt5p2**	**pt15p2**	**pt37p2**	**sq1_1p2**	**sq1_2p2**	**sq1_5p2**	**sq2_1p2**	**sq2_4p2**	**sq2_5p2**
1	23974.0	40161.3	58505.2	0.0	2087.1	23896.5	18220.6	16793.5	17517.4	24268.8
2	0.0	0.0	0.0	0.0	0.0	2.9	5.3	8.4	22.8	24410.3
3	64097.1	0.0	0.0	0.0	8532.0	17415.7	27162.0	23238.1	3780.6	24422.7
4	0.0	0.0	4269.2	0.6	2183.0	11427.0	15131.4	10438.9	25868.3	23424.9
5	996.5	0.0	0.0	0.0	3119.3	13600.8	22203.7	7199.1	24319.0	24811.2
6	0.0	0.0	31200.4	0.0	2078.8	23879.1	18203.3	16933.2	17505.5	24125.6
7	24045.6	41000.6	57303.4	0.0	2086.8	23895.8	18220.0	16828.8	17516.9	24125.6
8	0.0	0.0	0.0	0.0	0.0	7.8	35.9	84.0	0.0	24424.3
9	88379.5	45683.4	30521.0	0.0	5341.9	20734.2	14131.6	24959.0	38749.6	24138.1
10	61518.0	0.0	114488.5	0.0	6229.9	9900.9	17438.8	16554.7	44373.5	0.0
11	0.0	0.0	0.0	0.0	0.0	1.2	2.9	0.0	2.2	24414.9
12	3732.2	20281.9	21352.1	0.0	2075.8	23872.8	18196.9	16802.0	17501.2	23821.7
13	24030.8	41071.2	57090.0	0.0	2086.7	23895.6	18219.8	16830.8	17516.8	23194.2
14	54882.5	0.0	34407.2	0.0	5344.8	20737.1	14134.2	24959.0	38752.5	20984.1
15	4438.8	0.0	0.0	1.7	7236.5	13132.3	21709.9	24959.0	51068.6	16368.9
16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	24408.4
17	0.0	0.0	0.0	0.0	0.0	0.0	2.6	0.0	0.0	24415.3
18	26211.8	45683.4	51758.6	0.0	2085.4	23892.8	18217.0	16915.9	17514.9	22928.2
19	21052.8	0.0	39512.6	0.1	4266.0	13510.4	17214.8	12527.4	27951.7	23699.5
20	0.0	0.0	0.0	0.0	1.2	0.8	0.0	0.2	14.1	24413.9
21	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	24132.4
22	10033.2	0.0	54219.6	0.0	2085.9	23893.9	18218.1	16858.7	17515.6	23494.1
23	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1428.3	24627.1
24	56654.8	45683.4	0.0	0.0	7237.9	13133.7	21711.2	24959.0	51069.9	3213.2
25	0.0	0.0	23730.8	0.0	2076.7	23874.7	18198.8	16808.2	17502.4	24445.3
26	0.0	0.0	0.0	0.0	1956.8	23618.9	17943.0	16466.2	17328.1	0.0
27	93494.2	28.2	9281.0	0.0	8550.1	17433.7	27180.1	23256.1	3781.5	24357.9
28	56813.5	0.0	36951.3	0.0	5345.7	20738.0	14135.0	24959.0	38753.4	24129.4
29	0.0	0.0	0.0	0.0	0.1	4.5	0.0	0.0	0.0	24409.9
30	21132.7	0.0	41144.3	0.0	4265.0	13509.4	17213.8	12539.4	27950.7	23186.6
31	0.0	0.0	22761.1	0.0	4253.5	13497.9	17202.4	12481.2	27939.3	22904.3
32	35204.9	38267.7	0.0	0.0	7239.0	13134.8	21712.4	24959.0	51071.0	23565.8
33	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.9	0.0	24425.9
34	0.0	0.0	0.0	0.0	2606.0	5809.2	9323.4	7908.5	1339.8	24642.7
35	1800.0	0.0	48927.7	0.0	2084.4	23890.8	18214.9	16857.5	17513.4	23070.3
36	23752.2	39584.9	58209.7	0.0	2087.0	23896.3	18220.5	16799.7	17517.2	20362.4
37	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	24181.5
38	24377.2	41512.7	58717.1	0.0	2087.1	23896.4	18220.5	16798.3	17517.3	24385.7
39	52221.3	0.0	108968.7	0.0	6225.7	9897.5	17434.7	15780.9	44369.3	23216.9
40	132342.2	45683.4	0.0	0.0	0.9	21.6	0.0	1.2	10.1	24401.3
41	35837.3	0.0	49284.6	0.0	4270.6	13515.0	17219.4	12536.3	27956.4	23559.8
42	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	23975.2
43	0.0	0.0	0.0	0.0	8452.4	17336.0	27082.4	23158.4	3776.6	24909.5
44	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	24329.6
45	24271.9	41725.6	57275.2	0.0	2086.8	23895.8	18220.0	16829.1	17516.9	24206.4
46	0.0	0.0	0.0	0.0	0.0	33.6	0.0	0.0	244.6	24411.8
47	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	24418.0
48	23317.8	39833.7	53371.4	1.7	2085.8	23893.7	18217.9	16874.0	17515.4	18030.7
49	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	24428.6
50	24114.1	40597.9	58488.8	0.0	2087.1	23896.5	18220.6	16793.4	17517.4	24185.6

Table G.2 Solution of 50 Hypothetical Scenarios for High-VIF Model (Stage-2) (Continued).

Scenario No.	Emission Reduction (gm-mol)										
	sq3_4p2	sq3_5p2	sq5_1p2	pt2p2	pt3p2	pt4p2	pt6p2	pt21p2	pt23p2	pt63p2	pt64p2
1	55882.7	4122.4	9784.6	2535.4	25244.2	47047.9	50040.4	227.4	17.4	1165.4	2847.4
2	0.0	7.8	0.0	17.4	11.6	0.0	0.0	0.1	0.0	0.4	0.0
3	65536.1	17368.1	1490.6	105010.4	63528.6	87436.1	36271.5	301.9	0.0	408.8	4763.1
4	13159.5	6642.8	3463.0	65110.7	74407.2	75773.9	29737.0	55.0	0.0	518.8	0.0
5	11466.7	6235.7	11081.9	18855.9	117941.9	143674.0	30705.8	258.1	2.7	3075.3	6498.7
6	50522.0	4114.5	9767.3	2535.2	26050.7	47036.5	50183.5	210.0	1.4	1151.0	6705.8
7	56073.8	4122.1	9784.0	2535.4	25400.8	47047.4	51682.0	226.7	16.7	1164.9	6569.2
8	0.0	11.5	6.2	36.5	475.8	146.1	32.6	0.0	0.0	0.0	0.0
9	0.0	1912.5	8432.1	53559.0	8530.6	106221.6	51682.0	371.0	1.9	2334.9	0.0
10	54649.5	3821.0	9583.2	67966.1	98575.5	121590.6	31308.5	215.0	10.9	1089.2	0.0
11	0.0	0.0	1.2	0.0	0.0	6.4	1.3	0.0	0.0	0.0	6705.8
12	45361.4	4111.6	9760.9	2535.2	25286.6	47032.3	43399.8	203.6	0.0	1145.7	0.0
13	56083.8	4122.0	9783.8	2535.4	25436.9	47047.3	51682.0	226.5	16.5	1164.7	6705.8
14	0.0	1912.8	8435.0	53561.6	8538.3	106224.4	51682.0	373.9	2.2	2337.8	0.0
15	81956.9	14679.5	5321.5	16545.1	55341.5	140814.4	51682.0	261.7	13.8	1470.3	6705.8
16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	27.4	193.5	0.0
17	0.0	0.1	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
18	56237.8	4120.8	9781.0	2535.4	25903.8	47045.4	46703.9	223.7	13.7	1162.4	3883.5
19	42941.3	8726.1	5546.1	67194.2	76529.5	77857.2	32051.2	181.3	1.1	1555.4	6220.3
20	0.0	1.3	4.1	23.3	6.7	0.0	0.0	0.0	0.0	0.1	0.0
21	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
22	55807.4	4121.2	9782.1	2535.4	25599.1	47046.2	48727.4	224.8	15.1	1163.3	4932.3
23	0.0	0.0	0.0	64455.6	22456.0	46881.2	0.0	393.3	0.0	0.0	0.0
24	76729.8	14680.9	5322.9	16545.4	51928.9	140815.8	51682.0	263.1	15.1	1471.7	6705.8
25	47338.2	4112.5	9762.8	2535.2	25659.9	47033.5	48162.8	205.6	0.0	1147.3	0.0
26	0.0	3997.2	9507.0	2534.2	24348.1	46867.0	0.0	10.8	0.0	945.5	0.0
27	73646.8	17386.2	1493.8	105028.5	63545.4	87454.2	36289.5	319.9	14.3	411.9	4952.7
28	0.0	1912.9	8435.8	53562.4	8093.2	106225.4	51682.0	374.8	2.3	2338.6	0.0
29	0.0	1.9	0.9	0.0	12.4	17.6	0.0	0.0	0.0	0.4	0.0
30	42179.4	8725.1	5545.1	67193.1	76426.6	77856.3	31405.2	180.2	0.0	1554.3	6705.8
31	37134.1	8713.6	5533.6	67181.7	76450.8	77844.8	31704.1	169.0	0.0	1542.9	0.0
32	76199.3	14682.0	5324.0	16545.5	50637.1	140816.9	51682.0	264.2	16.3	1472.8	6705.8
33	0.0	0.8	0.0	0.0	0.6	0.0	0.0	0.0	0.0	0.0	4794.1
34	0.0	5792.0	456.1	37393.2	22468.5	31056.4	12606.1	0.0	0.0	74.0	0.0
35	55182.5	4119.8	9778.9	2535.4	25859.2	47044.2	51682.0	221.7	11.7	1160.6	6705.8
36	55907.0	4122.3	9784.5	2535.4	25275.7	47047.7	51682.0	227.2	17.2	1165.3	3704.3
37	0.0	0.0	0.0	0.0	0.0	0.0	0.0	393.3	0.0	281.4	0.0
38	55903.3	4122.4	9784.5	2535.4	25264.9	47047.7	51026.3	227.3	17.3	1165.3	5520.8
39	52342.3	3819.3	9579.0	67961.9	98388.5	121586.6	30516.9	210.8	6.8	1085.9	0.0
40	0.0	0.0	17.1	0.0	110.0	0.0	0.0	0.3	0.0	0.1	0.0
41	45157.2	8730.7	5550.7	67198.8	76582.3	77861.9	32329.2	185.9	3.3	1560.0	6705.8
42	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
43	29727.8	17288.5	1476.5	104930.7	63454.4	87356.5	36191.8	222.2	0.0	395.4	0.0
44	0.0	0.0	0.0	1014.3	5760.6	31013.5	0.0	64.6	0.0	0.0	0.0
45	56075.4	4122.1	9784.0	2535.4	25403.7	47047.4	51682.0	226.7	16.7	1164.9	6705.8
46	0.0	0.0	13.1	180.2	45.2	0.8	0.0	0.0	0.0	0.0	0.0
47	0.0	0.0	0.0	2207.4	6240.7	524.4	0.0	0.0	0.0	0.0	0.0
48	56043.6	4121.1	9781.9	2535.4	25709.0	47046.0	47962.5	224.6	14.6	1163.1	6705.8
49	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
50	55875.4	4122.4	9784.6	2535.4	25243.0	47047.9	50756.6	227.4	17.4	1165.4	5558.6

Table G.3 Solution of 50 Hypothetical Scenarios for High-VIF Model (Stage-3).

Scenario No.	Emission Reduction (gm-mol)									
	sq1_3p3	sq1_4p3	sq2_4p3	sq2_5p3	sq3_2p3	sq3_3p3	sq4_2p3	sq4_3p3	sq5_1p3	sq5_5p3
1	4245.437	6161.436	51494.51	1164.417	171525.7	479768.2	40497.59	145179.9	11622.53	34183.27
2	24177.41	39717.31	57417.17	0	226875.3	476278.2	40497.59	145179.9	11622.53	36429.26
3	16031.37	21133.15	28948.15	7436.964	226875.3	404498.7	40497.59	105948.3	11622.53	22972.7
4	16474.21	21275.42	28973.81	6406.47	226875.3	443095.6	40497.59	130615.6	11622.53	23865.83
5	15202.11	20863.72	28895.85	7539.213	226875.3	425518.7	40497.59	107265.9	11622.53	22883.41
6	14802.39	20730.64	28866.16	5581.045	226875.3	469551.1	40497.59	123271.5	11622.53	24579.53
7	24147.51	39707.2	57414.75	25507.29	217156.1	468039.8	40497.59	145179.9	11622.53	36429.26
8	24177.41	39717.31	57417.17	0	226875.3	473247.6	40497.59	145179.9	11622.53	36429.26
9	24177.41	39717.31	57417.17	0	226875.3	470753	40497.59	145179.9	11622.53	36429.26
10	16991.19	21444.96	29008.56	7993.947	226875.3	421112.7	40497.59	106954.4	11622.53	22488.13
11	14178.52	20528.87	28828.13	8718.911	153673.3	453887.1	40497.59	119351.4	11622.53	21850.4
12	16648.59	21334.04	28987.56	7965.018	226875.3	436559.1	40497.59	101129.8	11622.53	22514.34
13	15411.57	20930.42	28907.18	7237.672	184037	417354.2	40497.59	130069.7	11622.53	23142.51
14	24177.41	39717.31	32931.68	0	179996.7	470059.5	40497.59	145179.9	11622.53	36429.26
15	12160	19881.54	28712.67	12773.19	118167.3	254494.6	22008.98	74208	6096.307	18344.72
16	0	0	16020.65	0	226875.3	472842.5	40497.59	145179.9	11622.53	36429.26
17	19905.32	22387.67	29186.56	4495.645	226875.3	483613.5	40497.59	125146.5	11622.53	25523.84
18	14699.69	20700.8	28864.61	6496.521	226875.3	374806.7	40497.59	96203.77	11622.53	23791.52
19	14932.51	20774.3	28876.35	7512.045	180893.1	418886.9	40497.59	114550	11622.53	22902.54
20	17351.53	21559.45	29027.71	5381.105	226875.3	468997.2	40497.59	120206.2	11622.53	24755.83
21	24177.41	39717.31	57417.17	0	226875.3	475095.2	40497.59	145179.9	11622.53	36429.26
22	21338.69	22852.3	29275.39	4949.473	226875.3	468585.1	40497.59	130428.7	11495.15	25126.33
23	24177.41	24559.1	29596.77	0	226875.3	477375.8	40497.59	145179.9	11622.53	30673.32
24	14839.04	20746.2	28873.59	9916.505	210994.3	388443.1	40497.59	105403.1	11510.13	20815.67
25	16623.3	21325.69	28985.72	7919.488	226875.3	437801.5	40497.59	106070.5	11622.53	22553.54
26	13136.91	20190.96	28763.18	5662.419	226875.3	474638.7	40497.59	118576.3	11622.53	24511.92
27	15333.49	20906.94	28904.83	7860.024	226875.3	408788	40497.59	101986.5	11622.53	22605.7
28	24177.41	39717.31	57417.17	0	226875.3	477092.9	40497.59	145179.9	11622.53	36429.26
29	14699.04	20700	28863.75	6889.356	226875.3	440673.3	40497.59	110646.3	11622.53	23447.96
30	15116.26	20834.87	28889.12	7050.759	226875.3	420531.9	40497.59	112614.2	11622.53	23305.82
31	19401.62	22224.34	29155.26	5078.631	226875.3	473682.2	40497.59	124150.7	11622.53	25016.68
32	16110.08	21157.98	28952.06	9484.976	226875.3	420301.9	40497.59	112528.1	11622.53	21188.39
33	14801.25	20733.99	28871.28	7661.094	226875.3	407399	40497.59	105146.4	11622.53	22778.58
34	17323.57	21551.77	29027.89	6469.534	226875.3	458524.1	40497.59	117087.3	11622.53	23811.96
35	15762.12	21046.11	28931.75	8360.832	226875.3	413328.3	40497.59	105074.9	11622.53	22169.83
36	15401.98	20925.05	28903.44	5947.852	171491.8	458781.6	40497.59	145179.9	11622.53	24259.18
37	24177.41	39717.31	57417.17	0	226875.3	475924.4	40497.59	145179.9	11622.53	36429.26
38	18662.56	21984.72	29109.41	6264.881	218515.5	477244.1	39485.88	139281.3	11218	23985.49
39	16480.2	21278.33	28975.47	6919.71	226875.3	406336.3	40497.59	109751.9	11622.53	23421.09
40	13906.39	20443.59	28815.36	7852.539	226875.3	416138.8	40497.59	100422.9	11622.53	22612.64
41	17250.99	21529.13	29024.61	7951.68	226875.3	417161.6	40497.59	108085.4	11622.53	22524.34
42	17846.71	21720.43	29059.01	5474.6	226875.3	477573.4	40497.59	121074	11622.53	24674.8
43	16575.84	21309.05	28981.06	6511.491	226875.3	442091.8	40497.59	111460.5	11622.53	23775.42
44	17950.49	21752.35	29063.1	4173.384	226875.3	481667.1	40497.59	127516.2	11622.53	25803.16
45	24163.43	39712.69	57416.19	25784.77	225127.6	492758.9	40497.59	145179.9	11622.53	36429.26
46	18797.69	22030.29	29120.23	6365.602	226875.3	478660.1	40497.59	114368.1	11622.53	23901.94
47	11322.27	19459.17	28614.98	2327.203	226875.3	475511.3	40497.59	138921.3	11622.53	27577.53
48	14867.99	20754.84	28874.33	8015.676	179389.1	389659	40497.59	116667.3	11622.53	22468.09
49	19392.97	22221.04	29154.05	4310.83	226875.3	471637.6	40497.59	125772.9	11622.53	25683.9
50	16076.72	21145.29	28947.34	6581.107	226875.3	464079.8	40497.59	145179.9	11622.53	23710.41

Table G.3 Solution of 50 Hypothetical Scenarios for High-VIF Model (Stage-3) (Continued).

Scenario No.	Emission Reduction (gm-mol)									
	pt5p3	**pt30p3**	**pt37p3**	**pt63p3**	**pt64p3**	**sq2_1p3**	**sq2_2p3**	**sq2_3p3**	**sq3_4p3**	**sq4_1p3**
1	45683.38	4546.742	0.29297	2587.666	0	2279.124	3422.906	59640.74	92724.93	39155.12
2	6194.355	0	0	3141.544	6705.77	25879.1	0	64932.2	95090.77	39155.12
3	42096.14	5519.951	0	3141.544	0	25879.1	19418.22	64932.2	82538.69	39155.12
4	34743.17	825.8079	0	3141.544	6705.77	25879.1	19415.88	64932.2	87600.99	39155.12
5	45683.38	5519.951	0	3141.544	0	25879.1	19418.06	58031.04	79542	39155.12
6	30793.67	0	0	3141.544	6705.77	25879.1	19413.19	64932.2	65180.15	39155.12
7	43376.37	3894.856	1.6617	3139.12	6705.77	25878.5	38853.6	64932.2	95090.77	39155.12
8	6153.615	0	0	3141.544	6705.77	25879.1	0	64932.2	95090.77	39155.12
9	0	0	0	3141.544	6705.77	25879.1	0	64932.2	95090.77	39155.12
10	37115.92	5519.951	0	3141.544	0	25879.1	19418.26	57605.85	70769.92	39155.12
11	35752.42	5519.951	0	3141.544	0	25879.1	19414.48	64932.2	68113.38	39155.12
12	45683.38	5519.951	0	3141.544	0	25879.1	19418.84	35912.32	65129.27	39155.12
13	45683.38	5519.951	1.6617	0	0	12928.53	19416.08	33334.16	81392.17	39155.12
14	6163.549	0	0	3141.544	6705.77	25879.1	19137.05	64932.2	95090.77	39155.12
15	23437.54	5519.951	0	2455.63	1043.473	15851.1	19426.66	33586.21	48500.77	21925.89
16	0	0	0	3141.544	6705.77	25879.1	0	64932.2	95090.77	39155.12
17	15547.5	1279.655	0	3141.544	5151.214	25879.1	19412.73	64932.2	69877.04	39155.12
18	45683.38	5519.951	0	3141.544	0	12930.89	19418.41	33732.67	65337.84	39155.12
19	43942.15	5519.951	0	3141.544	0	25879.1	19415.3	35034.82	81780.54	39155.12
20	29507.85	1787.07	0	3141.544	4534.793	25879.1	19414.52	64932.2	79652.05	39155.12
21	6158.33	0	0	3141.544	6705.77	25879.1	24.44933	64932.2	95090.77	39155.12
22	22459.01	2226.2	0	3141.544	6705.77	25879.1	19411.36	64932.2	83545.53	39155.12
23	6779.404	0	0	3141.544	6705.77	25879.1	19400.19	64932.2	78461.7	39155.12
24	36837.56	5519.951	0	3141.544	0	25879.1	19418.61	64932.2	67945.69	39155.12
25	37559.34	5519.951	0	3141.544	0	25879.1	19418.61	35878.42	73150.81	39155.12
26	25694.93	1968.161	0	3141.544	4314.8	25879.1	19415.06	64932.2	62535.8	39155.12
27	45683.38	5519.951	0	3141.544	0	25879.1	19418.84	62673.43	73945.93	39155.12
28	6210.193	0	0	3141.544	6705.77	25879.1	7.202429	64932.2	95090.77	39155.12
29	38865.52	5519.951	0	3141.544	0	16765.27	19417.52	64932.2	57611.48	39155.12
30	37533.61	5519.951	0	3141.544	0	25879.1	19416.62	38156.97	78656.17	39155.12
31	26565.25	0	0	3141.544	6705.77	25879.1	19413.12	64932.2	93427.73	39155.12
32	39241.2	5519.951	0	3141.544	0	25879.1	19417.13	64932.2	63386.38	39155.12
33	35674.78	5519.951	0	3141.544	0	25879.1	19418.72	64932.2	55605.52	39155.12
34	33276.59	2541.158	0	1979.415	1579.605	25879.1	19416.58	64932.2	68839.62	39155.12
35	36860.45	5519.951	0	3141.544	0	25879.1	19418.8	64932.2	71643.75	39155.12
36	45683.38	1347.499	1.256056	766.8957	0	12925.21	19412.77	36395.6	84057.09	39155.12
37	6140.432	0	0	3141.544	6705.77	25879.1	0	64932.2	95090.77	39155.12
38	45241.19	3371.75	0.646686	1918.945	0	25879.1	19413.74	63096.59	76874.88	38391.75
39	36520.66	5519.951	0	3141.544	0	25879.1	19417.28	32458.16	88216.41	39155.12
40	45683.38	5519.951	0	3141.544	0	25879.1	19419.07	64932.2	57216.53	39155.12
41	37019.97	5519.951	0	3141.544	0	25879.1	19417.98	64932.2	81822.84	39155.12
42	22704.78	2305.243	0	3141.544	3905.304	25879.1	19414.75	64932.2	56585.77	39155.12
43	45200.64	5519.951	0	3141.544	0	25879.1	19416.78	64932.2	82225.98	39155.12
44	21497.42	2185.397	0	3141.544	5423.026	25879.1	19412.14	64932.2	77798.06	39155.12
45	45258.59	5192.211	1.6617	3141.327	6705.77	25878.99	38854.07	64932.2	95090.77	39155.12
46	26824.61	1909.737	0	3141.544	4385.775	25879.1	19416.23	64932.2	65750.69	39155.12
47	1125.514	135.9965	0	3141.544	6631.489	25879.1	19406.89	64932.2	63074.14	39155.12
48	45683.38	5519.951	0.526636	3141.544	0	12929.93	19417.48	33540.73	62852.81	39155.12
49	15483.78	0	0	3141.544	6705.77	25879.1	19412.42	64932.2	69872.75	39155.12
50	45683.38	0	1.6617	0	0	12926.79	19414.32	33407.68	66929.7	39155.12

Table G.3 Solution of 50 Hypothetical Scenarios for High-VIF Model (Stage-3) (Continued).

Scenario No.	**Emission Reduction (gm-mol)**									
	sq4_4p3	**sq4_5p3**	**sq5_3p3**	**pt1p3**	**pt2p3**	**pt3p3**	**pt4p3**	**pt6p3**	**pt15p3**	**pt23p3**
1	9546.765	1723.654	1673.711	21502.56	22541.06	30751.26	33203.89	51682	23987.54	0.58448
2	0	0	0	1.193467	0	0	0.780288	51682	0	0
3	54152.06	9780.141	9496.948	66162.21	67200.67	75411.09	77863.8	50282.39	68647.17	4.858139
4	54149.78	9777.807	9494.605	66159.82	67198.38	75408.82	77861.46	39053.41	68644.83	4.14868
5	54151.95	9779.984	9496.777	66162.08	67200.54	75410.94	77863.64	51682	68647.03	4.675757
6	54147.07	9775.139	9491.938	66157.17	67195.69	75406.1	77858.8	45285.03	68642.22	2.632332
7	108321.4	19577.47	19011.06	132341.7	134418.6	150839.4	155744.8	51682	137311.7	26.84096
8	1.953702	0	0	0	2.963147	0	1.87269	51682	2.476573	0
9	0	0	0	12308.49	13006.87	19302.38	21630.35	51682	13994.84	0
10	54152.17	9780.2	9497.005	66162.34	67200.81	75411.24	77863.8	49898.4	68647.31	4.919089
11	54148.37	9776.414	9493.214	66158.49	67196.9	75407.46	77860.05	51682	68643.45	2.74175
12	54152.71	9780.788	9497.577	66162.87	67201.35	75411.69	77864.42	51682	68647.86	5.483362
13	54149.89	9778.003	9494.795	66160.09	67198.52	75408.97	77861.61	51682	68645.11	3.910545
14	53870.84	9499.143	9215.964	65880.95	66919.44	75129.97	77582.58	43827.58	68366.08	0
15	54160.53	9788.616	9505.406	66170.69	67209.16	75419.55	77872.22	26680.44	68655.7	13.30816
16	0	0	0	23913.23	25990.17	42411.13	47316.48	51682	28883.31	27.43699
17	54146.53	9774.648	9491.443	66156.77	67195.15	75405.65	77858.34	50524.54	68641.67	2.700072
18	54152.28	9780.357	9497.158	66162.47	67200.94	75411.39	77863.95	51682	68647.44	5.073621
19	54149.13	9777.218	9494.033	66159.29	67197.71	75408.22	77860.83	41919.75	68644.28	3.888194
20	54148.37	9776.473	9493.252	66158.49	67197.04	75407.46	77860.05	51420.95	68643.59	3.1003
21	243.453	29.75943	26.5363	177.4287	446.6271	0	843.959	51682	122.3152	0
22	54145.22	9773.314	9490.109	66155.31	67193.8	75404.29	77856.93	51304.02	68640.43	2.022421
23	54134.04	9762.113	9478.908	66144.17	67182.62	75393.1	77845.85	51682	68629.15	1.339053
24	54152.49	9780.553	9497.348	66162.61	67201.08	75411.54	77864.27	44528.65	68647.58	5.263728
25	54152.49	9780.553	9497.348	66162.61	67201.08	75411.54	77864.27	49993.32	68647.58	5.252429
26	54148.91	9777.002	9493.786	66159.03	67197.57	75407.92	77860.68	49688.88	68644.14	3.441696
27	54152.71	9780.769	9497.577	66162.87	67201.35	75411.69	77864.42	48028.32	68647.86	5.477616
28	41.24482	1.196655	0	0	72.73179	0	150.5955	0.983926	6.053846	0
29	54151.41	9779.474	9496.262	66161.54	67200	75410.49	77863.17	51682	68646.48	4.157478
30	54150.54	9778.572	9495.367	66160.62	67199.06	75409.58	77862.24	42132.9	68645.66	3.283425
31	54146.96	9775.041	9491.843	66157.17	67195.55	75405.95	77858.65	51682	68642.08	2.478294
32	54150.98	9779.062	9495.862	66161.15	67199.59	75410.03	77862.7	43540.43	68646.21	3.786693
33	54152.6	9780.651	9497.443	66162.74	67201.21	75411.69	77864.27	46147.16	68647.72	5.347002
34	54150.43	9778.532	9495.329	66160.62	67199.06	75409.58	77862.24	51682	68645.66	4.072995
35	54152.71	9780.749	9497.539	66162.87	67201.35	75411.69	77864.42	47751.37	68647.86	5.447017
36	54146.63	9774.687	9491.481	66156.77	67195.15	75405.65	77858.34	51682	68641.8	1.389171
37	0	0	0.038099	14.3216	0	0	29.96304	51682	0	0
38	54147.61	9775.688	9492.49	66157.7	67196.23	75406.71	77859.43	46654.5	68642.77	3.364498
39	54151.19	9779.219	9496.015	66161.28	67199.73	75410.18	77862.86	51682	68646.34	3.941666
40	54152.93	9781.004	9497.805	66163.14	67201.61	75412	77864.73	51682	68648.13	5.704288
41	54151.84	9779.906	9496.719	66161.94	67200.4	75410.94	77863.64	51682	68647.03	4.621873
42	54148.59	9776.688	9493.481	66158.76	67197.17	75407.61	77860.36	49852.88	68643.73	3.1174
43	54150.65	9778.729	9495.519	66160.75	67199.19	75409.73	77862.39	42359.09	68645.79	3.431936
44	54145.98	9774.06	9490.871	66156.11	67194.61	75405.04	77857.71	51682	68641.12	2.209175
45	108321.8	19577.94	19011.54	132342.1	134419	150839.9	155745.2	51682	137312.1	27.32785
46	54150.11	9778.179	9494.967	66160.22	67198.65	75409.13	77861.77	51682	68645.24	4.128171
47	54140.77	9768.822	9485.613	66150.94	67189.36	75399.75	77852.41	51682	68635.89	1.478052
48	54151.3	9779.415	9496.205	66161.41	67200	75410.33	77863.02	51682	68646.48	5.219906
49	54146.31	9774.354	9491.138	66156.37	67194.88	75405.35	77858.02	51682	68641.39	2.244309
50	54148.15	9776.257	9493.062	66158.36	67196.77	75407.31	77859.9	51682	68643.32	1.516349

Table G.4 Solution of 50 Hypothetical Scenarios for High-VIF Model (Stage-4).

Scenario No.	Emission Reduction (gm-mol)											
	sq1_1p4	**sq1_3p4**	**sq1_4p4**	**sq2_5p4**	**sq3_2p4**	**sq3_3p4**	**sq4_2p4**	**sq4_3p4**	**pt1p4**	**pt6p4**	**pt15p4**	**pt64p4**
1	434.8648	1759.005	2899.2	2050.585	45764.4	219053.2	19526.12	17633.92	11100.3	5351.21	11252.72	100.8217
2	0	0	0	0	282611.6	656174.6	51779.39	0	0	51682	0	0
3	84.27125	1959.474	2408.607	2329.986	375.494	554511.6	12669.56	8903.965	6401.887	5568.813	0	0
4	0	0	8.098576	0	282611.6	614978.3	51779.39	0	0	7937.744	0	0
5	0	0	0	0.564588	0	603969.3	0	0	20.55415	7937.744	0	0
6	3.328727	10.36055	55.92517	0	32547.35	581929.6	38584.62	0	0	7937.692	0	0
7	3.534502	0.556686	0	0.10586	0	217961.7	2.179093	0	19.49329	6674.021	0	0
8	0	0	0	0	282611.6	656174.6	51779.39	0	0	51682	0	0
9	0	0	0	0	0	656174.6	0	0	0.132607	51682	0	0
10	1.634102	0	0	1.729052	0	656174.6	5.136433	0	0	51682	0	0
11	0	0	0	0	0	656174.6	0	0	0	51682	0	0
12	0	0	0	0	0	656174.6	0	0	0	51682	0	0
13	1.985131	1.948402	5.80398	3.211097	0	247822.3	0	0	0.663037	7227.246	0	0
14	0	0	0	0	172851.9	532245.7	51779.39	0	0	7937.744	0	0
15	0	2.938067	5.80398	35216.21	0	656174.6	6.277862	0	0	0	15.96014	0.315803
16	0	0	0	0	282611.6	656174.6	51779.39	0	0	51682	0	0
17	0	0	0	0	282611.6	656174.6	51779.39	0	0	51682	0	0
18	0	0	2.834502	0	17.84021	276183.8	0	0	0.53043	7622.163	0	0
19	0.072627	24.37049	74.28194	23.99501	30.8664	477528.1	0	0	12.4651	7937.951	0	0
20	2.25143	0	0	2.611222	282611.6	656174.6	51779.39	0	1.989111	51682	0	0
21	0	0	0	0	282611.6	656174.6	51779.39	0	0	51682	0	0
22	0.617327	5.102958	0.314945	5.398877	0	656174.6	0	0	0	19931.07	0	0
23	0	0	0	0	282611.6	656174.6	51779.39	0	0	51682	0	0
24	0	0.865957	0	1.411471	0	531647.4	0	0	5.569511	7937.744	0	0
25	0	4.608126	1.124802	0	30695.36	656174.6	20823.31	0	8.884696	51682	0	0
26	0	2.133964	0	4.587281	282611.6	656174.6	51779.39	0	0	51682	0	0
27	0	0	0	9.562717	33349.31	525822	51779.39	0	21.21718	7937.744	0	0
28	0	0	0	0	282611.6	656174.6	51779.39	0	0	51682	0	0
29	0.302612	0	0	1.129177	165709.3	656174.6	51779.39	0	0.132607	51682	0	0
30	0	0	2.834502	9.42157	0	495304.7	0	0	72.13843	7937.537	0	0
31	0.32682	4.577199	6.343885	0	32179.5	656174.6	23734.16	0	0	51682	0	0
32	2.941384	0	2.339589	2.293641	16.14115	520819.9	0	0	3.04997	7937.744	0	0
33	0.883626	0	2.15962	0	83935.09	656174.6	51779.39	0	0	51682	0	0
34	0	0	0	0	282611.6	656174.6	51779.39	0	0	51682	0	0
35	0	3.371045	0	5.116583	0	656174.6	0	0	5.702118	51682	0	0
36	3274.644	3608.812	5424.066	4056.78	66057.22	254908.7	20920.48	33561.11	17778.81	7391.406	18403.28	496.1799
37	0	0	1.214786	0	248598.6	656174.6	51779.39	0	0	51682	0	0
38	0	0	2.15962	1.834913	26974.69	656174.6	16670.99	0	0	51682	0	0
39	0	4.113294	3.689351	5.010723	32547.63	399054.1	49359.04	0	0	7937.744	0	0
40	0	0	0	0	282611.6	656174.6	51779.39	0	0	51682	0	0
41	1.912505	0	0	0.529302	0	650520.9	2.282859	0	0	7937.744	0	0
42	0	0	0	0	282611.6	656174.6	51779.39	0	0	51682	0	0
43	530.5506	1405.788	1853.674	1368.421	121564.6	571883.1	51757.76	1789.231	12502.62	8447.728	12442.3	0
44	0	0	0	0	282611.6	656174.6	51779.39	0	0	51682	0	0
45	0	0	4.274249	0	0	139660.7	4.461952	0	16.44332	4705.03	0	0
46	0	0	0	0	24940.34	656174.6	14922.38	0	1.989111	51682	0	0
47	1.585684	0	0	0.141147	282611.6	656174.6	51779.39	0	2.652148	51682	0	0
48	0	0	0	0	16.14115	369824.1	0.933897	0	0	7937.744	0	0
49	0	2.505089	0	0	131182.5	656174.6	51779.39	0	0	51682	0	0
50	6.73008	10.63889	17.95184	8.080673	6.229916	312800	0	0	51.9821	7906.621	0	0

APPENDIX H

SOLUTION OF 50 HYPOTHETICAL SCENARIOS FOR STEPWISE-PLS MODEL

Table H.1 Solution of 50 Hypothetical Scenarios for Stepwise-PLS Model (Stage-1).

Scenario No.	Emission Reduction (gm-mol)									
	sq1_2p1	sq1_3p1	sq1_4p1	sq2_1p1	sq2_2p1	sq2_3p1	sq2_4p1	sq3_1p1	sq3_2p1	sq3_3p1
1	28737.3	14676.0	7132.6	10852.3	22746.8	49234.6	16231.7	33800.9	136813.7	100767.4
2	23375.8	6119.8	4326.5	9623.7	31900.7	47142.3	15503.3	35133.2	133843.4	101261.9
3	22726.1	0.0	26094.7	0.0	10915.9	65564.4	6351.0	25979.9	56557.6	40090.0
4	9802.8	0.0	23700.9	0.0	48233.5	30475.9	7798.7	38938.4	175209.2	108521.4
5	25621.2	9543.4	10484.9	5227.1	24125.2	46417.7	16741.2	34301.8	142694.7	100958.5
6	0.0	0.0	29131.7	32978.8	0.0	81971.1	0.0	0.0	0.0	0.0
7	19946.6	0.0	16128.6	21504.1	48233.5	72094.1	13246.7	28599.6	63820.2	247935.9
8	24610.6	2003.4	7518.8	9264.2	25125.7	48221.7	15275.1	35270.6	141634.3	101736.7
9	28178.7	29842.9	13224.3	17217.6	9411.9	25865.4	0.0	38938.4	43730.5	295361.9
10	26540.8	0.0	0.0	0.0	27545.4	46992.9	13347.1	35298.0	141992.0	102862.8
11	30094.8	15555.5	7628.7	10205.1	21601.0	48294.1	16852.6	34022.9	142272.7	101048.4
12	25907.3	0.0	5542.4	10896.2	23401.4	46013.7	20208.3	34057.9	144503.5	100968.1
13	26492.0	8447.5	7781.8	11938.4	20689.7	49578.6	17791.1	34028.5	141932.6	104221.5
14	27501.3	4551.5	15713.9	6217.2	24010.6	46736.6	14448.2	35549.5	142088.6	101159.3
15	0.0	0.0	45991.1	32978.8	0.0	31785.0	0.0	38938.4	0.0	83409.2
16	25338.2	7817.3	3793.7	20391.3	33139.7	60773.3	10190.8	36075.2	82348.5	101957.2
17	20243.1	9237.8	0.0	13572.5	22894.1	48335.3	18436.0	34831.9	141183.0	101079.0
18	14352.9	3738.0	12638.4	8280.0	21242.4	41173.2	21630.0	35251.9	145912.0	100826.6
19	34150.4	0.0	0.0	32978.8	32430.2	26857.1	0.0	26180.6	32235.5	45162.9
20	15812.3	0.0	8103.3	4910.1	29417.6	46640.3	17639.0	35037.3	144545.5	101893.5
21	13115.1	1995.9	0.0	13065.4	42782.1	41999.4	31114.0	37893.6	131918.3	101490.7
22	7434.1	0.0	8413.4	0.0	28773.5	42758.7	18950.0	35703.5	144406.1	101938.1
23	27474.9	2022.7	11059.0	6274.9	29274.6	46310.0	15992.9	34465.0	143321.7	101715.0
24	29401.1	14265.0	9133.6	9923.1	22638.4	48416.0	16604.9	34095.0	142267.1	101093.7
25	30349.8	6387.0	2526.1	22813.9	18235.8	46494.9	13541.8	29066.5	71959.6	80453.4
26	30094.8	15555.5	7628.7	10205.1	21601.0	48294.1	16852.6	34022.9	142272.7	101048.4
27	21585.5	8609.5	1115.7	17134.4	30448.7	45293.2	11485.7	24365.3	75192.9	108049.8
28	26535.5	7678.9	10643.6	8987.4	24593.8	47523.7	16679.8	34407.4	142879.6	101302.7
29	27993.6	11179.0	7944.6	8471.9	23242.5	47731.1	16569.1	34143.9	142694.7	101302.1
30	22217.1	6174.9	8769.9	3157.0	20690.4	45905.8	18252.0	34506.7	142780.5	101678.1
31	18236.0	0.0	2483.2	0.0	34338.1	44547.2	11264.8	34783.3	133646.6	96875.4
32	29969.6	15466.5	7587.1	10296.4	21668.6	48296.5	16874.9	34032.1	142250.3	101052.9
33	11613.6	0.0	9520.1	2017.8	24950.6	44826.9	17658.8	34903.5	143956.2	102741.7
34	0.0	576.5	6464.0	1812.2	33768.6	54289.0	0.0	35252.5	130274.7	105764.4
35	29737.9	9982.4	14349.5	14144.2	26090.0	49980.7	17320.4	34089.4	142580.7	101325.0
36	21313.1	0.0	517.8	676.3	29932.8	47427.8	15187.6	34307.9	143848.9	102123.5
37	13169.5	0.0	11476.5	4899.1	47503.9	5290.8	16665.3	14170.8	138730.2	87349.0
38	4299.7	0.0	0.0	4343.9	7612.5	36314.8	21441.9	34371.4	140597.3	99465.4
39	23113.8	4546.8	10493.1	4520.6	22236.2	45386.7	17548.9	33700.4	142395.8	100805.6
40	10472.2	0.0	143.9	19039.6	44499.8	52694.9	20365.6	31285.1	130771.8	100622.7
41	18883.9	0.0	0.0	7975.1	7090.4	35971.7	23308.0	31577.2	139857.9	95783.0
42	28781.4	11135.5	9733.2	9347.5	22958.5	47840.7	16853.7	33986.9	142152.0	100870.6
43	14559.6	4580.7	5156.4	8143.2	10168.7	24723.3	23779.3	30864.4	153456.7	95751.8
44	26752.3	8483.9	10238.8	16734.4	23366.5	49075.2	15454.5	34583.9	141486.3	101450.5
45	28416.8	17529.0	6827.5	10301.2	21784.9	48321.1	17618.3	34145.1	142136.0	101876.3
46	25843.2	12099.8	4691.7	13447.2	26474.3	51144.0	18667.2	34688.5	128374.8	101326.9
47	22999.9	11566.5	7257.6	7232.4	28063.4	44647.1	13443.8	35018.1	142236.5	101689.5
48	29684.8	12276.4	6293.8	10240.9	24833.6	48593.0	17038.7	34204.3	141774.5	101015.9
49	25830.0	2545.9	3531.9	15289.5	19988.4	49180.4	16893.3	35179.4	136219.2	97478.3
50	29790.1	10215.8	5017.3	8322.7	30741.7	59764.9	14602.3	32019.6	93815.9	153208.9

Table H.1 Solution of 50 Hypothetical Scenarios for Stepwise-PLS Model (Stage-1) (Continued).

Scenario No.	Emission Reduction (gm-mol)									
	sq3_4p1	sq3_5p1	sq4_2p1	sq4_3p1	sq4_4p1	sq5_2p1	sq5_3p1	sq5_4p1	sq5_5p1	pt1p1
1	33714.5	9577.8	3763.3	43154.1	50220.1	14501.6	14526.6	15351.0	20459.7	77966.4
2	34687.0	19236.2	16970.2	39110.5	50321.5	9392.5	19254.9	11870.5	20519.5	79305.7
3	86064.8	0.0	14564.9	24733.5	55102.1	24259.5	0.0	62.4	1770.9	46940.1
4	29425.9	0.0	16077.7	61230.9	50660.1	19463.2	21842.2	14688.8	15718.5	61358.8
5	34956.4	8601.2	6644.7	39526.8	50235.6	12852.9	14487.7	15035.5	22433.1	76223.3
6	0.0	22570.2	0.0	0.0	119712.7	27430.3	0.0	48686.8	0.0	132342.2
7	10335.5	2064.2	22102.6	48179.5	13112.7	6398.0	21842.2	20249.8	1575.7	32074.8
8	33793.4	14438.4	7450.4	40910.9	50221.6	16124.2	20735.6	17105.2	22785.9	75595.1
9	0.0	4209.1	50196.2	73234.2	14672.6	1590.0	0.0	34193.8	26916.9	14545.6
10	30851.5	3563.7	3184.2	37871.3	50237.9	23501.4	11813.3	16560.2	25543.8	75313.7
11	35132.2	10057.3	4190.8	40635.3	50210.7	13812.0	14086.5	14067.7	19371.7	75782.5
12	37326.2	12078.3	507.2	39699.2	50198.4	160.3	16247.7	19307.5	25771.7	76743.2
13	34644.6	16591.6	12936.0	48337.4	50204.3	12024.1	6647.0	14904.6	16717.8	76604.2
14	30815.6	11149.0	9824.8	39414.4	50220.1	12105.7	11850.6	18047.5	25113.8	76658.0
15	0.0	22570.2	2787.6	0.0	79826.2	27430.3	0.0	48686.8	0.0	132342.2
16	20069.8	6024.8	2133.2	23457.7	51011.5	20090.9	17821.5	24325.6	15857.1	99829.9
17	32395.2	7902.2	0.0	40276.1	50194.8	19730.2	19866.8	17071.4	27298.3	76813.0
18	33879.4	2612.0	7789.6	44646.3	50237.5	7076.9	15331.8	16021.8	23978.1	77959.6
19	27215.5	22570.2	4752.1	0.0	48949.8	0.0	21842.2	0.0	0.0	132342.2
20	37684.9	9337.3	1947.7	40715.6	50223.5	16457.2	21299.7	18907.7	22345.7	73572.0
21	31917.7	8881.7	776.9	39567.7	50797.0	21563.8	21313.5	29082.4	16420.3	62852.6
22	33540.0	0.0	8854.8	44024.1	50274.5	14350.3	20833.2	15265.8	23431.5	76955.9
23	33548.8	12953.4	6606.9	41021.7	50213.1	9596.3	18465.8	16763.8	22270.2	77142.8
24	34766.2	8968.8	5129.4	40962.2	50210.6	14327.5	14906.5	14152.5	19469.5	75920.7
25	75534.5	19511.9	26077.7	20254.7	50526.6	15507.9	19277.9	31899.3	11833.8	104044.3
26	35132.2	10057.3	4190.8	40635.3	50210.7	13812.0	14086.5	14067.7	19371.7	75782.5
27	36232.1	22563.1	12088.1	18799.0	50185.9	6055.9	21842.2	9300.2	25525.2	98219.1
28	34033.7	6639.7	5900.2	41952.4	50208.5	14772.8	16340.7	14501.2	21063.6	76093.0
29	35127.3	9334.9	6306.3	40599.7	50223.9	14623.6	15664.7	14198.7	19849.9	76018.4
30	35161.0	5015.8	6324.7	42904.4	50221.9	8210.4	6181.9	15602.6	22517.6	75041.1
31	27461.2	14318.4	0.0	33644.4	50251.1	20236.1	7696.1	6376.8	29484.7	79789.5
32	35101.5	10136.0	4177.7	40669.0	50210.9	13838.1	14206.0	14114.3	19506.0	75798.8
33	31579.5	0.0	5978.0	44002.6	50215.4	9869.1	6439.9	16774.0	27263.2	77567.6
34	16595.8	22566.2	50196.2	45028.9	50284.8	26247.3	5043.1	9031.1	12514.6	87359.5
35	35597.7	4677.4	4889.1	41529.6	50219.0	15545.2	20372.8	13964.4	20615.7	76026.1
36	36712.9	0.0	113.4	40850.8	50236.2	11928.3	16605.2	12339.9	20758.6	74471.0
37	35022.9	11459.8	1921.4	35298.0	116005.2	6846.6	14460.2	14907.9	38802.6	72741.3
38	26416.3	1538.5	16685.4	53295.1	50418.4	3136.4	0.0	7257.5	17975.6	90734.9
39	36436.6	2880.1	8783.9	42270.7	50217.5	7854.7	7711.5	12517.6	23895.9	76646.0
40	26566.4	19338.5	5325.7	38744.1	50644.5	24479.4	21842.2	6643.9	6999.7	90931.5
41	36397.1	22570.2	3980.4	36611.6	50177.4	0.0	0.0	17866.0	23073.8	79414.9
42	34980.8	13087.7	5660.4	40047.9	50211.6	12388.6	13340.3	15010.0	20951.3	76199.8
43	38491.8	12567.8	9607.5	49501.1	50175.0	4457.7	14295.8	16470.3	26321.7	90702.1
44	32569.4	15059.7	12310.7	41721.2	50207.4	17262.3	15689.8	13892.6	22374.2	77114.9
45	35116.7	11015.7	4919.4	42741.3	50213.8	12556.6	13797.0	14748.1	19089.0	75866.2
46	31544.0	15886.9	10326.7	37663.2	50358.8	15436.6	17727.6	18311.5	21885.2	79093.8
47	28883.3	7372.8	2856.0	39203.0	50319.5	17155.2	16311.0	21484.1	20930.6	74211.1
48	34394.1	9496.5	799.2	40898.5	50229.0	16384.4	19179.6	14922.6	20911.7	75969.6
49	30080.3	1192.4	8691.2	37035.7	50137.1	11715.7	10640.2	15588.4	27265.4	76818.9
50	23149.2	6581.6	2988.4	33100.5	55015.2	18517.7	16833.8	9280.5	14953.3	95059.5

Table H.1 Solution of 50 Hypothetical Scenarios for Stepwise-PLS Model (Stage-1) (Continued).

Scenario	**Emission Reduction (gm-mol)**								
No.	**pt2p1**	**pt3p1**	**pt4p1**	**pt5p1**	**pt6p1**	**pt12p1**	**pt30p1**	**pt63p1**	**pt64p1**
1	31366.0	53413.4	155518.5	6085.2	40019.1	53442.2	5004.9	3141.5	4450.9
2	24938.5	50322.4	155745.4	13216.5	39034.3	53450.4	5520.0	3141.5	906.5
3	64181.8	113149.7	99718.1	0.0	5493.6	56307.4	0.0	1257.3	1552.7
4	31565.1	43832.9	142291.8	0.0	28121.2	52046.5	1768.4	3141.5	6183.8
5	29838.5	53547.6	155424.4	5228.4	40383.7	53488.4	0.0	3141.5	0.0
6	0.0	0.0	0.0	45683.4	39765.2	46620.8	5520.0	3141.5	6705.8
7	78900.8	2870.2	129978.7	19807.8	26995.9	37055.4	5520.0	3141.5	6705.8
8	28033.9	54110.8	154781.9	7578.7	39892.2	53509.5	3156.6	3141.5	781.1
9	0.0	0.0	5779.0	42181.4	0.0	31097.5	5520.0	938.8	820.3
10	28902.0	55521.2	155745.4	6661.8	37623.9	53304.5	1115.4	3141.5	6705.8
11	28775.7	53942.4	155456.7	6409.6	40345.6	53520.9	3103.1	2225.4	5668.4
12	31440.7	54359.2	155745.4	7608.5	45073.1	53427.4	0.0	0.0	1094.5
13	28813.6	54745.7	154959.6	13123.6	40059.8	53509.2	5375.4	101.7	4115.0
14	28282.6	53022.8	154889.9	3348.9	40428.6	53516.7	1775.3	3141.5	4064.3
15	0.0	0.0	0.0	45683.4	0.0	58009.5	0.0	0.0	0.0
16	42530.0	32241.4	155745.4	4469.7	30898.0	53248.0	5520.0	3141.5	4951.2
17	30311.6	54579.8	155745.4	3599.1	36087.4	53408.2	5520.0	3141.5	5414.5
18	32098.4	55196.3	155745.4	754.5	37576.3	53397.8	0.0	444.6	0.0
19	0.0	97820.4	0.0	0.0	4379.5	23459.9	5520.0	3141.5	6705.8
20	30999.8	55319.6	155574.5	7023.0	37055.1	53387.2	703.9	3141.5	4072.9
21	20095.3	69975.9	155745.4	1169.5	12140.1	52770.1	5520.0	3141.5	6146.1
22	32260.1	53133.6	154902.7	0.0	36401.0	53420.1	1909.0	2741.3	5491.5
23	30291.6	52050.8	154633.6	5336.7	42091.1	53427.4	1828.9	3141.5	340.9
24	28874.7	53773.0	155323.2	6071.7	40554.5	53534.5	5520.0	3141.5	1765.6
25	15136.3	27419.2	148935.8	25740.1	20936.6	51470.3	5520.0	3141.5	1032.0
26	28775.7	53942.4	155456.7	6409.6	40345.6	53520.9	3103.1	2225.4	5668.4
27	11498.9	47848.5	155741.2	28086.9	35727.4	54090.2	5520.0	2214.4	0.0
28	29905.2	53894.6	155293.4	4204.5	40613.5	53510.1	1361.9	3141.5	0.0
29	29202.6	53688.2	155107.0	6262.2	40121.1	53500.6	3003.5	3141.5	0.0
30	29655.7	54779.7	155745.4	8551.3	41668.2	53485.9	0.0	0.0	0.0
31	23416.9	48108.7	155745.4	12572.1	31485.4	53271.2	5520.0	3141.5	1228.8
32	28792.6	53958.3	155487.1	6421.2	40364.6	53520.5	4239.7	3141.5	5185.5
33	31522.5	53988.5	155745.4	7213.9	38642.2	53377.1	205.3	0.0	0.0
34	13316.1	45745.8	155354.0	37656.7	22571.3	53561.9	5520.0	3141.5	6693.2
35	29772.0	54335.2	155471.7	5782.5	42423.5	53607.0	4420.1	3141.5	0.0
36	30336.2	54255.7	155745.4	9535.7	42659.9	53426.2	4597.9	3141.5	1120.1
37	93551.8	127355.5	75449.6	5977.1	12108.5	52389.5	0.0	3141.5	6705.8
38	27871.6	53847.2	155745.4	2296.3	18440.9	52960.2	5520.0	0.0	6049.7
39	29892.5	54283.4	155745.4	10937.0	42683.7	53468.4	0.0	261.4	0.0
40	23133.0	51544.2	155745.4	6303.2	12113.5	53243.9	5520.0	3141.5	6705.8
41	22918.1	60446.6	155745.4	15095.3	33915.8	53170.7	5520.0	191.8	0.0
42	29183.6	53472.0	155609.5	6598.2	41069.0	53521.7	5520.0	3141.5	1029.4
43	35285.6	46417.0	155745.4	12953.7	35730.1	52295.9	2633.1	0.0	773.4
44	28416.6	53305.3	155200.1	6339.6	39415.8	53534.8	5520.0	3141.5	2668.8
45	28834.1	54293.8	155503.8	8028.1	40189.7	53507.9	5520.0	708.8	910.2
46	25959.1	58517.6	155745.4	8783.7	35287.4	53351.2	5520.0	3141.5	2523.2
47	32260.6	51874.0	155152.8	4762.0	42786.4	53471.9	4205.2	3141.5	3632.8
48	28959.6	54183.6	155745.4	5436.1	41027.7	53525.2	5520.0	3141.5	2672.1
49	26050.9	56526.8	155745.4	10942.5	38895.4	53493.9	5520.0	1278.9	1395.5
50	37296.1	35568.9	155520.2	4190.5	44214.4	35291.0	4544.5	3141.5	4499.2

Table H.2 Solution of 50 Hypothetical Scenarios for Stepwise-PLS Model (Stage-2).

Scenario No.	Emission Reduction (gm-mol)									
	sq1_1p2	sq1_2p2	sq1_3p2	sq1_4p2	sq1_5p2	sq2_1p2	sq2_3p2	sq2_4p2	sq3_2p2	sq3_3p2
1	4993.7	0.0	23306.1	0.0	34460.4	24959.0	5419.3	16463.5	24748.1	474850.0
2	8562.8	0.0	23306.1	6062.5	31447.4	24959.0	19627.6	773.6	60063.5	334371.4
3	8562.8	5126.4	23306.1	38690.0	34460.4	24959.0	63289.9	41001.8	84067.8	190799.5
4	8562.8	14296.6	23306.1	38690.0	34460.4	24959.0	32862.1	0.0	96732.8	338320.1
5	8562.8	8029.7	23306.1	38690.0	11906.6	22145.5	27033.4	30625.9	28647.8	388020.9
6	0.0	7479.0	23306.1	0.0	33159.6	18144.8	6323.0	32374.5	69149.4	414315.9
7	0.0	27051.6	8832.7	0.0	9291.3	0.0	21364.3	0.0	97228.9	482243.5
8	0.0	21929.3	19861.2	7983.2	30380.5	19809.0	37584.1	46129.5	57485.0	442191.6
9	0.0	0.0	23306.1	0.0	34460.4	11040.1	0.0	11046.8	157844.2	169524.7
10	5061.3	10842.7	14852.1	6665.5	10409.8	12160.6	7107.6	42591.1	88729.9	262216.2
11	8562.8	0.0	23306.1	23140.9	34460.4	23465.3	0.0	24982.7	114534.7	373855.0
12	8562.8	0.0	23306.1	0.0	34460.4	24959.0	38199.6	3435.0	61936.9	377504.4
13	8562.8	0.0	23306.1	38690.0	34460.4	24959.0	0.0	31536.5	110324.2	304654.1
14	8562.8	21063.1	23306.1	38690.0	34460.4	24174.0	56604.0	9494.6	38410.3	322243.9
15	3717.8	6701.2	23306.1	2765.6	34460.4	24959.0	31506.8	55934.3	85854.6	264755.3
16	4367.2	0.0	23306.1	0.0	34460.4	13805.6	21250.3	13141.2	18427.8	436156.1
17	8562.8	0.0	23306.1	13178.4	34460.4	24959.0	8737.1	16424.3	32654.2	456528.1
18	8562.8	0.0	23306.1	31289.4	34460.4	24959.0	1564.4	3649.3	113800.3	407010.1
19	7486.6	0.0	23306.1	0.0	34460.4	3757.8	5388.6	0.0	0.0	486464.7
20	8562.8	1904.9	23306.1	38690.0	34460.4	24074.4	63289.9	0.0	39358.4	444008.2
21	4896.7	0.0	23306.1	0.0	34460.4	5978.6	31986.0	3471.6	6206.5	379793.9
22	8503.0	6019.5	23306.1	38690.0	34453.8	18764.0	47884.4	29340.5	24038.6	371666.8
23	8562.8	0.0	23306.1	38173.2	34460.4	24959.0	24445.1	52696.1	86543.3	370495.5
24	8562.8	27051.6	23306.1	38495.0	34460.4	24959.0	13642.4	589.4	56898.9	460340.4
25	8562.8	0.0	23306.1	0.0	34460.4	18658.3	8803.6	0.0	7513.4	486464.7
26	8562.8	20341.4	23306.1	33240.7	34085.1	24959.0	63289.9	15488.8	67549.5	486464.7
27	0.0	0.0	23306.1	0.0	34460.4	24838.8	512.7	51057.7	87291.3	327302.0
28	0.0	24318.5	23306.1	0.0	34460.4	24314.0	0.0	25821.5	46010.9	486464.7
29	4597.9	0.0	23306.1	14396.0	34460.4	24959.0	0.0	580.2	120754.7	411123.6
30	8562.8	27051.6	23306.1	38690.0	34460.4	24959.0	1032.1	0.0	58898.5	486464.7
31	0.0	0.0	23306.1	0.0	34460.4	10243.7	4912.1	5658.4	73746.7	424764.1
32	8562.8	0.0	0.0	0.0	34460.4	24959.0	0.0	0.0	126815.1	415988.3
33	8435.6	0.0	22667.6	28428.6	34460.4	16905.4	14554.9	19146.6	120037.0	337873.6
34	8100.8	805.1	23306.1	28819.2	34460.4	24959.0	11972.6	0.0	54643.0	327120.7
35	8562.8	0.0	23306.1	38675.2	34460.4	24959.0	16340.1	0.0	28628.6	416033.6
36	4050.3	0.0	23306.1	38690.0	34460.4	24959.0	0.0	82.3	59557.6	486464.7
37	8562.8	19334.5	23306.1	38690.0	34460.4	24959.0	60309.9	0.0	54428.6	322865.4
38	8562.8	0.0	23306.1	11629.1	34460.4	18565.2	8520.6	14355.9	120764.0	354305.7
39	8562.8	0.0	23306.1	8854.3	34460.4	24959.0	29124.7	10519.1	132274.2	396476.5
40	8562.8	0.0	23306.1	1053.9	34460.4	24959.0	57888.7	0.0	54328.9	415222.5
41	530.4	0.0	23306.1	0.0	34460.4	24959.0	63289.9	28474.5	49512.2	253831.7
42	0.0	0.0	23306.1	0.0	19152.3	17963.0	21067.0	20955.8	32425.5	401707.3
43	7838.1	1101.8	16187.2	31867.8	33380.2	15262.9	15923.3	21905.1	118906.5	328963.7
44	0.0	0.0	23306.1	0.0	34460.4	24959.0	0.0	21707.1	103925.6	329812.8
45	8562.8	0.0	23306.1	15735.0	34460.4	24481.0	7613.6	18176.7	120536.3	380497.3
46	8562.8	0.0	23306.1	12901.1	34460.4	24959.0	638.0	25466.7	119572.3	390338.2
47	8562.8	0.0	23306.1	0.0	34460.4	24959.0	60221.8	11568.8	95941.7	468958.8
48	0.0	0.0	23306.1	10533.1	34460.4	24959.0	0.0	1672.8	121865.0	385242.5
49	7703.2	1144.8	15944.0	31885.9	33291.8	15246.3	15906.8	21921.7	118896.3	328878.4
50	6511.6	0.0	23306.1	0.0	34460.4	24959.0	0.0	0.0	97791.6	393383.3

Table H.2 Solution of 50 Hypothetical Scenarios for Stepwise-PLS Model (Stage-2) (Continued).

Scenario No.	Emission Reduction (gm-mol)									
	sq3_4p2	sq3_5p2	sq4_2p2	sq4_3p2	sq5_1p2	sq5_4p2	pt1p2	pt2p2	pt3p2	pt4p2
1	52468.5	17483.0	39352.9	112151.5	0.0	7803.4	83362.6	46595.9	0.0	37402.5
2	30927.8	17483.0	38770.8	106150.8	0.0	18766.3	41279.8	33031.5	0.0	25070.0
3	33758.4	17483.0	39352.9	70589.6	10534.7	9605.3	104465.9	38787.1	53677.3	85344.6
4	28054.0	17483.0	28255.5	103767.8	5347.3	10927.8	89266.1	58474.6	69722.8	69626.1
5	86862.7	17483.0	9799.4	123643.4	0.0	3891.0	36435.2	121214.5	8007.4	28905.0
6	82762.6	17483.0	29677.0	134636.0	0.0	0.0	41654.2	2836.7	0.0	51437.2
7	36873.8	17483.0	39352.9	141864.6	0.0	7605.5	24777.7	2307.2	0.0	0.0
8	55081.2	16308.9	31232.9	125270.7	2295.1	10709.5	36615.7	15578.5	6013.6	18996.4
9	8080.9	17483.0	39352.9	55068.5	0.0	8872.7	78247.6	15689.6	40141.1	64524.6
10	16594.1	17360.5	18523.5	86080.3	3517.8	33432.2	69932.0	89923.4	47242.2	147983.2
11	25682.9	17483.0	35944.0	49310.6	11123.0	0.0	16108.6	25144.5	135121.5	87900.9
12	38267.1	17483.0	39352.9	121014.5	0.0	14222.8	55801.2	30999.0	172.2	26659.5
13	15486.9	17483.0	39352.9	100244.5	992.3	244.3	83410.2	0.0	19126.5	79877.4
14	47544.5	17483.0	39352.9	108685.5	0.0	16785.0	72726.0	43504.4	15403.5	37396.8
15	93096.1	17483.0	39352.9	84099.4	50.8	23626.0	62048.2	32043.3	38967.1	45446.6
16	62836.2	17483.0	28049.7	132964.5	0.0	1813.3	24848.0	76411.1	315.7	16705.2
17	25624.7	17483.0	39352.9	141864.6	3269.8	11443.5	16007.6	0.0	0.0	21538.6
18	12924.5	17483.0	39352.9	60496.2	126.4	0.0	24563.7	22943.8	132910.6	79939.8
19	38847.6	17483.0	39352.9	131625.6	807.3	2902.7	15236.9	31563.3	0.0	3387.5
20	54472.0	17483.0	0.0	141864.6	0.0	0.0	89273.2	36852.9	0.0	48164.7
21	43482.9	17483.0	39352.9	115426.6	0.0	5449.3	24616.8	18508.2	0.0	11508.5
22	41208.1	10180.4	38580.8	119456.7	3338.2	8584.6	56328.7	40414.9	6243.5	45484.5
23	50829.4	17483.0	31946.1	114620.5	2172.4	8901.8	69801.1	32963.1	66055.8	76403.7
24	39299.2	17483.0	22129.3	141864.6	0.0	7160.4	47114.5	0.0	14008.9	17082.2
25	1961.3	17483.0	39352.9	141864.6	0.0	3397.7	38475.8	22351.3	0.0	16945.5
26	15842.1	17483.0	39352.9	141864.6	0.0	0.0	61539.0	55811.7	5380.1	30898.0
27	46553.6	17483.0	39352.9	103121.2	0.0	714.2	39984.6	0.0	0.0	66591.9
28	42526.2	17483.0	34732.6	141864.6	0.0	6672.4	29051.9	0.0	0.0	29015.5
29	18493.5	17483.0	39352.9	60736.5	6830.3	0.0	18957.3	16870.9	131461.3	79132.7
30	6979.9	17483.0	39352.9	141864.6	0.0	0.0	132342.2	26610.3	40501.9	0.0
31	18708.5	17483.0	39352.9	83092.3	0.0	0.0	27322.6	17711.0	79047.9	53187.5
32	0.0	13867.1	38612.9	122869.2	11123.0	23799.9	0.0	11460.2	36858.8	33302.2
33	27981.9	17483.0	26093.1	37310.5	4754.8	493.9	21736.3	40413.3	141656.2	90447.6
34	51105.6	17483.0	38483.3	105277.3	0.0	16858.9	48473.4	32298.2	0.0	30058.4
35	6088.4	17483.0	39352.9	132704.2	0.0	8489.3	58061.6	25511.9	0.0	26451.4
36	93096.1	17483.0	39352.9	141864.6	0.0	0.0	57848.5	0.0	0.0	0.0
37	37801.2	17483.0	39352.9	107033.1	3200.8	15709.8	79222.7	64402.1	14699.3	40577.4
38	25833.3	17483.0	33675.3	41647.6	0.0	0.0	19338.9	35740.9	137098.5	87746.8
39	32085.6	17483.0	39352.9	50955.4	0.0	0.0	17508.0	33531.4	124282.3	81908.7
40	55808.7	17483.0	39352.9	124351.9	0.0	10711.2	38780.8	42238.9	0.0	19754.7
41	55456.5	17483.0	38859.6	81264.8	0.0	23833.5	50495.4	62852.3	12539.8	45968.5
42	85490.4	17483.0	13736.1	55418.6	5346.8	23034.5	105393.7	122639.3	5880.9	32172.5
43	29166.5	16998.9	23699.9	34896.1	9738.2	932.2	21819.0	42294.6	143396.0	91782.9
44	42680.2	17483.0	39352.9	96552.8	0.0	14078.7	47758.7	38047.6	52173.3	66864.7
45	27151.5	17483.0	39352.9	49532.2	0.0	0.0	16610.1	27753.9	130658.6	85357.8
46	28731.3	17483.0	37436.9	52912.7	5577.0	0.0	11320.0	21869.5	128621.8	83339.7
47	49074.0	17483.0	39352.9	141864.6	0.0	8736.1	39714.6	19278.5	0.0	7100.0
48	21855.3	17483.0	39352.9	115505.4	0.0	0.0	35387.5	0.0	0.0	36357.3
49	29173.5	16826.0	23661.0	34874.7	9836.6	939.4	21815.0	42305.4	143415.1	91787.6
50	3125.1	17483.0	38087.9	124070.0	11123.0	0.0	54251.0	0.0	0.0	46889.5

Table H.2 Solution of 50 Hypothetical Scenarios for Stepwise-PLS Model (Stage-2) (Continued).

Scenario No.	**Emission Reduction (gm-mol)**							
	pt5p2	**pt6p2**	**pt9p2**	**pt21p2**	**pt23p2**	**pt37p2**	**pt63p2**	**pt64p2**
1	45683.4	51682.0	13168.4	0.0	11.4	0.0	3141.5	6705.8
2	45683.4	29078.7	13168.4	0.0	27.4	0.0	3141.5	6705.8
3	45683.4	51682.0	13168.4	393.3	18.9	0.0	0.0	6705.8
4	45683.4	51682.0	13168.4	393.3	27.4	0.0	0.0	6705.8
5	24263.9	51682.0	13168.4	393.3	26.3	0.0	0.0	6705.8
6	0.0	41464.4	13168.4	142.0	27.4	0.0	222.3	6705.8
7	45683.4	29121.1	13168.4	0.0	27.4	0.0	0.0	6705.8
8	36257.2	41018.1	13168.4	0.0	27.4	0.0	2493.3	5322.1
9	45683.4	26119.6	13168.4	0.0	0.0	1.7	3141.5	6705.8
10	27150.3	11538.3	13168.4	393.3	0.0	1.7	3141.5	6705.8
11	42953.6	26269.0	13168.4	0.0	27.4	0.0	3141.5	6705.8
12	45683.4	38186.0	13168.4	0.0	27.4	0.0	3141.5	6705.8
13	45683.4	49754.6	13168.4	0.0	20.4	0.0	0.0	6705.8
14	45683.4	51682.0	13168.4	16.5	27.4	0.0	0.0	6705.8
15	45683.4	0.0	13168.4	0.0	27.4	0.0	3141.5	6705.8
16	37065.7	51682.0	13168.4	0.0	27.4	0.0	213.2	6705.8
17	45683.4	51682.0	13168.4	0.0	27.4	0.0	3141.5	6705.8
18	45683.4	42833.0	13168.4	0.0	27.4	0.0	0.0	6705.8
19	45683.4	51682.0	13168.4	0.0	27.4	0.0	0.0	6705.8
20	45683.4	51682.0	13168.4	393.3	24.3	0.0	3141.5	6705.8
21	45683.4	51682.0	13168.4	0.0	27.4	0.0	3141.5	6705.8
22	45676.2	41885.9	7685.2	393.3	13.2	0.4	1306.2	6698.0
23	45683.4	51593.2	13168.4	0.0	6.2	0.0	709.7	6705.8
24	45683.4	51682.0	13168.4	0.0	27.4	0.0	3141.5	6705.8
25	45683.4	51682.0	13168.4	0.0	27.4	0.0	0.0	6705.8
26	45456.1	51682.0	13168.4	108.9	26.2	0.0	869.9	6705.8
27	45683.4	51682.0	13168.4	0.0	27.4	0.0	3141.5	6705.8
28	44848.7	41758.8	13168.4	0.0	27.4	0.0	3141.5	6705.8
29	45683.4	18960.0	13168.4	0.0	27.4	0.0	3141.5	6705.8
30	45683.4	0.0	13168.4	0.0	27.4	0.0	0.0	6705.8
31	42138.6	37626.7	13168.4	0.0	27.4	0.0	1940.9	6705.8
32	45683.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0
33	15982.1	21407.3	13168.4	0.0	16.9	0.0	2283.5	6705.8
34	45683.4	17356.1	13168.4	0.0	14.6	0.0	3141.5	6705.8
35	45683.4	51682.0	13168.4	393.3	0.0	0.0	3141.5	6705.8
36	45683.4	20362.1	13168.4	0.0	5.1	0.0	3141.5	6705.8
37	45683.4	38516.9	13168.4	393.3	21.8	0.0	0.0	6705.8
38	23845.0	19312.4	13168.4	0.0	27.4	0.0	2746.2	6705.8
39	45683.4	35279.6	13168.4	0.0	27.4	0.0	0.0	6705.8
40	45683.4	51682.0	13168.4	0.0	27.4	0.0	3056.0	6705.8
41	45683.4	27775.9	13168.4	0.0	27.4	0.0	0.0	6705.8
42	45683.4	51682.0	13168.4	0.0	27.4	0.0	0.0	6705.8
43	10776.6	19442.2	7015.0	315.0	0.0	0.0	353.8	6089.4
44	45683.4	25951.8	13168.4	0.0	1.8	0.0	3141.5	6705.8
45	45683.4	30941.4	13168.4	0.0	0.0	0.0	3141.5	6705.8
46	45683.4	30147.3	13168.4	0.0	18.2	0.0	3141.5	6705.8
47	45683.4	51682.0	13168.4	0.0	27.4	0.0	3141.5	6705.8
48	45683.4	51682.0	13168.4	0.0	27.4	0.0	3141.5	6705.8
49	10706.4	19402.8	6832.8	257.4	21.9	0.7	267.2	4841.9
50	45683.4	51682.0	13168.4	0.0	27.4	0.0	3141.5	6705.8

Table H.3 Solution of 50 Hypothetical Scenarios for Stepwise-PLS Model (Stage-3).

Scenario No.	Emission Reduction (gm-mol)											
	sq1_3p3	**sq1_4p3**	**sq2_1p3**	**sq2_3p3**	**sq2_4p3**	**sq3_2p3**	**sq3_3p3**	**sq3_4p3**	**sq4_1p3**	**sq4_2p3**	**sq4_3p3**	**sq4_4p3**
1	24177.41	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
2	24177.41	39717.31	0	64932.2	41190.37	226875.3	497934.8	95090.77	0	40497.59	114317.8	0
3	24177.41	39717.31	0	64932.2	57417.17	226875.3	497934.8	95090.77	1177.125	40497.59	145179.9	0
4	24177.41	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	39155.12	40497.59	145179.9	0
5	24177.41	39717.31	25879.1	64932.2	0	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
6	24177.41	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	0	40497.59	0	0
7	24177.41	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	0	40497.59	38279.19	0
8	24177.41	39717.31	6598.911	64932.2	22960.77	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
9	24177.41	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
10	24177.41	39717.31	0	64932.2	57417.17	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
11	0	35273.82	25879.1	12147.72	3803.571	226875.3	497934.8	95090.77	0	31260.33	131080.8	0
12	24177.41	39717.31	25879.1	64932.2	0	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
13	16978.35	39717.31	25514.3	63333.74	57225.53	226875.3	497934.8	95090.77	33794.6	39746.28	144665	107126.6
14	24177.41	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	39155.12	40497.59	145179.9	0
15	24177.41	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	8639.433	40497.59	145179.9	0
16	24177.41	39717.31	25879.1	64932.2	0	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
17	24177.41	39717.31	25879.1	64932.2	0	226875.3	497934.8	95090.77	0	40497.59	53000.98	0
18	24177.41	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
19	24177.41	39717.31	0	64932.2	0	226875.3	497934.8	95090.77	0	0	145179.9	0
20	24177.41	39717.31	25879.1	64932.2	0	226875.3	497934.8	28208.42	0	40497.59	145179.9	0
21	24177.41	39717.31	4341.854	64932.2	0	226875.3	497934.8	95090.77	0	0	145179.9	0
22	0	39717.31	20283.74	0	0	226875.3	497934.8	83016.15	0	4915.588	120763.2	0
23	24177.41	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
24	24177.41	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
25	24177.41	39717.31	3990.152	64932.2	0	226875.3	497934.8	95090.77	0	0	145179.9	0
26	24177.41	39717.31	0	64932.2	0	226875.3	497934.8	0	0	40497.59	145179.9	0
27	24177.41	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
28	24177.41	39717.31	24913.35	64932.2	52423.94	226875.3	497934.8	95090.77	0	40497.59	61024.71	0
29	0	37507.38	25879.1	19532.55	57417.17	226875.3	497934.8	95090.77	0	39149.12	135224.9	0
30	24177.41	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
31	24177.41	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
32	24177.41	39717.31	0	64932.2	57417.17	226875.3	497934.8	95090.77	0	40497.59	126039	0
33	0	39717.31	25879.1	46623.59	52232.88	226875.3	497934.8	93357.03	0	40497.59	145179.9	75304.9
34	24177.41	39717.31	0	64932.2	0	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
35	0	39717.31	25879.1	0	57417.17	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
36	24177.34	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	39155.08	40497.59	145179.9	108321.9
37	24177.41	39717.31	25879.1	64932.2	0	226875.3	497934.8	73991.48	0	40497.59	145179.9	0
38	24177.41	39717.31	25879.1	64932.2	0	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
39	24177.41	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
40	24177.41	39717.31	25879.1	64932.2	0	226875.3	497934.8	0	0	40497.59	145179.9	0
41	24177.41	39717.31	11457.08	64932.2	0	226875.3	497934.8	16365.14	0	0	145179.9	0
42	24177.41	39717.31	0	64932.2	0	226875.3	497934.8	95090.77	0	0	145179.9	0
43	12900.1	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	0	40497.59	145179.9	95549.7
44	24177.41	39717.31	15967.79	64932.2	57417.17	226875.3	497934.8	94750.23	0	40497.59	145179.9	21859.32
45	0	39717.31	0	0	57417.17	226875.3	497934.8	95090.77	0	10205.15	145179.9	0
46	0	39717.31	25879.1	0	55243.02	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
47	24177.41	39717.31	25879.1	64932.2	53227.27	226875.3	497934.8	95090.77	0	40497.59	108247	0
48	24177.41	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	0	40497.59	145179.9	0
49	0	39717.31	0	0	0	226875.3	497934.8	95090.77	0	0	0	0
50	24177.41	39717.31	25879.1	64932.2	57417.17	226875.3	497934.8	95090.77	0	40497.59	145179.9	0

Table H.3 Solution of 50 Hypothetical Scenarios for Stepwise-PLS Model (Stage-3) (Continued).

Scenario	Emission Reduction (gm-mol)											
No.	sq4_5p3	sq5_5p3	pt1p3	pt2p3	pt3p3	pt4p3	pt5p3	pt6p3	pt15p3	pt23p3	pt30p3	pt63p3	pt64p3
1	0	1.46009	132342.2	134419.1	150840	155745.4	45683.38	17093.17	137312.2	0	5519.951	3141.544	0
2	0	0.511032	132342.2	134419.1	150840	0	45683.38	31973.76	137312.2	0	5519.951	3141.544	4362.587
3	19578.06	17626.32	132342.2	134419.1	150840	0	0	51682	0	0	5519.951	3141.544	0
4	19578.06	0	132342.2	134419.1	150840	0	0	51682	0	0	5519.951	3141.544	0
5	0	0	132342.2	134419.1	0	155745.4	45683.38	51682	137312.2	0	5519.951	3141.544	0
6	0	0	132342.2	134419.1	150840	155745.4	45683.38	51682	137312.2	0	5519.951	3141.544	0
7	0	0.730045	132342.2	134419.1	150840	155745.4	45683.38	51682	137312.2	0	5519.951	3141.544	0
8	0	0.584036	132342.2	134419.1	150840	155745.4	45683.38	20555.76	137312.2	0	5519.951	3141.544	0
9	0	0	132342.2	134419.1	150840	155745.4	45683.38	51682	137312.2	0	5519.951	3141.544	0
10	0	0	132342.2	134419.1	150840	155745.4	45683.38	51682	137312.2	0	5519.951	0	0
11	0	36203.38	132342.2	134419.1	150840	155745.4	45683.38	51682	127955.6	0	0	3141.544	6705.77
12	0	0	132342.2	134419.1	150840	155745.4	45683.38	0	137312.2	0	5519.951	3141.544	0
13	10544.29	36429	132342.2	134419.1	150840	155745.4	45683.38	51682	137312.2	0	0	3141.544	6705.77
14	19578.06	0	132342.2	134419.1	150840	0	0	51682	0	0	5519.951	3141.544	0
15	4319.825	16688.43	132342.2	134419.1	150840	81943.45	35603.51	51682	63538.96	0	5519.951	3141.544	0
16	0	0	132342.2	134419.1	0	0	45683.38	51682	135985.7	0	5519.951	3141.544	0
17	0	2.153633	132342.2	134419.1	150840	88639.41	45683.38	5891.126	6411.573	0	5519.951	3141.544	0
18	0	0	132342.2	64571.01	150840	155745.4	45683.38	0	137312.2	0	5519.951	3141.544	0
19	0	0	132342.2	134419.1	150840	155745.4	45683.38	51682	83753.99	0	5519.951	2167.165	6705.77
20	0	2.117131	132342.2	134419.1	150840	155745.4	45683.38	51682	0	0	5519.951	3141.544	0
21	0	5.32933	132342.2	134419.1	0	0	45683.38	51682	0	0	5519.951	3141.544	6705.77
22	0	36287.59	132342.2	134419.1	150840	155745.4	45683.38	51634.41	137312.2	0	0	3141.544	3525.998
23	0	0	132342.2	0	150840	155745.4	45683.38	0	137312.2	0	5519.951	3141.544	0
24	0	0	132342.2	134419.1	150840	155745.4	45683.38	51682	137312.2	0	5519.951	3141.544	0
25	0	0	132342.2	134419.1	0	0	45683.38	51682	0	0	5519.951	3141.544	6705.77
26	0	0	132342.2	134419.1	0	0	45683.38	51682	0	0	5519.951	3036.246	6705.77
27	0	0	132342.2	134419.1	150840	155745.4	45683.38	51682	137312.2	0	5519.951	3141.544	0
28	0	18126.37	132342.2	97443.36	87304.63	87516.73	45683.38	49342.02	92893.65	0	5519.951	3141.544	0
29	0	14745.27	132342.2	134419.1	150840	155745.4	45683.38	43138.78	137312.2	0	0	3141.544	6705.77
30	0	0	132342.2	134419.1	150840	43875.1	45683.38	2336.824	137312.2	0	5519.951	3141.544	0
31	0	0	132342.2	134419.1	150840	155745.4	45683.38	51682	137312.2	0	5519.951	3141.544	0
32	0	0.438027	132342.2	134419.1	150840	26879.97	45683.38	51682	137312.2	0	5519.951	3141.544	0
33	0	36336.98	132342.2	134419.1	150840	155745.4	45683.38	0	137312.2	0	5519.951	3141.544	6705.77
34	0	0	132342.2	134419.1	150840	0	45683.38	31950.14	137312.2	0	5519.951	3141.544	1846.096
35	0	15488.49	132342.2	1036.024	150840	155745.4	45683.38	0	137312.2	0	5519.951	3141.544	6705.77
36	19577.96	36429.26	132342.2	134419.1	150840	155745.4	45683.38	51682	137312.2	0	5519.879	3141.544	6705.77
37	0	0.474529	132342.2	134419.1	150840	155745.4	45683.38	51682	137312.2	0	5519.951	171.5919	0
38	0	0	132342.2	134419.1	150840	155745.4	45683.38	0	137312.2	0	5519.951	3141.544	0
39	0	0.657041	132342.2	134419.1	150840	106958.8	45683.38	0	137312.2	0	5519.951	3141.544	0
40	0	5.292828	132342.2	134419.1	0	0	45683.38	51682	0	0	5519.951	3141.544	5565.137
41	0	1.606099	132342.2	134419.1	0	0	45683.38	51682	0	0	5519.951	3141.544	6705.77
42	0	7.847986	132342.2	134419.1	6669.154	0	45683.38	51682	0	0	5519.951	1562.685	6705.77
43	0	36423.38	132342.2	134419.1	150840	155745.4	45683.38	49624.61	137312.2	0	5519.951	3141.544	4031.108
44	0	18189.22	108636.1	79090.97	91767.56	90906.93	45683.38	51682	85084.32	0	5519.951	936.4698	0
45	0	18108.77	132342.2	134419.1	150840	155745.4	45683.38	51682	137312.2	0	0	1890.974	6705.77
46	0	0	132342.2	134419.1	150840	155745.4	45683.38	51682	137312.2	0	5519.951	3141.544	6705.77
47	0	0.620538	132342.2	134419.1	150840	155745.4	45683.38	26041.77	137312.2	0	5519.951	3141.544	0
48	0	0	132342.2	134419.1	150840	106592.1	45683.38	51682	137312.2	0	5519.951	3141.544	0
49	0	0	132342.2	134419.1	150840	155745.4	45683.38	51682	137312.2	0	0	3141.544	6705.77
50	0	0	132342.2	134419.1	150840	155745.4	45683.38	51682	137312.2	0	5519.951	3141.544	0

Table H.4 Solution of 50 Hypothetical Scenarios for Stepwise-PLS Model (Stage-4).

Scenario No.	**Emission Reduction (gm-mol)**						
	sq1_1p4	**sq1_3p4**	**sq1_4p4**	**sq3_2p4**	**sq3_3p4**	**sq4_2p4**	**sq4_3p4**
1	0	0.896884	0	282611.6	396217	51779.39	0
2	0	3.742169	2.519557	282611.6	385864.9	51779.39	0
3	0	0	0	282611.6	656174.6	51779.39	0
4	0	3.154556	3.284423	282611.6	560637.4	51779.39	0
5	1.295177	0	3.464391	282611.6	422400.9	51779.39	0
6	0	0	0	282611.6	656174.6	51779.39	0
7	0	0.030927	3.464391	30207.16	623745.3	40624.51	0
8	1.46464	0	0	282611.6	319708.3	51779.39	0
9	0	0	0	282611.6	656174.6	51779.39	0
10	0	0	0	282611.6	656174.6	51779.39	0
11	0	4.515345	0	282611.6	518442.4	51779.39	0
12	0.871521	0	0	282611.6	436991.3	51779.39	0
13	0.012104	0	0	282611.6	439721.2	51779.39	13.87582
14	0	0.773176	0	282611.6	500737.5	51779.39	0
15	0	0	0	282611.6	656174.6	51779.39	0
16	0	0	1.664707	282611.6	537510.2	51779.39	0
17	0.919939	0	0	282611.6	388579.6	51779.39	0
18	0.738372	0.587613	0	282611.6	409723.2	51779.39	0
19	0	0	0	282611.6	656174.6	51779.39	0
20	0.859417	1.979329	2.249604	282611.6	503836.3	51779.39	0
21	0	0	0	282611.6	461597.1	51779.39	7.125422
22	0	3.340118	0	282611.6	290589.4	51779.39	3.187689
23	0.762581	0	0.494913	282611.6	478820.7	51779.39	6.937911
24	0.823103	4.020513	0	282611.6	492962.7	51779.39	0
25	0	1.731913	0	282611.6	517070.2	51779.39	0
26	0	0	0	282611.6	529185.8	51779.39	0
27	0	0	0.85485	282611.6	400066	51779.39	4.125244
28	0	0	0	30207.16	446396	49770.22	0
29	0	0	1.844676	282611.6	454287.8	51779.39	0
30	0.435761	0	0	282611.6	519069.6	51779.39	0
31	0	0	0	282611.6	517956.5	51779.39	0
32	0	0	0	282611.6	656174.6	51779.39	0
33	1.343595	0	3.104454	282611.6	404342.3	51779.39	0
34	0	1.298935	0	282611.6	487490.4	51779.39	0
35	1.258864	0	0	282611.6	528384.3	51779.39	0
36	0	0	1.979652	282611.6	499248.3	51779.39	0
37	0	0	0	282611.6	538216.4	51779.39	6.562889
38	0	1.670059	1.844676	282611.6	378988.2	51779.39	0
39	1.525162	0	0.764866	282611.6	443559.6	51779.39	9.375555
40	0	0.865957	0	282611.6	559586.1	51779.39	0
41	0.375238	0	0	282611.6	536684.4	51779.39	2.250133
42	0.980461	0	0.629889	282611.6	415489.4	51779.39	6.937911
43	0	0	0	282611.6	336820.1	51779.39	4.125244
44	1.22255	0	0	29956.27	578606.6	24048.73	0
45	0	0	0	282611.6	457269.6	51779.39	0
46	0.133149	0	2.249604	282611.6	535116.3	51779.39	0
47	0.447865	0.061854	0	282611.6	437758.5	51779.39	10.50062
48	0	0	0	30207.16	543227.8	49448.02	0.750044
49	0	0	5.129098	282611.6	600703.5	51779.39	0
50	1.68252	0	0	226956.7	656174.6	51779.39	0

REFERENCES

Adda, J., & Cooper, R. W. (2003). *Dynamic economics*. Cambridge: MIT Press.

Ariyajunya, B., Chen, V. C. P., & Kim, S. B. (2010, June). Orthogonalized dynamic programming state space for efficient value function approximation. In *Proceedings of the 2010 IE Research Conference*, Cancun, Mexico.

Benjamini, Y., & Hochberg, Y. (1995). Controlling the false discovery rate-a practical and powerful approach to multiple testing. *Journal of The Royal Statistical Society Series B-Methodological*, *57*(1), 289-300.

Bellman, R. (1957). *Dynamic programming*. Princeton: Princeton University Press.

Bertsekas, D. (2005). *Dynamic programming & optimal control*. Belmont, Mass: Athena Scientific.

Bertsekas, D. & Tsitsiklis, J. (1996). *Neuro-dynamic programming*. Belmont: Athena Scientific.

Breiman, L., Friedman, J. H., Olshen, R. A., and Stone, C. J. (1984). *Classification and regression trees*. New York, N.Y: Chapman & Hall.

Burkhauser, R. V., Butler, J. S. & Gumus, G. (2004). Dynamic programming model estimates of Social Security Disability Insurance application timing. *Journal of Applied Econometrics*, *19*(6), 671–685. doi: 10.1002/jae.804

Chen, V. C. P., Tsui, K.-L., Barton, R. R., & Meckesheimer, M. (2006). Design, modeling, and applications of computer experiments, *IIE Transactions*, *38*(4), 273–291.

Chen, V. C. P., Ruppert, D., & Shoemaker, C. A. (1999). Applying experimental design and regression splines to high-dimensional continuous-state stochastic dynamic programming. *Operations Research*, *47*(1), 38–53.

Hocking, R. R. (1976). The analysis and selection of variables in linear regression, *Biometrics*, *32*(1), 1-49.

Kim, S. B. (2009). Feature extraction/ selection in high-dimensional spectral data. In Wang, J. (Ed.), *Encyclopedia of Data Warehousing and Mining*. (Vol. 2, pp. 863-869). Hershey, PA: Information Science Reference.

Kutner, M. H., Nachtsheim, C. J., Neter, J., & Li, W. (2005). *Applied linear statistical models*. Boston: McGraw-Hill Irwin.

Martinez, N. M., Martinez, D. L., Rosenberger, J. M., & Chen, V. C. P. (2011, May). Global optimization for a piecewise linear regression spline function. In *Proceedings of the 2011 IE Research Conference*, Reno, NV.

Powell, W. (2011). *Approximate dynamic programming: solving the curses of dimensionality*. Hoboken, N.J: Wiley.

Shih, D. T., Martinez, D. L., Chen, V. C. P., & Kim, S. B. (2012). A convex version of multivariate adaptive regression splines (COSMOS Technical Report 12-01). The University of Texas at Arlington. Arlington, TX.

Shih, D. T., Pilla, V. L., Kim, S. B., Rosenberger, J. M., & Chen, V. C. P. (2006, November). Efficient computer experiment-based optimization through variable selection. In *Proceedings of INFORMS Workshop on Artificial Intelligence and Data Mining*, Pittsburgh, PA.

Shih, D. T. (2006). Convex versions of multivariate adaptive regression splines and implementations for complex optimization problems. (Doctoral dissertation). Retrieved from Dissertations and Theses database. (UMI No. 3242658)

Si, J., Barto, A. G., Powell, W. B., & Wunsch, D. (2004). *Handbook of learning and approximate dynamic programming*, Piscataway, NJ: IEEE Press Wiley-Interscience.

SIP (2001). *Georgia's State Implementation Plan for the Atlanta Ozone Non-attainment Area*, Environmental Protection Division, Georgia Department of Natural Resources, Atlanta, Georgia.

Sobol´, I. M. (1967). The distribution of points in a cube and the approximate evaluation of integrals. *USSR Computational Mathematics and Mathematical Physics, 7*(4), 86-112.

Sule, N., Chen, V. C. P., & Sattler, M. L. (2011). A decision-making framework for assessing control strategies for ground-level ozone. *Atmospheric Environment*, *45*(28), 4996–5004.

NAG Inc. (2002). *The NAG C Library Manual (Mark 7)*. Oxford, UK: Author.

NAG Inc. (1991). *The NAG Fortran Library Manual (Mark 15)*. Oxford, UK: Author.

Tejada-Guibert, J. A., Johnson, S. A., Stedinger, J. R. (1993). Comparison of two approaches for implementing multi-reservoir operating policies derived using dynamic programming. *Water Resources Research*, *29*(12), 3969-3980.

Tsai, J. C. C., Chen, V. C. P., Beck, M. B., Chen, J. (2004). Stochastic dynamic programming formulation for a wastewater treatment decision-making framework. *Annals of Operations Research*, *132*(1–4), 207–221. doi:10.1023/B:ANOR.0000045283.86576.62.

van der Voet, H. (1994). Comparing the predictive accuracy of models using a simple randomization test. *Chemometrics and Intelligent Laboratory Systems*, *25*(2), 313–323.

Wold, S., Sjöström, M., & Eriksson, L. (2001). PLS-regression: a basic tool of chemometrics. *Chemometrics and Intelligent Laboratory Systems*, *58*(2), 109-130.

Yang, Z., Chen, V. C. P., Chang, M. E., Sattler, M. L., & Wen, A. (2009). A decision-making framework for ozone pollution control. *Operations Research*, *57*(2), 484-498.

Yang, Z., Chen, V. C. P., Chang, M. E., Murphy, T. E., & Tsai. J. C. C. (2007). Mining and modeling for a metropolitan Atlanta ozone pollution decision-making framework. *IIE Transactions*, *39*(6), 607–615.

Yang, Z. (2004). A decision-making framework for ozone pollution control. (Doctoral dissertation). Retrieved from Dissertations and Theses database. (UMI No. 3145840)

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Bancha Ariyajunya was born in Chonburi, Thailand in 1977. He received his Bachelor of Engineering degree in Industrial Engineering from Burapha University, Thailand in 1999. He received his Master of Engineering degree in Manufacturing Systems Engineering from Asian Institute of Technology, Thailand, in 2002 on the thesis topic of "Geometric Error Identification and Compensation in Five-Axis CNC Milling Machines" (Advisor: Associate Professor Erik L. J. Bohez). In 2008, he started his Doctor of Philosophy degree in Industrial Engineering at the University of Texas at Arlington and his dissertation topic was “Adaptive Dynamic Programming for High-Dimensional, Multicollinear State Spaces”. During his doctoral study at UTA, he has worked as a Graduate Research Assistant with Dr. Victoria Chen in the National Science Foundation (NSF) funded project of “Statistically Parsimonious Adaptive Dynamic Programming for Minimizing the Environmental Impact of Airport Deicing Activities”. His current research interest is in the area of statistical modeling and data mining.