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Sensitivity Analysis of the UNO Activated Sludge Model

A Thesis

Submitted to the Graduate Faculty of the
University of New Orleans
in partial fulfillment of the
requirements for the degree of

Master of Science
in
Environmental Engineering

by

Ysabel Vilorio

B.S., Universidad de Zulia, 2001

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Abstract

Different types of mathematical models have been proposed to predict the activated sludge process final effluent quality. La Motta (2004b) developed a mathematical model linking the operating parameters of an activated sludge system and the classical limiting flux sludge settling theory.

This project studies the estimation of the unknown parameters of La Motta's model and also the model's sensibility. To obtain unknown parameters true values Full Information Maximum Likelihood (FIML) estimator is used, it will converge on a set of values that satisfy all the estimating equation simultaneously. Favorable results were obtained when correlations are applied between predicted values using estimated kinetics parameters and the observed values obtained from activated sludge pilot plant located within installations of the Marrero Wastewater Treatment Plant, New Orleans, Louisiana.

Constructive results about the sensibility of the model are also obtained demonstrated that the model is affected significantly to the variation of some kinetics parameters.

1. Introduction

1.1 Background

Mathematical modeling is a useful tool for the design, analysis and control of wastewater treatment systems. The activated sludge process is one of the most common processes used in wastewater treatment, and therefore, it is a particularly important candidate for the application of mathematical models.

In the 1980s, a task group organized by the International Association on Water Quality (IAWQ) developed a conceptual model of the activated sludge process, which has become an industry-wide standard for the development of computer-based activated sludge models. All these models, including the commercial versions that are widely used by industry, have ignored the role of biological flocculation on the removal of colloidal particles from wastewater. La Motta et al. (2007) recently published a new steady state mathematical model of suspended growth reactors linked with a one-dimensional settling tank model, which takes into consideration the kinetics of biological flocculation. This model was tested using experimental data collected at a pilot plant; the kinetic coefficients used for testing the model accuracy were selected using previous batch kinetic studies, as well as by trial and error.

There are two major methods for parameter estimation in process modeling: the three-stage least squares method (3SLS) and the full information maximum likelihood method (FIML). Both of these methods provide parameter estimators that have many

good properties. When the parameter estimates have been made, the model is then cautiously evaluated to see if the basic assumptions of the analysis appear reasonable.

This present investigation will use FIML method to determine the kinetic coefficients of the UNO Activated Sludge Model, and will develop a sensitivity analysis to assess the relative importance of such coefficients in predicting the quality of the final effluent.

1.2 Objectives and scope

The main objective of this research is to a conduct sensitivity analysis of the UNO Activated Sludge Model. This research was developed using the data previously collected by Rojas (2004), and the following software packages: TSP/Give Win2, and the 1D UNO Activated Sludge Model software prepared by Homes and La Motta (2004).

The specific objectives of this project are the following:

- Introduce the three-stage least squares method (3SLS) and the full information maximum likelihood method (FIML) for parameter estimation when solving systems of simultaneous equations.
- Introduce the statistical software TSP to the environmental engineering community. This software is a world-wide standard for econometric estimation.
- Conduct a statistical regression analysis on existing activated sludge pilot plant data to determine the kinetic coefficients of the UNO model.
- Conduct the respective sensitivity analysis and provide a set of recommendations regarding the importance of certain kinetic coefficients when

making decisions related to the design and operation of activated sludge systems.

2. Literature Review

2.1 Activated Sludge Model

2.1.1 Activated Sludge Treatment Process:

The activated sludge process was developed around 1913 at the Lawrence Experiment Station in Massachusetts by Clark and Gage (Metcalf and Eddy, 1930), and by Arden and Lockett (1914) at the Manchester Sewage Works in Manchester, England. The activated-sludge process was so named because it involved the production of an activated mass of microorganisms capable of stabilizing a waste under aerobic conditions.

An important feature of the activated sludge process is the formation of floc particles, which can be removed by gravity settling, leaving a relatively clear liquid as the treated effluent (Metcalf and Eddy, 2003).

The activated sludge system is by far the most commonly employed biological process used for treatment of industrial and municipal wastewaters (Dwight et al., 1997).

Engineering innovation, technological advances in equipment and better understanding of microbiological processes have resulted in different configurations of the activated sludge process (Mecalf & Eddy., 2003).

Three major processes take place in an activated sludge system: First, microorganisms grow in an aeration tank using the substrate available in the wastewater, flocculate themselves, and become settleable particles. Second, the settleable particles are removed by gravity in a sedimentation tank. Third, solids removed from the sedimentation tank are returned through a recycle line to the aeration basin (La Motta et al., 2007).

2.1.2 Flocculation in Wastewater Treatment

Flocculation is a transport step that brings about the collisions between the destabilized particles needed to form larger particles that can be removed readily by settling or filtration. The purpose of wastewater flocculation is to form aggregates or flocs from finely divided particles and from chemically destabilized particles.

There are two types of flocculation: microflocculation and macroflocculation. Microflocculation, also known as perikinetic flocculation, is the term used to refer to the aggregation of particles brought about by the random thermal motion of fluid molecules. Its size range from 0.001 to about 1 μm . Macroflocculation, also known as orthokinetic flocculation, is the term used to refer to the aggregation of particles greater than 1 or 2 μm (Mecalf & Eddy., 2003).

According to Clauss et al. (1998), several parameters such as floc size and density provide an indication as to how to achieve good activated biomass separation from the treated wastewater. In order for the activated sludge to operate successfully, a

flocculent biomass that settles rapidly and compacts correctly in the clarifier must be developed. (Grady, 1999).

2.1.3 Microbial Growth Kinetics

The performance of biological processes used for wastewater treatment depends on the dynamics of substrate and microbial growth. Biological flocculation takes place due to action of bacterial exocellular polymers on colloids and other finely divided particles. The most common mechanism of particle flocculation is chemical bridging. This process occurs when a coagulant substance (exocellular polymers) forms threads or fibers, which attach to several colloids, capturing and binding them together (Spicer et al., 1996, Metcalf and Eddy, 2003). A review of the equations developed by La Motta (2004) is presented below.

Rate expressions for production and consumption of soluble substrate

- Rate of biomass growth in the aeration tank

La Motta (2004) considered that the growth of MLSS in the aerator takes place by microbial growth (net growth) and by biological flocculation of inorganic and organic particles contained in the wastewater. Under steady-state conditions, there is an existing mass of SS in the reactor, which is already flocculated. The equation that follows this assumption is given by:

$$r_g = r_{ng} + r_f \quad (2.1)$$

Parker et al. (1970) demonstrated that the rate of biological flocculation in suspended growth reactors follows a first-order expression, such as Eq. (2). This was confirmed later by La Motta and coworkers (La Motta et al. 2007; Jimenez et al 2005).

$$r_f = k_x(X_e - a_x) \quad (2.2)$$

Where:

r_{ng} = net rate of growth of microorganisms, Kg SS/ Kg MLSS day

r_f = rate of flocculation of particles, Kg SS/ Kg MLSS day

a_x = kinetic parameter of TSS flocculation, Kg/m³

k_x = first order constant of TSS flocculation, m³/day Kg

X_e = suspended solids concentration in the final effluent, Kg/m³

- Rate of disappearance of dissolved COD

As indicated by Metcalf and Eddy (2003), the rate of disappearance of dissolved COD is given by:

$$-U = \frac{1}{Y} \cdot (r_{ng} + k_d) \quad (2.3)$$

Where:

k_d = endogenous respiration coefficient, day⁻¹

U = rate of uptake of dissolved COD, Kg COD/Kg MLSS day

Y = true yield coefficient, Kg biomass/Kg DCOD consumed

Knowing that hydrolysis is a slow process and that it would not be released to the bulk of the liquid, a mass balance on dissolved COD, S , around the aeration yields the following equation:

$$-U = \frac{(1 - f_p) \cdot (S_{T_i} - S_T)}{X \cdot \bar{t}} \quad (2.4)$$

Where:

f_p = PCOD/TCOD

S_T = total COD concentration in the aerator, Kg/m³

S_{Ti} = total COD concentration in the influent stream, Kg/m³

Subsequently, a combination of equations yields equation 2.5:

$$r_g = \frac{Y}{X \cdot \bar{t}} \cdot (1 - f_p) \cdot (S_{Ti} - S_T) + k_x \cdot (X_e - a_x) - k_d \quad (2.5)$$

2.1.4 Solids Retention Time

La Motta's activated sludge model assumes that the settling tank can be described by the one-dimensional limiting flux theory, under steady-state conditions. This analysis will refer to a completely mixed activated sludge system, as sketched in Figure 2.1. A steady-state mass balance on suspended solids in the reactor yields the following relationship (La Motta et al., 2007):

$$X \cdot \bar{t} \cdot r_g + X_i = (1 + \alpha) \cdot X - \alpha \cdot X_R \quad (2.6)$$

The equilibrium of solids in the overall system can be written as follows: mass produced – mass removed = accumulation. Assuming no accumulation of solids, the following equation is applicable:

$$X \cdot \bar{t} \cdot r_g + X_i - w \cdot X_R - (1 - w)X_e = 0 \quad (2.7)$$

Where:

r_g = rate of growth of suspended solids, Kg SS/Kg MLSS day

V_r = reactor (aerator) volume, m³

V_s = settling tank volume, m³

\bar{t} = hydraulic retention time (V_r/Q), days

X = MLSS concentration in the influent to the aerator, Kg/ m³

X_e = SS concentration in the final effluent, Kg/ m³

X_R = SS concentration in the recycle line, Kg/ m³

X_w = SS concentration in the waste stream, Kg/ m³

α = recycle ratio, $\frac{Q_R}{Q}$

w = waste ratio, $\frac{Q_w}{Q}$

Q = influent flow rate, m³/d

Q_R = recycle flow rate, m³/d

Q_w = waste sludge flow rate, m³/d

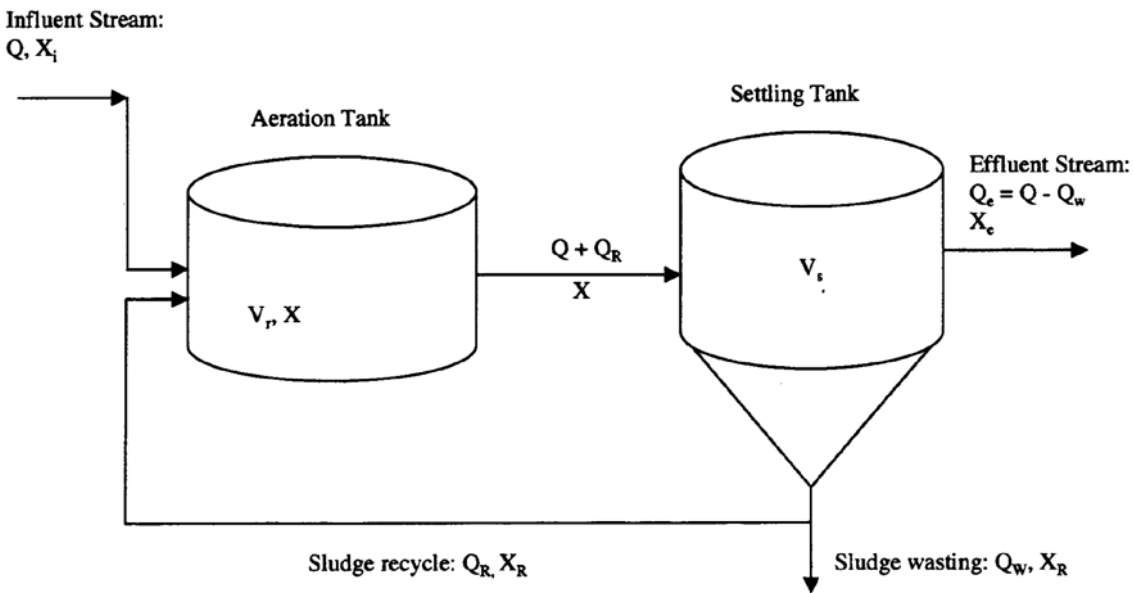


Figure 2.1 Complete-Mix Aerator Tank with Sludge Recycle. (La Motta, 2004)

Using the basic assumption of one-dimensional limiting flux theory, under steady-state conditions and under the assumption of no biological growth in the settling tank, the following definition of solids retention time is appropriate:

$$\bar{t}_c = \frac{X \cdot \bar{t} \cdot \left(1 + \frac{V_s}{V_r}\right)}{w \cdot X_R + (1-w) \cdot X_e} \quad (2.8)$$

La Motta (2004) developed a combination of equations from equation 2.1 all the way through equation 2.8 and found the following equation on solids retention time:

$$\bar{t}_c = \frac{\bar{t} \cdot X \cdot \left(1 + \frac{V_s}{V_r}\right)}{X_i + Y \cdot (1 - f_p) \cdot (S_{T_i} - S_T) + \bar{t} \cdot X \cdot [k_x \cdot (X_e - a_x) - k_d]} \quad (2.9)$$

2.1.5 The Sludge Settling Characteristics

For a settling tank with cross sectional area A to be able to handle an activated sludge suspension with a concentration X_R and with a limiting flux F_L , applied at a flow rate $Q(\alpha+w)$, the following relationship must hold:

$$\frac{F_L \cdot A}{Q} = (\alpha + w) \cdot X_R \quad (2.10)$$

The sludge settling characteristics are commonly expressed by equation 2.11 (Vesilind, 1968).

$$F_B = X \cdot v_0 \cdot e^{n \cdot X} \quad (2.11)$$

Where:

F_B = batch sludge flux, Kg/d.m²

v_0 = settling velocity parameter, m/d

n = empirical parameter, m³/Kg ($n < 0$)

The limiting flux for settling tank design is found by drawing a tangent through the batch flux plot, starting on the horizontal axis at an underflow concentration X_R . La Motta (2004) demonstrated that the limiting flux is given by:

$$F_L = \frac{v_0 e^{nX_L}}{\frac{1}{X_L} - \frac{1}{X_R}} \quad (2.12)$$

Also, it can be shown that the abscissa of the point of tangency is given by:

$$X_L = \frac{1}{2} \left(X_R + \sqrt{X_R^2 + \frac{4X_R}{n}} \right) \quad (2.13)$$

La Motta (2004) also established that the limiting flux can be expressed as a function of the sludge concentration in the recycle line and the sludge settling characteristics, as presented in equation 2.14:

$$F_L = \frac{v_0 \cdot e^{\left[\frac{n}{2} \left(X_R + \sqrt{X_R^2 + \frac{4X_R}{n}} \right) \right]}}{\frac{1}{\frac{1}{2} \left(X_R + \sqrt{X_R^2 + \frac{4X_R}{n}} \right)} - \frac{1}{X_R}} \quad (2.14)$$

2.1.6 Mass Balance into the Aeration Tank

Mass balance on non-settleable solids:

According to La Motta et al. (2007) two factors must be taken in consideration into the mass balance of unflocculated particles. The unflocculated particles will appear as suspended solids in the final effluent, so the supernatant suspended solids (SSS) can be used to get an estimate of the value of the effluent suspended solids concentration, X_e . These two factors affecting the concentration of SSS are: the rate of

growth of colloidal particles (r_{gc}) and the rate of flocculation (r_f). r_{gc} is given by the following equation:

$$r_{gc} = k_g X_e \quad (2.15)$$

Where:

r_{gc} = rate of growth of colloidal particles, Kg SSS/Kg MLSS. day

k_g = first order constant of TSS growth, m³/d

X_e = supernatant suspended solids, Kg/m³

A mass balance on nonsettleable solids results in the following equation for X_e :

$$X_e = \frac{X_i + \alpha.(SSS)_R + \bar{t}.k_x.a_x.X}{1 + \alpha + \bar{t}.(k_x - k_g).X} \quad (2.16)$$

Where:

$(SSS)_R$ is the concentration of non-settleable solids in the recycle line which is the same to the respective concentration in the supernatant suspended solids.

In addition, if $\bar{t} = 0$ in equation 2.15, the following plotting point can be obtained:

$$X_0 = \frac{X_i + \alpha.(SSS)_R}{1 + \alpha}$$

(2.17)

Finally, combining equations 2.15 and 2.16 yields the following expression:

$$X_e = \frac{(1 + \alpha).X_0 + \bar{t}.X.k_x.a_x}{1 + \alpha + \bar{t}.X.(k_x - k_g)} \quad (2.18)$$

Mass Balance on Particulate COD

La Motta (2004) obtained the following equation from a mass balance on particulate COD:

$$S_p = \frac{S_{p_i} + \alpha.S_{p_R} + k_p.a_p.\bar{t}.X}{1 + \alpha + (k_g - k_{gp}).\bar{t}.X} \quad (2.19)$$

Where:

S_p = particulate COD concentration in the aerator, kg/m^3

S_{p_i} = particulate COD concentration in the influent stream, kg/m^3

S_{p_R} = particulate COD concentration in the recycle line, kg/m^3

k_p = first order constant of PCOD flocculation, $\text{m}^3/\text{d.kg}$

a_p = kinetic parameter of PCOD flocculation, kg/m^3

k_{gp} = first order constant of PCOD growth, $\text{m}^3/\text{d.Kg}$

Additionally, if $\bar{t} = 0$, $S_p = S_{p0}$, from Eq. 2.19 the following relationship can be written:

$$S_p = \frac{S_{p_i} + \alpha.S_{p_R} + k_p.a_p.\bar{t}.X}{1 + \alpha + (k_g - k_{gp}).\bar{t}.X} \quad (2.20)$$

Next, La Motta (2004) combined those two equations (2.19-2.20) and used the relationship $S_p = f_p.S_T$, which gives equation 2.21 as a result.

$$S_T = \frac{S_{T0}.(1 + \alpha) + \frac{k_p.a_p}{f_p}.\bar{t}.X}{1 + \alpha + \bar{t}.X.(k_p - k_{gp})} \quad (2.21)$$

2.1.7 Brief History of Activated Sludge Models

During the last decade, many models have been proposed to describe behavior of wastewater treatment plants using the activated sludge process (e.g., Henze et al.

2000). In these models, kinetic parameters that depict the activity of biomass in the processes are assumed constant. The representation of active biomass can therefore be regarded as a static picture of its particular metabolic state. Authors of these models stated that these constant kinetic parameters depend on the type of substrate, process configuration, and sludge age (Henze et al. 2000).

Different types of mathematical models have been proposed to predict the activated sludge process final effluent quality, ranging simple models to complex ones, such as the International Water Association activated sludge model. Simple models have fewer parameters and are easy to apply while advanced models generally required software to solve differential equations for dynamic simulations and the level of complexity exceeds the capacity of a designer and an operator of an activated sludge systems. (Shahriari et al., 2006).

Most simple models are based on the Lawrence and McCarty (1970) model, which makes no distinction between particulate and soluble substrates. Lawrence and McCarty (1970) used Monod expression (Monod, 1949) for substrate removal, and a first order expression for biomass growth. Even though the standard Monod relationship yielded the best fit, predictions of reactor performance by this kinetic model has been generally poor. One remedy for this poor fit has been to include a non-biodegradable portion of influent COD in the formulation. With this modification, predictions of effluent soluble COD have much lower error values (Shahriari et al., 2006).

Acknowledgment of the fact that a large amount of solids in the system is debris associated with endogenous decay of biomass was one of the first advances to basic

models. As a result, all subsequent kinetic formulations were modified to include a non-biodegradable component.

Since 1982, the International Association on Water Pollution Research and Control (IAWPRC), established a Task Group on Mathematical Modeling for Design Operation of Activated Sludge Processes, which has published the Activated Sludge Models N° 1 (ASM1), ASM2, ASM2d, ASM3 since 1987 (Gujer et al., 1999; Henze et al., 2000).

An important contribution of ASM1 (Henze et al., 1986) is death-regeneration concept to describe reactions such as death, and growth occurring during the endogenous phase. The major difference between ASM1 and ASM2 is that ASM2 includes biological removal of phosphorus (Henze et al., 1995).

Simulation of the behavior of activated sludge system treating municipal wastewater of mainly domestic origin are currently implemented in various computer codes for the mathematical models related to ASM1. However, some defects of this model have become apparent. Considering these defects and the advance in experimental evidence on storage of organic compounds, the task group has proposed the Activated Sludge N° 3 (ASM3), which should correct for these defects and which could become a new standard for future modeling (Gujer et al., 1999). Compared to ASM1 and ASM2, AMS3 (Gujer et al.,1999) introduced the storage of readily biodegradable substrate in the form of cell internal storage product. In ASM3, all substrate first become stored material and then are converted to biomass. Despite all

these improvements, ASM3 still does not consider any relationship between the settling behavior and the aerator performance.

According to La Motta et al. (2007) no existing model considers simultaneously the effect of biological flocculation on the removal of particulate COD and the sludge settling characteristics in defining the activated sludge operating characteristics under steady state conditions. Some of the few researchers that have been taken flocculation into account as an important process in the performance of suspended-growth reactor system are Parker et al. (1970), Wahlberg et al. (1994), and La Motta et al. (2004).

Settling tank mathematical models can be classified by their spatial resolution according to Ekama et al., (1997); the models can simulate steady-state or non-steady conditions in the settling tank.

One dimensional models (1D) are based on the flux theory. It is assumed that in clarifiers, the profiles of horizontal gradients are uniform and that horizontal gradients in concentration are negligible. Based on the solid flux concept, Takacs et al., (1991) presented a multi-layer model of clarification/thickening process that is designed to predict the solids profile and underflow suspended solids. This model provides a unified framework for simulation of clarification and thickening processes under both steady state and dynamic conditions. Later, Henze et al., (1995) studied Takacs model and concluded that it is the most reliable to fit the data for steady state and dynamic conditions. However, the main disadvantage of this model is the relatively long calculation time required for convergence.

Another settling tank model is presented by Dupont et al., (1995). This is a dynamic, one-dimensional flux model for the secondary settling tank that predicts -the suspended sludge concentration profile near the effluent weirs and the return sludge concentration of a secondary settling tank, when density current and short-circuiting are included.

On the other hand, LaMotta et al. (2007) developed a model that can be used for activated sludge system preliminary design and operation, based on the one-dimensional limiting flux theory.

2.2 Parameter Estimation of the Mathematical Model

There are two main groups of mathematical techniques that can be used to estimate the parameters of the any particular model: single equation techniques and simultaneous equation techniques.

2.2.1 Single equation techniques

These are techniques that are applied to one equation at time. The most important are: the classical least squares or ordinary least squares method, the indirect least squares or reduced- form technique; the two-stage least squares method, the limited information maximum likelihood method and various methods of mixed estimation.

2.2.2 Simultaneous equation techniques

These are techniques that are applied to all equations of the system at once, and give estimates of the coefficients of all the functions simultaneously. The most important are the three-stage least squares method (3SLS) and the full information maximum likelihood method (FIML) (Koutsoyiannis,1977).

Three-stage Least Squares method:

This method was developed by Theil and Zellera as a logical extension of Theil's two-stage Least Squares (2SLS). It involves the application of the method of least squares in three successive stages. It utilizes more information than the single-equation techniques, that is, it takes into account the entire structure of the model with all the restrictions that this structure imposes on the values of the parameter (Koutsoyiannis.,1977).

The first stage is the estimation of all structural coefficients using the least-squares estimator; the second stage is estimation of all structural coefficients by applying 2SLS to each of the structural equations. Finally, the third stage is the generalized least-squares estimation of all the structural coefficients of the system, using a covariance matrix for the stochastic disturbance terms of the structural equations that is estimated from the second stage residuals. Using the information contained in this covariance matrix has the effect of improving efficiency (Intriligator., 1978).

Properties of the 3SLS estimates

1. The 3SLS estimates are biased but consistent.
2. They are more efficient than 2SLS, since in their estimation we use more information than in 2SLS.

The method is simpler than Full Information Maximum Likelihood. However, it requires complete knowledge of the specification of the entire model and a large amount of data (Koutsoyiannis.,1977).

Full Information Maximum Likelihood (FIML):

Maximum likelihood (ML) is a very popular estimation and testing approach. Its essence is the estimation of unknown parameters that underlie an assumed model (variable distribution) by values that maximize the probability of observing the data at hand (probability density). The principle of ML is of fundamental relevance for applied statistics as well as social, behavioral, and educational research (Mokhtari et al., 2006).

Maximum likelihood (ML) estimation has been widely known in statistics at least since the 1950s, with impact of R.A. Fisher's work. However, in the social sciences, it has only rather gained ground as a method for estimating parameters since 1993. ML estimation systematically searches over different possible population values, finally selecting parameter estimates that are more likely (have the "maximum likelihood") to be true, given the sample observation (Eliason,1993). Each observation of the sample has a certain probability of occurring in any random drawing (Koutsoyiannis,1977). The

leading alternative estimation procedure, of course, is ordinary least squares (OLS) regression. (Eliason, 1993).

The maximum likelihood method chooses among all possible estimates of the parameters those values make the probability of obtaining the observed sample as large as possible. The function which defines the joint (total) probability of any sample being observed is called the *likelihood function* of the variable X .

Full Information Maximum Likelihood is a system method, that is, this method is applied to all the equations of the model and yields estimates of all the structure parameters contemporaneously. It is a straightforward extension of the maximum likelihood method.

The method in its most general form is based on two main assumptions, namely:

1. The FIML assumes full information, that is, full knowledge of the complete specification of all the equations of the model. We need to know not only the variables appearing in the model, but also the mathematical form of all the equations.
2. The FIML assumes that the random disturbances of the various equations of the model are normally distributed with zero means and constant variances. (Koutsoyiannis.,1977).

In this approach, FIML, the likelihood function for the entire system, is maximized by choice of all system parameters, subject to all a priori identifying restrictions. Maximizing the system is equivalent to minimizing the sum of squared errors (Eliason,

1993). The resulting estimators are consistent and asymptotically efficient. They also have the same asymptotic properties as 3SLS, including the same asymptotic covariance matrix (Intriligator, 1978).

The following are properties of the maximum information likelihood estimates: For small samples the maximum information likelihood estimates are biased. However, for large samples they possess the desirable properties of efficiency and consistency.

A major advantage of FIML over 3SLS, however, is that with this technique it is possible to use in the estimation process a wide range of a priori information, pertaining not only to each equation individually but also to several equations simultaneously, such as constraints involving coefficients of different structural equations and certain restriction on the error structure. The major disadvantage of FIML, however, is that it is difficult and expensive to compute, involving the estimation of rather awkward simultaneous nonlinear equations, which usually must be computed via iteration (Intriligator, 1978).

The full-information techniques, specifically 3SLS and FIML, generally provide the most desirable estimators in terms of both bias and mean squared error when the model is correctly specified and the variables are correctly measured. FIML is, however, extremely sensitive to both specification error and measurement error. Such sensitivity to specification error and measurement error may be expected in this approach, where because of its computation via a system of nonlinear equations, an error in one equation or in one variable will propagate throughout the whole system in the process of estimation (Intriligator, 1978).

Theory-based maximum likelihood (ML) approaches for treating missing data have been known in the technical literature for some time and have recently begun to appear in statistical packages.

2.3 Sensitivity Analysis

Sensitivity analysis (SA) is one of the key issues in today's engineering that has been becoming increasingly recognized as an integral part of model development and a tool for helping to answer key policy questions (McCarthy et al. 1995; Helton 1997). This challenge is to reduce design problem set in a complex engineering world to a simple mathematical problem. Mathematical programming techniques can be use to compute the sensitivity of the basic design. By computing gradients, sensitivity analysis measures the variation of performance induced by small perturbation of the control parameters. Gradients are also major ingredient in reliability analysis for computing a random model (Laporte and Le Tallec, 2003).

SA can be used in the study of the stability of an inverse problem, in that whenever a computational model is employed to simulate an underlying, physical process, it is of interest to ascertain whether experimental measurements, with their related uncertainties, allow the extraction, or estimation, of some parameters embedded into the simulation model (Saltelli and Scott, 1997).

Sensitivity analysis can be used for quantifying the impact of changes in input values on model output (Cullen and Frey, 1999); evaluating how the variation in the output of a model can be apportioned, qualitatively or quantitatively, among model

inputs (Saltelli, 2002); and for identifying factors contributing to particular outcomes (i.e., worst or best) of interest (Mishra et al., 2003). Sensitivity analysis can provide insights regarding the key controllable sources of variability and key sources of uncertainty among model inputs. Knowledge of key sources of variability is useful in identifying control measures to reduce exposure/risk, whereas knowledge of key sources of uncertainty can help prioritize additional data collection and research (Cullen and Frey, 1999).

SA in this research involves an exploration of the UNO 1D Activated Sludge Model to determine the effects of individual components such as: X , X_R , t_c , X_e and St on the analysis outcomes

2.4 The Modeling Process and the Role of Sensitivity Analysis

The quality and reliability of the model is often difficult to judge, since they are multi-attribute, but the sensitivity analysis process encourages the modeler to explore and gain greater understanding of the constructed model (Saltelli et al., 2000).

Selecting the best mathematical model is the largest problem when designing any process. In addition, advanced models contain many parameters; consequently, sensitivity analysis becomes crucial to determine the most important parameters. A correct model should predict an activated sludge system over a wide variety of operating conditions (Shahriari et al., 2006).

3. Experimental Phases

3.1 Description of the Database

The database was obtained from Rojas (2004) bibliographical source. This database was generated at the experimental activated sludge pilot plant located within the installations of the Marrero Wastewater Treatment Plant, 6250 Lapalco Boulevard, Marrero, Louisiana. The full-scale facility is a 34 000 m³/d trickling filter/solid contact process that treats domestic sewage with a design average flow rate of 24,226 m³/d (6.4 mgd), and that has operated overloaded with more than 37 854 m³/d (10 mgd) for several years.

The activated sludge pilot plant operated by Rojas (2004) has the following characteristics: an inlet mechanism, a rotating screen, a reservoir tank, an aeration basin, a secondary clarifier and a final effluent collection tank.

The pilot plant was fed by pumping the wastewater from a grit chamber splitter tank of the full scale plant to a rotational screen; this rotating cylindrical screen removes the solids larger than 0.5 mm, which fall into an external collection basin. A submersible centrifugal pump sent the wastewater to the aeration basin. Diffusers in the aeration tank maintained the required dissolved oxygen levels and to provide uniform mixing. The aeration basin effluent flowed into the secondary clarifier that delivered the mixed liquor tangentially into center well to minimize the inflow energy and to create a circular motion that provided additional flocculation to the mixed liquor solids. The scrapper avoided the formation of solids clumps in the conical section of the secondary clarifier. The clarifier had three effluent collectors, 3.81 cm in diameter. They were placed

vertically on the surface of the water in opposite locations of the tank. Part of the sludge that settled in the bottom of the secondary clarifier was recycled to the aeration basin and another part was wasted and sent to a collection tank using two different lines. Figure 3.1 illustrates a diagram of the pilot plant operated by Rojas.

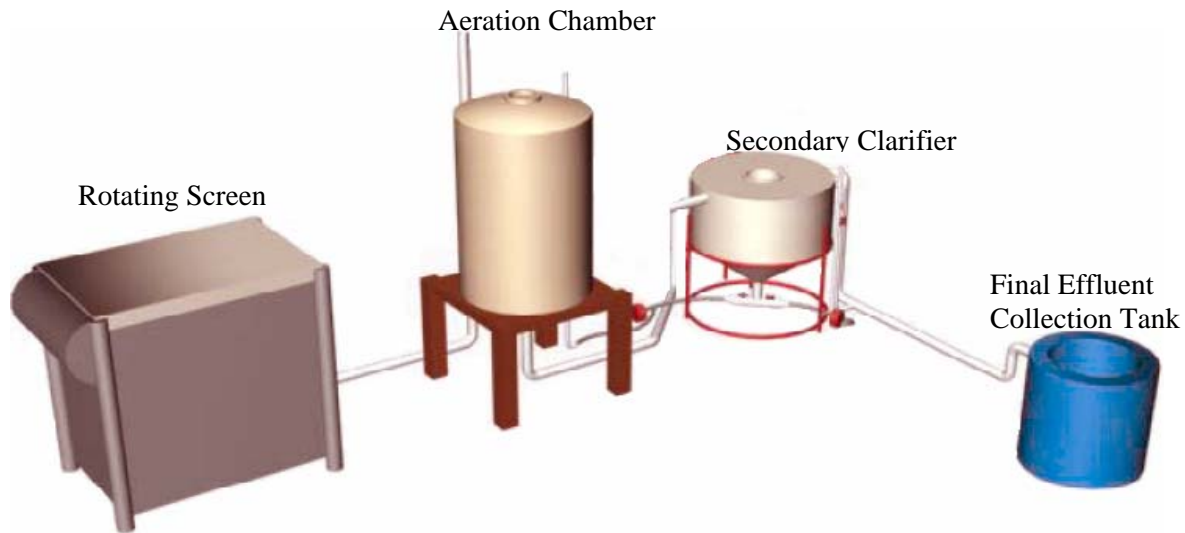


Figure 3.1 Pilot Plant Diagram (Jimenez 2002)

Rojas operated the aeration basin at two different hydraulic retention times and maintained the following parameters constant: recirculation ratio, and sludge wasting ratio. Raw and treated wastewater samples were taken during the period March 2004 to October 2004 in order to test the validity of La Motta’s model.

Table 3.1 Recirculation Ratio and Waste Ratio Used during the Rojas (2004) Experimental Phase

HRT (min)	α	w
45	0.701	0.019
30	0.712	0.035

Rojas measured some parameters right at the pilot plant such as recirculation flow rate, dissolved oxygen, temperature, pH, and sludge settling parameters, and took some samples to measure total suspended solids (TSS), total and particulate COD at the Environmental Engineering Laboratory located at the Center for Energy Resources Management (CERM).

Rojas (2004) found the numerical values of the kinetic constants of La Motta's model by trial and error, first using the UNO 1D Activated sludge Model to predict the value of effluent characteristics, and then comparing these results with the actual values observed at the pilot plant. Rojas accepted the set of kinetic constants that yielded the closest agreement between the observed and the predicted effluent characteristics. A similar approach was used by La Motta et al. (2007), who performed a sensitivity analysis on the predicted values of the final effluent TSS and total COD to test the effect of changing the kinetics constants using the recirculation ratio of 0.377 at 45 minutes of retention time at the Marrero Wastewater Treatment Plant. The following kinetic constants were reported.

Table 3.2 Kinetics Parameter Values found by La Motta et al (2007)

Kinetics constant	Value
$K_p, m^3/dayKg$	500
$K_x, m^3/dayKg$	500
$K_g, m^3/dayKg$	0.5
$K_{gp}, m^3/dayKg$	0.5
$a_p, m^3/dayKg$	0.03
$a_x, m^3/dayKg$	0.015
$K_d, m^3/dayKg$	0.06
$Y, m^3/dayKg$	0.5

La Motta et al. (2007) then performed a linear regression analysis between the MLSS observed and MLSS predicted and found the following linear relationship between them: $X_{\text{pred}}=1.316 X_{\text{osb}}$, with a coefficient of determination (R^2) of 0.88. Additionally, La Motta et al. (2007) found the following relationship between the observed and predicted values of X_R : $X_{R\text{pred}}=1.325 X_{R\text{obs}}$ with a coefficient of determination of 0.78.

3.2 Data Analysis

Several newer approaches for dealing with missing values exist, and most software programs now offer options that are more reasonable than traditional approaches. When missing values cannot be avoided, multiple imputation and full information maximum likelihood methods offer substantial improvements (Acock, 2005). The full information maximum likelihood estimation method was applied to find the numerical values of the unknown kinetic constants in this research.

The statistical software called TSP/Give Win2 was used for the estimation of the unknown parameters. This software is a complete econometric software package, with easy input of commands and data, all the standard estimation methods (including nonlinear), regression, forecasting, and a flexible language for programming your own estimators. It uses convenient loading of raw data from free format, fixed format, binary, Lotus or Excel files.

TSP estimate single equations using a variety of techniques such as OLSQ Ordinary least squares (with extensive diagnostics), 2SLS Two stage least squares

(instrumental variables), LIML Limited Information Maximum Likelihood, AR1 Regression with first-order serial correlation, and others.

TSP also estimates the parameters of systems of equations by simultaneous methods, such as: LSQ least squares, minimum distance, nonlinear least squares, multivariate regression and three-stage least squares, both linear and nonlinear, GMM Generalized method of moments estimation (multiple equation, nonlinear, panel data), and FIML estimation of a complete nonlinear simultaneous model by the full information maximum likelihood method are also include in this software (Hall et al., 2005).

The maximum likelihood method, as stated before, consists of the maximization of the likelihood function. From the general conditions of maximization we know that the maximum value of the function is that value where the first derivatives of the function with respect to its parameters are equal to zero. Therefore, TSP takes the partial derivatives of the likelihood function with respect to μ and σ^2_x , it equates them to zero and solves for the unknown parameters.

The analysis approach proceeds in three steps. The first step consists of the estimation of the unknown parameters; this is accomplished by solving an optimization problem in which the objective functions are maximized by full information maximum likelihood. That way, it will produce parameter estimates that will be close to the true, unknown parameter values. The unknown parameters are treated as variables to be solved for in the optimization, and the data serve as known coefficients of the objective function in this stage of the process. As stated before these unknown parameters will be generated by TSP/GiveWin2, which will read observed values from a Microsoft Excel

file, will solve the system of equations and by FIML methods it will get the unknown parameters that minimizes error in the system of equations.

Stages of the maximum likelihood method are the following:

1. Form the likelihood function, which gives the total probability of the particular sample values being observed.
2. Take the partial derivatives of the likelihood function with respect to the parameters which we want to estimate and equate them to zero
3. Solve the equations of the partial derivatives for the unknown parameters, to obtain their maximum likelihood estimates (Koutsoyiannis, 1977).

To run TSP some initial values are need, thus La Motta's et al (2007) kinetic parameters are used as starting point. The numerical values of the kinetic parameter were varied until a favorable answer was found. In other words, each answer from TSP/GiveWin2 was taken to run the 1D UNO Activated Sludge Model. Then, the predicted values from the 1D UNO Activated Sludge Model were compared to the observed values. The closest agreement between the predicted and observed values yielded the selected set of kinetic constants.

When the parameter estimation has been made, the 1D UNO Activated Sludge model is then carefully assessed to see if the underlying assumptions of the kinetics parameters appear plausible. Statistical analyses were conducted to determine the reliability of the predicted values versus the observed values. One of the most widely used statistical criteria is the correlation coefficient (R^2) which was applied to select the parameters. Here, regression analyses were conducted between predicted and observed values using Microsoft Office Excel.

Once the kinetic parameters seem to be valid, the third step corresponds to the sensitivity analysis. The 1D UNO Activated Sludge mathematical model was used to establish the sensitivity of output to various parameters that served as kinetic parameters in the model. The best group of the kinetic constants obtained from previous step was taken to run 1D UNO Activated Sludge model. The data sets used for sensitivity analysis were generated from model runs by disturbing model kinetics parameter randomly and carrying out model simulations for each set of perturbed parameters. All kinetic parameters were intended to vary individually from 0.00001 to 1000000.

4. Results and Discussion

4.1 Kinetics Parameters

The kinetic parameters of the UNO Activated Sludge Model were estimated using the TSP/GiveWin2 software package according to the methodology described in Chapter III.

Table 4.1 shows the constant parameters used in the program, which correspond to the dimensions of the pilot plant used by Rojas (2004) to collect his experimental data.

Table 4.1 Constant Parameters Used in the Project

HRT, minutes	45
Plant Flow Rate (Q), m ³ /d	5.599
Aeration Tank volume (V _r), m ³	0.175
Sedimentation tank volume (V _s), m ³	0.145
Recirculation ratio, α	0.701
Particulate chemical oxygen demand fraction, f_p PCOD/TCOD)	0.899

Table 4.2 shows Rojas' (2004) summary of the results from laboratory analyses of the following parameters: TSS in the mixed liquor (MLSS), recycled sludge (X_R), influent (X_i), the supernatant of the mixture of 1000 ml of the raw wastewater and 1000 ml of the recycled sludge multiplied by the recirculation ratio (X_0) and also the TCOD in the influent (S_{ti}) and in the supernatant of the mixture (S_0).

Table 4.2 Parameters obtained in the Activated sludge system by Rojas 2004

HRT (min)	TSS (kg/m ³)				TCOD (kg/m ³)		<i>n</i> (m ³ /kg)	<i>V₀</i> (m/d)
	MLSS	<i>X_R</i>	<i>X_i</i>	<i>X₀</i>	<i>S_{ii}</i>	<i>S₀</i>		
45	1.978	5.225	0.289	0.046	0.257	0.052	-0.9192	414.80
	2.376	6.720	0.293	0.032	0.301	0.115	-0.7907	400.30
	2.470	6.015	0.203	0.024	0.255	0.093	-0.8998	450.24
	2.836	6.320	0.115	0.036	0.115	0.078	-0.7684	348.48
	3.014	6.235	0.471	0.029	0.361	0.068	-0.6692	344.54
	3.242	7.790	0.520	0.040	0.356	0.115	-0.6442	224.15
	3.348	7.975	0.357	0.017	0.381	0.138	-0.5721	298.91
	4.645	9.145	0.438	0.041	0.438	0.118	-0.4080	214.85

The following two tables illustrate the best values found by the TSP/GiveWin2 program. Table 4.3 shows the output from the first trial run with its respectively standard errors and t-statistic. The t-statistic measures how many standard errors the coefficient is away from zero. Generally, any t-value greater than +2 or less than - 2 is acceptable. The higher the t-value, the greater the confidence we have in the coefficient as a predictor. Low t-values are indications of low reliability of the predictive power of that coefficient. In the model there are six unknown kinetic parameters: the asymptote of TSS remaining in the effluent (*a_x*), the first-order constant of TSS flocculation (*k_x*), the first order constant of TSS growth (*k_g*), the asymptote of PCOD remaining in the effluent stream (*a_p*), the first order constant of PCOD flocculation (*k_p*), the first order constant of PCOD growth (*k_{gp}*). In the first trial, *k_g* and *k_{gp}* were chosen randomly as constants to find out the other parameters. Results are show in Table 4.3.

Table 4.3 Parameters estimation from TSP/GiveWin2 program, 1st trial

Parameter	Estimate	Standard Error	t-statistic
k_x	501.894	2.11E-03	238373
a_x	0.015	1.03E-08	1.45E+06
k_p	7.051	6.02E-05	117151
a_p	0.037	5.92E-07	62627.1

As can be seen in Table 4.3, the asymptotes a_p and a_x have very low standard error. Therefore, for the second trial these parameter were chosen to be constant to detect the values of k_g and k_{gp} . Table 4.4 illustrates the values found when a_p and a_x were chosen as constants, and shows that k_x and k_p did not change at all. Therefore, for subsequent calculations, k_x and k_p were chosen from Table 4.3.

Table 4.4 Parameters estimation from TSP/GiveWin2 program, 2nd trial

Parameter	Estimate	Standard Error	t-statistic
k_x	507.109	1.89E-03	268674
k_g	1.248	5.36E-04	5480.61
k_p	8.141	2.60E-04	31270.7
k_{gp}	0.247	2.01E-04	5208.11

Tables 4.5 and 4.6 show the results obtained from 1D UNO Activated Sludge System when using the kinetic parameters determined by TSP and the respectively regression analysis between observed and predicted values. Table 4.5 shows regression analysis and predicted values on mixed liquor suspended solids (MLSS), recycled sludge (X_R) and solids retention time (t_c), while Table 4.6 shows regression analysis and predicted values on supernatant suspended solids (X_e) and TCOD in the effluent (St).

Table 4.5 Observed Values and Predicted Values and its Regression Analysis

MLSS observed	MLSS predicted	X_R observed	X_R predicted	tc observed	tc predicted
1.978	3.0939	5.225	7.0134	0.93	0.5108
2.376	3.5369	6.720	8.1159	0.96	0.6187
2.47	3.1442	6.015	7.3119	1.15	0.8080
2.836	3.4564	6.320	8.1760	1.18	1.3390
3.014	4.1184	6.235	9.2743	1.19	0.4674
3.242	3.9434	7.790	8.7561	1.06	0.3959
3.348	4.5822	7.975	10.5933	1.16	0.7116
4.645	5.9814	9.145	13.8128	1.34	0.6961
Regression Statistics		Regression Statistics		Regression Statistics	
Multiple R	0.9975	Multiple R	0.9947	Multiple R	0.9371
R Square	0.9949	R Square	0.9894	R Square	0.8782
Adjusted R Square	0.8521	Adjusted R Square	0.8465	Adjusted R Square	0.7354
Standard Error	0.3096	Standard Error	1.0319	Standard Error	0.2784
Observations	8	Observations	8	Observations	8
Equation: X _{pred} =1.319 X _{osb}		Equation: X _{Rpred} =1.324 X _{Rosb}		Equation: tc _{pred} =0.60 tc _{osb}	

Regression analysis on the output model indicates that the determination coefficients (R^2) are really high, very close to 1. Thus, the R^2 between the observed MLSS and predicted MLSS is 0.995, and the R^2 between observed X_R and predicted X_R is 0.989. By comparison, La Motta et al. (2007) reported a linear relationship between the MLSS observed and MLSS predicted with the coefficient of determination (R^2) of 0.88, a linear relationship between the X_R observed and predicted with the coefficient of determination of 0.78.

Consequently, it can be stated that the kinetic coefficients predicted by TSP are much more reliable than those obtained by the trial and error procedure used by La Motta et al. (2007).

Table 4.6 Continuation of Observed Values and Predicted Values and its Regression Analysis

X_e observed	X_e predicted	St observed	St predicted
0.023	0.0161	0.040	0.0490
0.014	0.0155	0.021	0.0928
0.009	0.0153	0.038	0.0788
0.018	0.0157	0.026	0.0673
0.028	0.0154	0.040	0.0594
0.027	0.0157	0.058	0.0911
0.014	0.0151	0.048	0.1033
0.026	0.0155	0.051	0.0858
Regression Statistics		Regression Statistics	
Multiple R	0.9506	Multiple R	0.9531
R Square	0.9036	R Square	0.9084
Adjusted R Square	0.7607	Adjusted R Square	0.7655
Standard Error	0.0051	Standard Error	0.0259
Observations	8	Observations	8
Equation: $X_{e_{pred}}=0.70 X_{e_{osb}}$		Equation: $St_{pred}=1.83 St_{osb}$	

4.2 Interpretation of the Sensitivity Analysis

A sensitivity analysis of the kinetic parameters k_p , k_x , a_p , a_x , k_g , k_{gp} was performed with the experimental data collected by Rojas when the activated sludge system was operated at a HRT of 45 min. The idea of this analysis is to observe the impact of changing the values of the kinetic parameters of the 1D UNO Activated Sludge model on its output. Analysis of the results will be based on the first day of experiments due to every day have roughly same performance (Appendix C).

Figure 4.1 shows variations on the first order constant of PCOD flocculation (k_p) from 0.00001 to 1000000. Changing this kinetic constant does not significantly make any change to the predicted values. It can be noticed that the predicted values remains almost constant; there is a maximum change around 0.01 units on predicted values that

can be calculated by Appendix C. In other words, individual perturbations on k_p will not affect results of the model output. In the figure also, it can be observed the best predicted value which is $k_p = 7.01 \text{ m}^3/\text{Kg.d}$

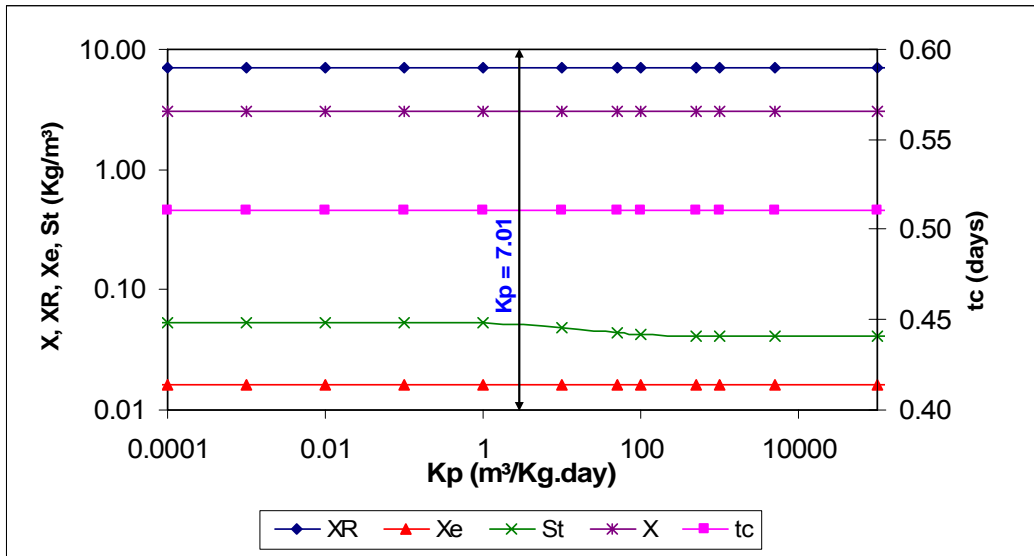


Figure 4.1 Effect of Changing First Order Constant of PCOD Flocculation (k_p)

Similar effect is observed in Figure 4.2, where the predicted values remain roughly constant despite the substantial changes in k_x . The kinetic constant k_x does not affect any model output when it is perturbed individually. In Appendix C it can be seen that the predicted values of X and X_R have a maximum change of 2% when k_x is perturbed. Similarly, the predicted values of St remain constant, X_e changes around 3.4 %, and t_c has a maximum change of around 7%. X_e values are constants until k_x gets 10 then it changes little by little until k_x gets 1000 and then X_e remains constant at 0.015. It can be noticed that the best value of the First Order Constant of TSS Flocculation is $501 \text{ m}^3/\text{Kg.d}$

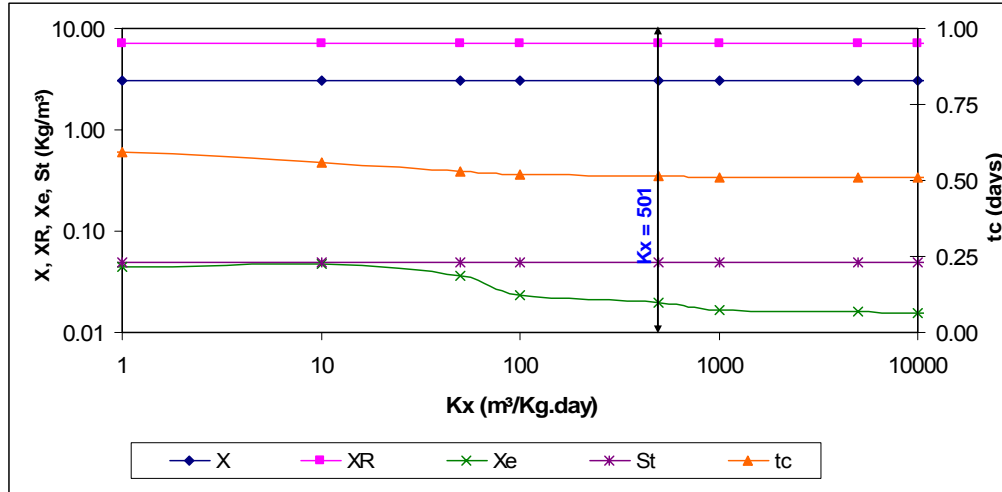


Figure 4.2 Effect of Changing First Order Constant of TSS Flocculation (k_x)

It can be observed in Figure 4.3 that perturbations on kinetic parameter of PCOD flocculation (a_p) can cause radical changes on the predicted values. First, a_p is directly proportional to S_t . Second, X and X_R have a maximum change of 10% and 2% respectively, and X_e does not have any change when a_p is perturbed. Third, it can be noticed in Figure 4.3 that t_c is the parameter that is the most affected when a_p is perturbed. Specifically, for values of a_p between 0.00001 and 10, the predicted values of t_c do not change at all. But, after a_p is equal to 10 it can be observed that the predicted values of t_c go up until 20, then they go down through zero, become negative, and remain negative. Even when the curve starts to go up again, it never gets values greater than zero again. As it is known, t_c is the solids retention time, which in real life would never get negative values. Same behavior is observed for the rest of the experiment's days, the predicted values of t_c start to fluctuate when a_p has taken values greater than 10 (Appendix C). Figure 4.4 shows the best value of Kinetic Parameter of PCOD Flocculation obtained.

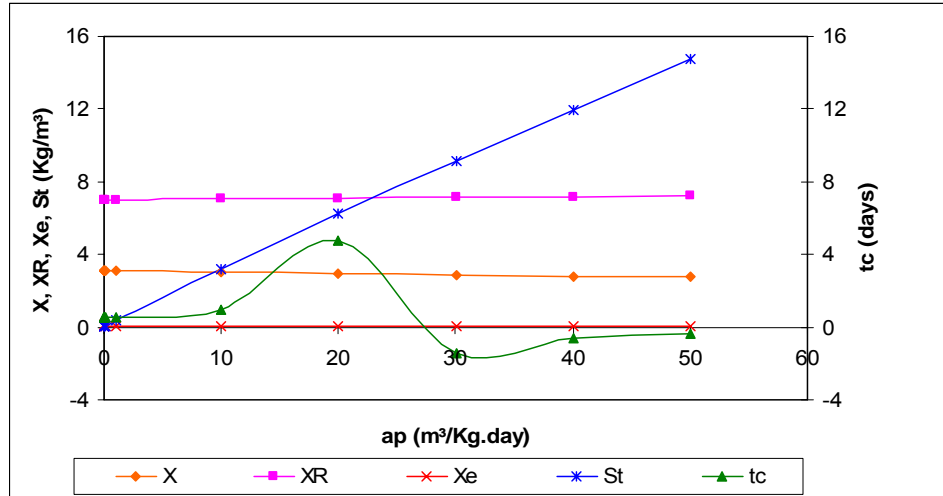


Figure 4.3 Effect of Varying Kinetic Parameter of PCOD Flocculation (a_p)

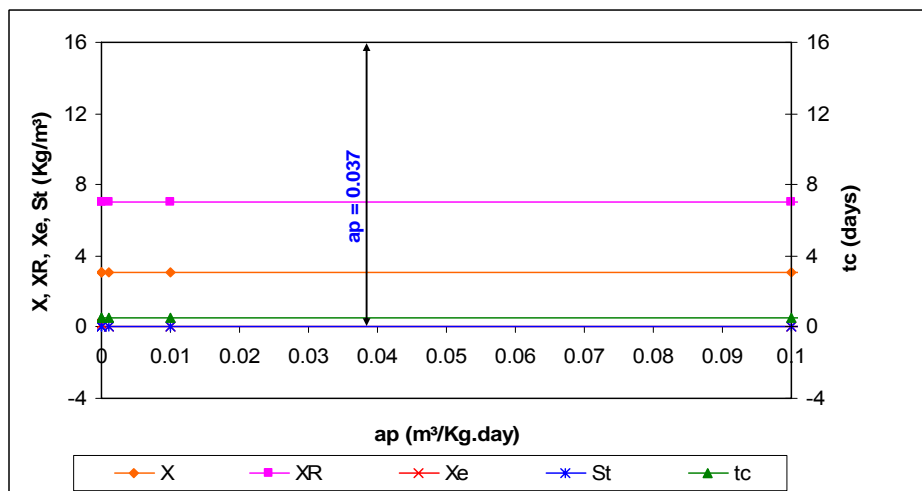


Figure 4.4 Best Value of a_p when it is changed.

The effect of changes in a_x can be observed in Figure 4.5. The predicted values of X are affected with a maximum difference of 6.5% and the predicted values of X_R are affected with a maximum of difference of 3.5%. Perturbing a_x does not change the predicted values of St , but it does affect X_e and t_c . X_e can increase progressively with respect to a_x (Appendix D-4) and t_c has the same behavior observed when a_p is disturbed. Predicted values of t_c reach a peak when a_x is 0.2, turn negative at $a_x = 0.27$,

and do not become positive anymore. Thus, the system is much more sensitive to changes in a_x than to changes in a_p , because while t_c turns negative when a_p reaches a value of approximately 27, it turns negative when a_x reaches a value 100 times smaller.

Figure 4.6 shows the best value found of the kinetic parameter a_x .

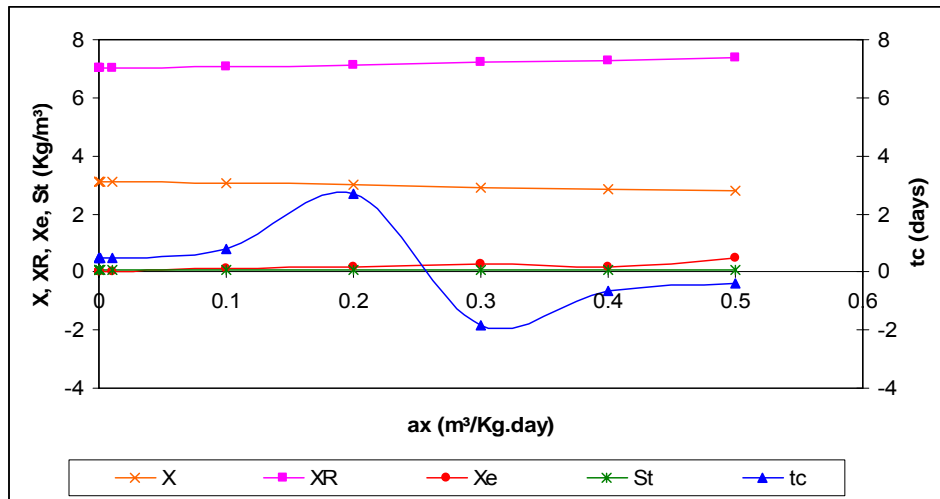


Figure 4.5 Effect of Varying Kinetic Parameter of TSS Flocculation (a_x)

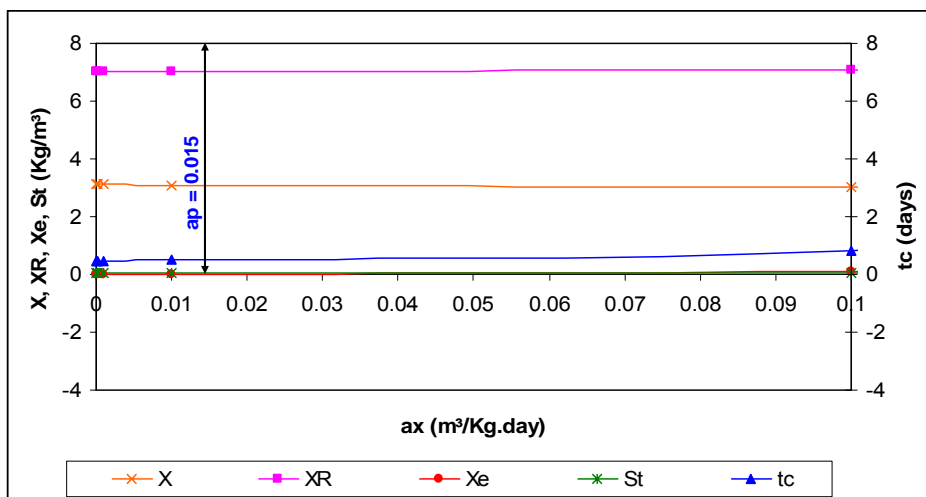


Figure 4.6 Best Value of a_x when it is changed.

Figure 4.7 shows the effect of changing k_g on the model output. It can be seen that X starts to change from a constant straight line to a convex form. When k_g has taken values greater than 100, X increases exponentially until k_g gets a value equal to 420, which yields the maximum value of X . After that, X goes down until k_g gets to 450, beyond which the predicted values on X start to go up again. The behavior of X_R is completely different. The predicted values of X_R remain practically constant through $k_g = 420$, and turn negative when k_g exceeds 450.

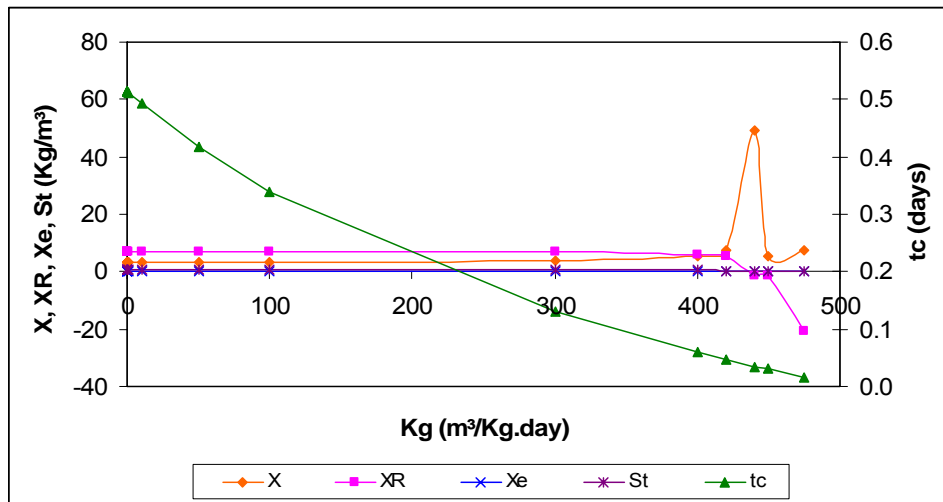


Figure 4.7 Effect of Changing First Order Constant of TSS Growth (k_g)

In addition, changing k_g also affects t_c ; predicted values of the cell retention time decrease progressively until they get close to zero when k_g is equal to 475. Better look of the t_c performance is shown in Figure 4.8. It can be observed from this figure that k_g affects X_e increasing predicted values exponentially.

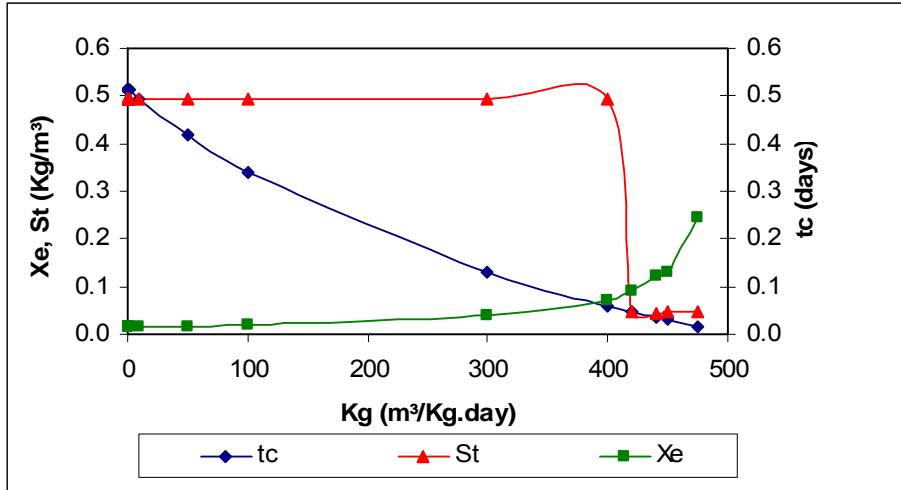


Figure 4.8 Closer look on Xe, St and tc when k_g is varied

Different behavior can be seen for St, where predicted values remains constant until k_g get 400, the major changes is observed between 400 and 420 and after this predicted values remains constant again. By figure 4.9 it can be observed the best value of the First Order Constant of TSS Growth found by TSP software.

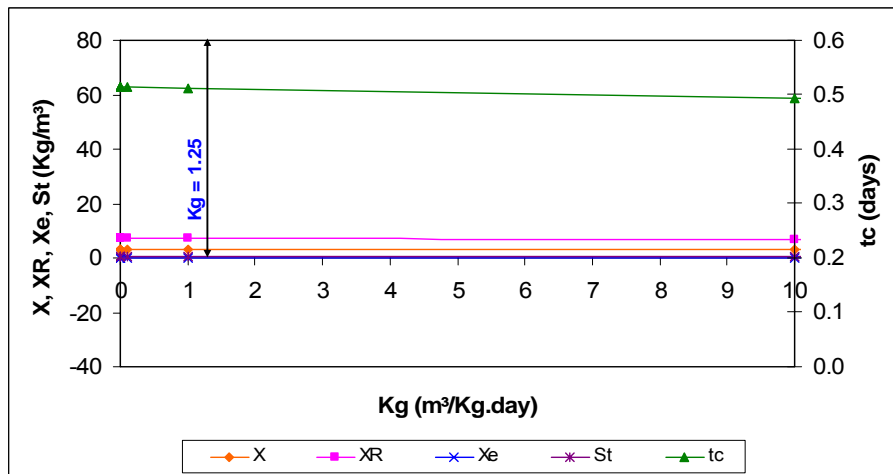


Figure 4.9 Best Value of k_g when it is changed

Fig. 4.10 shows the effect of changing k_{gp} from 0 to 50 on the model output. Although some system parameters remain almost constant, such as X , X_R and X_e , with a maximum change of 0.05%, other parameters, such as S_t , are substantially affected. Thus, if k_{gp} is greater than 25, S_t turns negative, this cannot occur in real life. As it can be noticed by the figure 4.11 the best value of the First Order Constant of PCOD Growth was $0.25\text{m}^3/\text{Kg.d}$

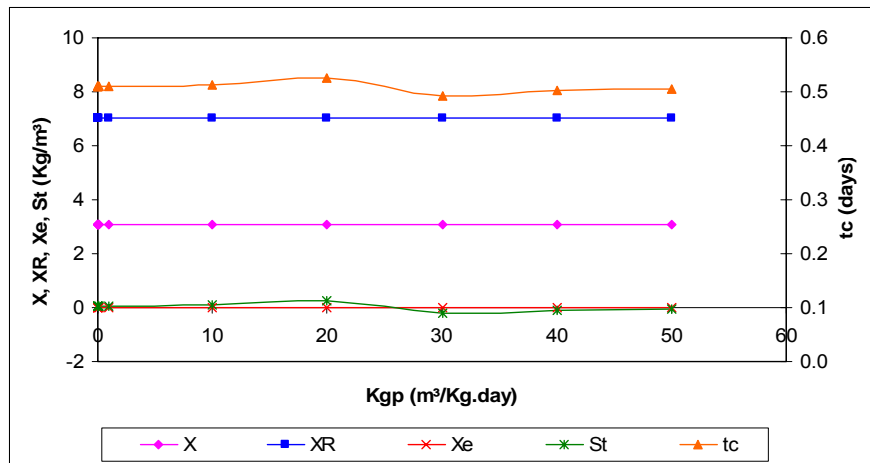


Figure 4.10 Effect of Varying First Order Constant of PCOD Growth (k_{gp})

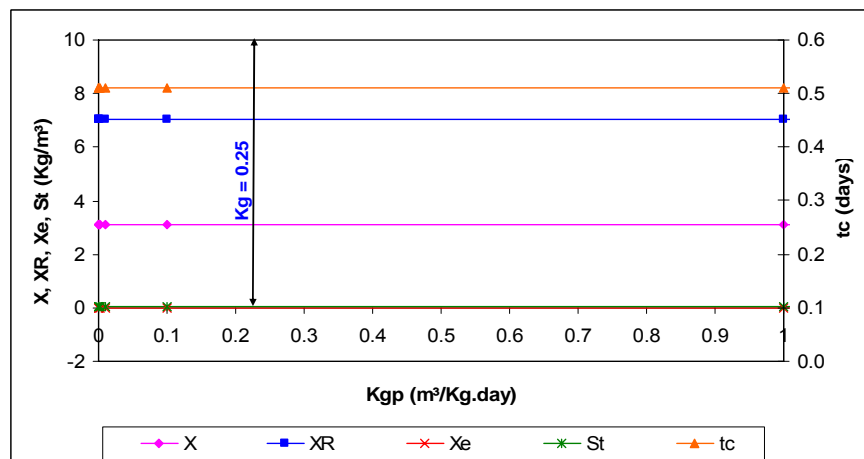


Figure 4.11 Best Value of k_{gp} when it is changed

5. Conclusions and Recommendations

5.1 Conclusions

The following conclusions can be drawn from this research project:

- The software TSP proved to be a very efficient tool for estimating parameters in cases that involve the simultaneous solution of several non-linear equations, such as the UNO Activated Sludge Model.
- The kinetic coefficients predicted by TSP/GiveWin2 using FIML as parameter estimator are very reliable.
- Regression analyses between predicted values and observed values provided very good results, with the lowest value of the coefficient of determination (R^2) being 0.88.
- Based on optimum results from regression analysis, it can be concluded that the ideal values of each kinetic parameter are: $k_p=7.1$, $k_x=500$, $k_g=1.25$, $k_{gp}=0.25$, $a_p=0.037$ and $a_x=0.015$ for a design and operation of an activated sludge system.
- Variations on the first order constant of PCOD flocculation (k_p) do not affect any predicted value of the 1D UNO Activated Sludge model.
- When first order constant of TSS flocculation (k_x) is perturbed only small changes on recycled sludge (X_R) are observed.
- Varying the asymptote of PCOD remaining in the effluent stream (a_p) affects two of the five of the activated sludge output model; the others remains almost constant. Predicted values of S_T increase gradually as a_p

increases, while the predicted values of t_c fluctuate and then turn negative when a_p reaches a value of approximately 27. Since the best-fit value of a_p is 0.037, this coefficient would not be expected to be greater than 1 in other systems.

- Changing the kinetic parameter of TSS flocculation (a_x) will affect t_c and X_e substantially but not X , X_R , and neither St .
- Individually alterations of the first order constant of TSS growth (k_g) have an effect on all predicted values of the 1D UNO Activated Sludge model. X remains almost constant but when k_g gets 420 starts to oscillate. X_R has same behavior of X but when k_g gets 440 values become negative going down. t_c is affected going down gradually. Finally, X_e is affected increasing exponentially and St has a jump down change when k_g takes values between 300 and 420.
- Varying k_{gp} only affects significantly St , which gets negative values when k_{gp} reaches around 25.
- The system is much more sensitive to changes in a_x than to changes in a_p respect to t_c . Fluctuations of t_c are 100 times smaller varying a_x than varying a_p .
- The kinetic parameter of TSS flocculation (a_x) is the most sensitive to changes. Significant variation of the system output occurs when a_x takes values over 0.1.

- The first order constant of TSS growth (k_g) is the parameter that has the most important impact on the model performance, especially on the predicted value of t_c .

5.2 Recommendations for Further Research

- It would be highly desirable to extend this study to the case of a full-scale activated sludge system, such as the new system recently built at the Marrero wastewater treatment plant. For such a study, a long-term data collection program should be implemented.
- Perform a complete sensitivity analysis changing parameters simultaneously.

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7. Appendices

Appendix A

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| for use by: |
StudentTSP/GiveWin User#45AGT0002

TSP Version 4.5
(07/16/01) Student GWin 2.2MB
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In case of questions or problems, see your local TSP
consultant or send a description of the problem and the
associated TSP output to:

TSP International
P.O. Box 61015
Palo Alto, CA 94306
USA

PROGRAM

```
COMMAND *****  
1 options crt MEMORY=20;  
2  
2  
2 smpl 1 8; ? number of observations  
3 read(file='data_obs.xls');  
4 ?X Xr tc Xe St  
4  
4 alpha = 0.701;  
5  
5  
5 list vars Xr tc Xe St n Xo Xi;  
6 ?corr Vars; stop;  
6  
6 ? define constants  
6  
6 const  
6 Vs 0.14537  
6 Vr 0.175  
6 Q 5.599  
6 t 0.03125  
6 A 0.4389353  
6 Kg 1.2484  
6 Kgp 0.247  
6  
6 Y 0.5  
6 Kd 0.06  
6 fp 0.899;  
7  
7 ? define parameters  
7 param  
7 ax 0.015  
7 ap 0.037  
7 Kx 500  
7 Kp 7  
7 ;  
8  
8
```

```

8
8 ?msd X Xr tc Xe St;
8
8 ?Generate Fl and w with the observed data
8 Fl = (Vo*exp(n/2*
  ((Xr^2+4*Xr/n)^(0.5))))/(1/((0.5)*(Xr+((Xr^2+4*Xr/n)^(0.5))))-1/Xr);
9 w = 1-(Fl*A/Q)*(1-X/Xr)/(X-Xe);
10 Xr = (X/alpha*(1+alpha-t/tc*(1+Vs/Vr)));
11
11
11 ? write system of equations
11 frml eq1 tc - (t*X*(1+Vs/Vr))/(Xi+Y*(1-fp)*(Sti-St)+t*X*(kx*(Xe-ax)-
kd));
12
12 frml eq2 Fl - (Vo*exp(n/2* (
(Xr^2+4*Xr/n)^(0.5))))/(1/((0.5)*(Xr+((Xr^2+4*Xr/n)^(0.5))))-1/Xr);
13
13 frml eq3 alpha -((Fl*A/(Q*X))-1+(Xe/X)*(1-(X*(t/tc)*(1+Vs/Vr)-Xe)/(Xr-
Xe)));
14
14 frml eq4 Xe - (((1+alpha)*Xo+t*X*kx*ax)/(1+alpha+t*X*(kx-kg)));
15
15 frml eq5 St - ((So*(1+alpha)+kp*ap*t*X/fp)/(1+alpha+t*X*(kp-kgp)));
16
16 frml eq6 w - 1-(Fl*A/Q)*(1-X/Xr)/(X-Xe);
17
17 frml eq7 X - (Xe+(Fl*A/(Q*(1+alpha)))*(1-Xe/((X/alpha)*(1+alpha-
t/tc*(1+Vs/Vr)))));
18
18
18 list Equations eq1 eq2 eq3 eq4 eq5 eq6 eq7;
19
19 ?get the parameters that minimizes error in the system of equations!
19 fiml(maxit=500,endog=(X,St,Xe,tc,fl,w,Xr)) Equations; ?stop;
20
20 end;
EXECUTION
*****
**

```

Current sample: 1 to 8

Full Information Maximum Likelihood
=====

Equations: EQ1 EQ2 EQ3 EQ4 EQ5 EQ6 EQ7

Endogenous variables: TC FL ALPHA W X XE ST

CONSTANTS:

	T	VS	VR	Y
FP				
VALUE	0.031250	0.14537	0.17500	0.50000
0.89900				
	KD	A	Q	KG
KGP				
VALUE	0.060000	0.43894	5.59900	1.24840
0.24700				

STARTING VALUES

VALUE	KX	AX	KP	AP
500.00000		0.015000	7.00000	0.037000

F= -254.33492879	FNEW= -262.53309335	ISQZ= 2	STEP= 2.00	CRIT= 3.1912
F= -262.53309335	FNEW= -264.45309999	ISQZ= 4	STEP= 8.00	CRIT= .54858
F= -264.45309999	FNEW= -267.82859874	ISQZ= 2	STEP= 2.00	CRIT= 1.9635
F= -267.82859874	FNEW= -273.04289532	ISQZ= 5	STEP= 16.0	CRIT= .43263
F= -273.04289532	FNEW= -282.05898739	ISQZ= 2	STEP= 2.00	CRIT= 3.3035
F= -282.05898739	FNEW= -283.87041994	ISQZ= 3	STEP= 4.00	CRIT= .55032
F= -283.87041994	FNEW= -285.67537724	ISQZ= 3	STEP= 4.00	CRIT= .57229
F= -285.67537724	FNEW= -287.47628252	ISQZ= 3	STEP= 4.00	CRIT= .59763
F= -287.47628252	FNEW= -289.26980665	ISQZ= 3	STEP= 4.00	CRIT= .62677
F= -289.26980665	FNEW= -291.05751687	ISQZ= 3	STEP= 4.00	CRIT= .66014
F= -291.05751687	FNEW= -292.83650831	ISQZ= 3	STEP= 4.00	CRIT= .69830
F= -292.83650831	FNEW= -294.60737798	ISQZ= 3	STEP= 4.00	CRIT= .74168
F= -294.60737798	FNEW= -296.36768267	ISQZ= 3	STEP= 4.00	CRIT= .79085
F= -296.36768267	FNEW= -298.11726233	ISQZ= 3	STEP= 4.00	CRIT= .84625
F= -298.11726233	FNEW= -299.85357858	ISQZ= 3	STEP= 4.00	CRIT= .90841
F= -299.85357858	FNEW= -301.57744395	ISQZ= 3	STEP= 4.00	CRIT= .97757
F= -301.57744395	FNEW= -303.30262580	ISQZ= 2	STEP= 2.00	CRIT= 1.0545
F= -303.30262580	FNEW= -312.77149462	ISQZ= 5	STEP= 16.0	CRIT= .41513

Full Information Maximum Likelihood
=====

Residual Covariance Matrix

	EQ1	EQ2	EQ3	EQ4
EQ1	0.62936			
EQ2	0.000011245	2.45456D-09		

EQ3	-37.01902	-0.00079572	3024.45826	
EQ4	0.0052225	5.58749D-08	-0.23598	0.000056461
EQ5	-0.028813	-9.08655D-07	2.16398	-0.00014851
EQ6	-2.52043D-07	2.41208D-11	0.000026612	-1.36732D-09
EQ7	-61.07758	-0.0015196	4609.44479	-0.40221

	EQ5	EQ6	EQ7
EQ5	0.0021153		
EQ6	9.30676D-09	9.63541D-13	
EQ7	3.55657	0.000030783	7299.45677

Number of observations = 8 Log likelihood = 314.690
 Schwarz B.I.C. = -306.640

Parameter	Estimate	Standard Error	t-statistic	P-value
KX	501.894	.210550E-02	238373.	[.000]
AX	.014979	.103411E-07	.144845E+07	[.000]
KP	7.05074	.601848E-04	117151.	[.000]
AP	.037060	.591762E-06	62627.1	[.000]

Standard Errors computed from covariance of analytic first derivatives(BHHH)

Appendix B

Table B-1 Summary of regression analysis respect to X

<i>Regression Statistics</i>	
Multiple R	0.997477482
R Square	0.994961328
Adjusted R Square	0.852104185
Standard Error	0.309642803
Observations	8

<i>ANOVA</i>					
	<i>df</i>	<i>SS</i>	<i>MS</i>	<i>F</i>	<i>Significance F</i>
Regression	1	132.5287477	132.5287477	1382.25482	2.52698E-08
Residual	7	0.671150659	0.095878666		
Total	8	133.1998983			

	<i>Coefficients</i>	<i>Standard Error</i>	<i>t Stat</i>	<i>P-value</i>	<i>Lower 95%</i>	<i>Upper 95%</i>
Intercept	0	#N/A	#N/A	#N/A	#N/A	#N/A
X Variable 1	1.319822067	0.035499426	37.17868771	2.64784E-09	1.235879264	1.40376487

Table B-2 Summary of regression analysis respect to X_R

<i>Regression Statistics</i>	
Multiple R	0.994669143
R Square	0.989366703
Adjusted R Square	0.84650956
Standard Error	1.03195913
Observations	8

ANOVA

	<i>df</i>	<i>SS</i>	<i>MS</i>	<i>F</i>	<i>Significance F</i>
Regression	1	693.6052689	693.6052689	651.3094625	2.38499E-07
Residual	7	7.454577527	1.064939647		
Total	8	701.0598464			

	<i>Coefficients</i>	<i>Standard Error</i>	<i>t Stat</i>	<i>P-value</i>	<i>Lower 95%</i>	<i>Upper 95%</i>
Intercept	0	#N/A	#N/A	#N/A	#N/A	#N/A
X Variable 1	1.32450284	0.051899025	25.52076532	3.62305E-08	1.201781146	1.447224533

Table B-3 Summary of regression analysis respect to tc

<i>Regression Statistics</i>	
Multiple R	0.937154068
R Square	0.878257747
Adjusted R Square	0.735400604
Standard Error	0.27837213
Observations	8

ANOVA

	<i>df</i>	<i>SS</i>	<i>MS</i>	<i>F</i>	<i>Significance F</i>
Regression	1	3.913183371	3.913183371	50.49852516	0.000390207
Residual	7	0.542437299	0.077491043		
Total	8	4.45562067			

	<i>Coefficients</i>	<i>Standard Error</i>	<i>t Stat</i>	<i>P-value</i>	<i>Lower 95%</i>	<i>Upper 95%</i>
Intercept	0	#N/A	#N/A	#N/A	#N/A	#N/A
X Variable 1	0.619929289	0.087237419	7.106231432	0.000192605	0.413645572	0.826213006

Table B-4 Summary of regression analysis respect to Xe

<i>Regression Statistics</i>	
Multiple R	0.950567438
R Square	0.903578455
Adjusted R Square	0.760721312
Standard Error	0.005158649
Observations	8

ANOVA

	<i>df</i>	<i>SS</i>	<i>MS</i>	<i>F</i>	<i>Significance F</i>
Regression	1	0.001745668	0.001745668	65.59788229	0.000189997
Residual	7	0.000186282	2.66117E-05		
Total	8	0.00193195			

	<i>Coefficients</i>	<i>Standard Error</i>	<i>t Stat</i>	<i>P-value</i>	<i>Lower 95%</i>	<i>Upper 95%</i>
Intercept	0	#N/A	#N/A	#N/A	#N/A	#N/A
X Variable 1	0.704722617	0.087010828	8.099251959	8.42411E-05	0.498974704	0.910470531

Table B-5 Summary of regression analysis respect to St

<i>Regression Statistics</i>	
Multiple R	0.953089709
R Square	0.908379994
Adjusted R Square	0.765522851
Standard Error	0.025990827
Observations	8

ANOVA

	<i>df</i>	<i>SS</i>	<i>MS</i>	<i>F</i>	<i>Significance F</i>
Regression	1	0.046883008	0.046883008	69.40252714	0.000162387
Residual	7	0.004728662	0.000675523		
Total	8	0.05161167			

	<i>Coefficients</i>	<i>Standard Error</i>	<i>t Stat</i>	<i>P-value</i>	<i>Lower 95%</i>	<i>Upper 95%</i>
Intercept	0	#N/A	#N/A	#N/A	#N/A	#N/A
X Variable 1	1.828011404	0.219427603	8.330817916	7.03073E-05	1.309147573	2.346875235

Appendix C

Table C-1 Effect of changing K_p on the output model (Day 1)

Day 1 (29-Jul-04)					
K_p	X	Xr	tc	Xe	St
0.00001	3.0939	7.0134	0.5111	0.0161	0.0527
0.0001	3.0939	7.0134	0.5111	0.0161	0.0527
0.001	3.0939	7.0134	0.5111	0.0161	0.0527
0.01	3.0939	7.0134	0.5111	0.0161	0.0527
0.1	3.0939	7.0134	0.5111	0.0161	0.0527
1	3.0939	7.0134	0.5111	0.0161	0.0527
10	3.0940	7.0134	0.5111	0.0161	0.0485
50	3.0940	7.0133	0.5105	0.0161	0.0441
100	3.0941	7.0133	0.5105	0.0161	0.0429
500	3.0941	7.0133	0.5105	0.0161	0.0415
1000	3.0941	7.0133	0.5105	0.0161	0.0413
5000	3.0941	7.0133	0.5105	0.0161	0.0412
100000	3.0941	7.0133	0.5105	0.0161	0.0412
500000	3.0941	7.0133	0.5105	0.0161	0.0412
1000000	3.0941	7.0133	0.5105	0.0161	0.0412

Table C-2 Effect of changing K_p on the output model (Day 2)

Day 2 (30-Jul-04)					
K_p	X	Xr	tc	Xe	St
0.00001	3.5363	8.1162	0.6211	0.0155	0.1168
0.0001	3.5363	8.1162	0.6211	0.0155	0.1168
0.001	3.5363	8.1162	0.6211	0.0155	0.1168
0.01	3.5363	8.1162	0.6211	0.0155	0.1168
0.1	3.5363	8.1162	0.6211	0.0155	0.1168
1	3.5363	8.1162	0.6206	0.0155	0.1122
10	3.5370	8.1158	0.6183	0.0155	0.0867
50	3.5377	8.1154	0.6158	0.0155	0.0588
100	3.5377	8.1154	0.6151	0.0155	0.0512
500	3.5377	8.1154	0.6144	0.0155	0.0434
1000	3.5377	8.1154	0.6143	0.0155	0.0423
5000	3.5377	8.1154	0.6143	0.0155	0.0423
100000	3.5377	8.1154	0.6143	0.0155	0.0423
500000	3.5377	8.1154	0.6143	0.0155	0.0423
1000000	3.5377	8.1154	0.6143	0.0155	0.0423

Table C-3 Effect of changing K_p on the output model (Day 3)

Day 3 (31-Jul-04)					
K_p	X	Xr	tc	Xe	St
0.00001	3.1438	7.3121	0.8109	0.0153	0.0943
0.0001	3.1438	7.3121	0.8109	0.0153	0.0943
0.001	3.1438	7.3121	0.8109	0.0153	0.0943
0.01	3.1438	7.3121	0.8109	0.0153	0.0943
0.1	3.1438	7.3121	0.8109	0.0153	0.0943
1	3.1438	7.3121	0.8109	0.0153	0.0943
10	3.1443	7.3118	0.8074	0.0153	0.0747
50	3.1447	7.3116	0.8039	0.0153	0.0547
100	3.1447	7.3115	0.8029	0.0153	0.0489
500	3.1450	7.3114	0.8020	0.0153	0.0441
1000	3.1450	7.3114	0.8020	0.0153	0.0441
5000	3.1450	7.3114	0.8020	0.0153	0.0441
100000	3.1450	7.3114	0.8020	0.0153	0.0441
500000	3.1450	7.3114	0.8020	0.0153	0.0441
1000000	3.1451	7.3114	0.8015	0.0153	0.0441

Table C-4 Effect of changing K_p on the output model (Day 4)

Day 4 (1-Aug-04)					
K_p	X	Xr	tc	Xe	St
0.00001	3.4561	8.1767	1.3450	0.0157	0.0792
0.0001	3.4561	8.1767	1.3450	0.0157	0.0792
0.001	3.4561	8.1767	1.3450	0.0157	0.0792
0.01	3.4561	8.1767	1.3450	0.0157	0.0792
0.1	3.4561	8.1767	1.3450	0.0157	0.0792
1	3.4561	8.1767	1.3442	0.0157	0.0769
10	3.4561	8.1765	1.3385	0.0157	0.0643
50	3.4568	8.1763	1.3322	0.0157	0.0502
100	3.4568	8.1763	1.3305	0.0157	0.0463
500	3.4570	8.1762	1.3288	0.0157	0.0424
1000	3.4570	8.1762	1.3285	0.0157	0.0418
5000	3.4570	8.1762	1.3285	0.0157	0.0418
100000	3.4570	8.1762	1.3285	0.0157	0.0418
500000	3.4570	8.1762	1.3285	0.0157	0.0418
1000000	3.4570	8.1762	1.3282	0.0157	0.0412

Table C-5 Effect of changing K_p on the output model (Day 5)

Day 5 (2-Aug-04)					
K_p	X	Xr	tc	Xe	St
0.00001	4.1182	9.2745	0.4678	0.0154	0.0693
0.0001	4.1182	9.2745	0.4678	0.0154	0.0693
0.001	4.1182	9.2745	0.4678	0.0154	0.0693
0.01	4.1182	9.2745	0.4678	0.0154	0.0693
0.1	4.1182	9.2745	0.4678	0.0154	0.0693
1	4.1182	9.2745	0.4678	0.0154	0.0693
10	4.1185	9.2745	0.4673	0.0154	0.0673
50	4.1187	9.2742	0.4669	0.0154	0.0571
100	4.1187	9.2742	0.4667	0.0154	0.0470
500	4.1188	9.2741	0.4667	0.0154	0.0444
1000	4.1188	9.2741	0.4667	0.0154	0.0419
500000	4.1188	9.2741	0.4667	0.0154	0.0419
1000000	4.1188	9.2741	0.4667	0.0154	0.0412

Table C-6 Effect of changing K_p on the output model (Day 6)

Day 6 (3-Aug-04)					
K_p	X	Xr	tc	Xe	St
0.00001	3.9428	8.7565	0.3969	0.0157	0.1170
0.0001	3.9428	8.7565	0.3969	0.0157	0.1170
0.001	3.9428	8.7565	0.3969	0.0157	0.1170
0.01	3.9428	8.7565	0.3969	0.0157	0.1170
0.1	3.9428	8.7565	0.3969	0.0157	0.1170
1	3.9429	8.7564	0.3967	0.0157	0.1118
10	3.9435	8.7559	0.3958	0.0157	0.0848
50	3.9442	8.7556	0.3949	0.0157	0.0574
100	3.9443	8.7554	0.3947	0.0157	0.0503
500	3.9445	8.7553	0.3945	0.0157	0.0432
1000	3.9445	8.7553	0.3945	0.0157	0.0422
500000	3.9445	8.7553	0.3945	0.0157	0.0422
1000000	3.9445	8.7553	0.3944	0.0157	0.0412

Table C-7 Effect of changing K_p on the output model (Day 7)

Day 7 (4-Aug-04)					
K_p	X	Xr	tc	Xe	St
0.00001	4.5813	10.5939	0.7153	0.0151	0.1409
0.0001	4.5813	10.5939	0.7153	0.0151	0.1409
0.001	4.5813	10.5939	0.7153	0.0151	0.1409
0.01	4.5813	10.5939	0.7153	0.0151	0.1409
0.1	4.5813	10.5939	0.7153	0.0151	0.1409
1	4.5815	10.5938	0.7145	0.0151	0.1330
10	4.5824	10.5932	0.7109	0.0151	0.0948
50	4.5832	10.5927	0.7077	0.0151	0.0600
100	4.5834	10.5926	0.7069	0.0151	0.0520
500	4.5836	10.5925	0.7061	0.0151	0.0435
1000	4.5836	10.5925	0.7061	0.0151	0.0435
5000	4.5836	10.5925	0.7061	0.0151	0.0435
10000	4.5836	10.5925	0.7061	0.0151	0.0435
500000	4.5836	10.5925	0.7061	0.0151	0.0435
1000000	4.5837	10.5924	0.7059	0.0151	0.0412

Table C-8 Effect of changing K_p on the output model (Day 8)

Day 8 (5-Aug-04)					
K_p	X	Xr	tc	Xe	St
0.00001	5.9806	13.8134	0.6987	0.0155	0.1210
0.0001	5.9806	13.8134	0.6987	0.0155	0.1210
0.001	5.9806	13.8134	0.6987	0.0155	0.1210
0.01	5.9806	13.8134	0.6987	0.0155	0.1210
0.1	5.9806	13.8134	0.6987	0.0155	0.1210
1	5.9807	13.8133	0.6981	0.0155	0.1130
10	5.9816	13.8128	0.6958	0.0155	0.0788
50	5.9822	13.8124	0.6940	0.0155	0.0533
100	5.9823	13.8123	0.6936	0.0155	0.0477
500	5.9824	13.8122	0.6933	0.0155	0.0426
1000	5.9824	13.8122	0.6932	0.0155	0.0419
5000	5.9824	13.8122	0.6932	0.0155	0.0419
10000	5.9824	13.8122	0.6932	0.0155	0.0419
500000	5.9824	13.8122	0.6932	0.0155	0.0419
1000000	5.9824	13.8122	0.6932	0.0155	0.0412

Table C-9 Effect of changing K_x on the output model (Day 1)

Day 1 (29-Jul-04)					
K_x	X	Xr	tc	Xe	St
0.00001	3.0721	7.0356	0.5885	0.0495	0.0494
0.0001	3.0721	7.0356	0.5885	0.0495	0.0494
0.001	3.0721	7.0356	0.5885	0.0495	0.0494
0.01	3.0721	7.0356	0.5885	0.0495	0.0494
0.1	3.0721	7.0356	0.5978	0.0493	0.0494
1	3.0734	7.0342	0.5924	0.0450	0.0494
10	3.0806	7.0269	0.5607	0.0475	0.0494
50	3.0891	7.0183	0.5279	0.0364	0.0494
100	3.0915	7.0158	0.5194	0.0235	0.0494
500	3.0935	7.0138	0.5125	0.0198	0.0494
1000	3.0939	7.0134	0.5109	0.0168	0.0494
5000	3.0943	7.0130	0.5097	0.0161	0.0494
10000	3.0946	7.0130	0.5088	0.0155	0.0494
1000000	3.0946	7.0130	0.5088	0.0155	0.0494

Table C-6 Effect of changing K_x on the output model (Day 2)

Day 2 (30-Jul-04)					
K_x	X	Xr	Tc	Xe	St
0.00001	3.5245	8.1288	0.6792	0.0348	0.0929
0.0001	3.5245	8.1288	0.6792	0.0348	0.0929
0.001	3.5245	8.1288	0.6792	0.0348	0.0929
0.01	3.5245	8.1288	0.6792	0.0348	0.0929
0.1	3.5245	8.1288	0.6792	0.0348	0.0929
1	3.5253	8.1279	0.6748	0.0335	0.0929
10	3.5298	8.1233	0.6521	0.0266	0.0929
50	3.5344	8.1184	0.6299	0.0194	0.0929
100	3.5356	8.1171	0.6243	0.0174	0.0929
500	3.5369	8.1159	0.6189	0.0155	0.0929
1000	3.5370	8.1157	0.6181	0.0153	0.0929
5000	3.5372	8.1155	0.6175	0.0150	0.0929
10000	3.5372	8.1155	0.6175	0.0150	0.0929
1000000	3.5372	8.1155	0.6175	0.0150	0.0929

Table C-7 Effect of changing K_x on the output model (Day 3)

Day 3 (31-Jul-04)					
K_x	X	Xr	Tc	Xe	St
0.00001	3.1373	7.3189	0.8714	0.0259	0.0788
0.0001	3.1373	7.3189	0.8714	0.0259	0.0788
0.001	3.1373	7.3189	0.8714	0.0259	0.0788
0.01	3.1373	7.3189	0.8714	0.0259	0.0788
0.1	3.1373	7.3189	0.8714	0.0259	0.0788
1	3.1377	7.3184	0.8673	0.0252	0.0788
10	3.1400	7.3161	0.8452	0.0217	0.0788
50	3.1427	7.3134	0.8212	0.0176	0.0788
100	3.1434	7.3127	0.8147	0.0165	0.0788
500	3.1442	7.3119	0.8081	0.0153	0.0788
1000	3.1442	7.3119	0.8081	0.0153	0.0788
5000	3.1442	7.3119	0.8081	0.0153	0.0788
10000	3.1442	7.3119	0.8081	0.0153	0.0788
1000000	3.1442	7.3119	0.8081	0.0153	0.0788

Table C-8 Effect of changing K_x on the output model (Day 4)

Day 4 (1-Aug-04)					
K_x	X	Xr	Tc	Xe	St
0.00001	3.4418	8.1933	1.7749	0.0391	0.0674
0.0001	3.4418	8.1933	1.7749	0.0391	0.0674
0.001	3.4418	8.1933	1.7749	0.0391	0.0674
0.01	3.4418	8.1933	1.7749	0.0391	0.0674
0.1	3.4419	8.1932	1.7709	0.0389	0.0674
1	3.4427	8.192	1.7375	0.0375	0.0674
10	3.4479	8.1863	1.5618	0.0293	0.0674
50	3.4534	8.1799	1.4096	0.0204	0.0674
100	3.4549	8.1782	1.3739	0.0180	0.0674
500	3.4564	8.1766	1.3399	0.0157	0.0674
1000	3.4566	8.1763	1.3352	0.0153	0.0674
5000	3.4566	8.1763	1.3352	0.0153	0.0674
10000	3.4566	8.1763	1.3352	0.0153	0.0674
1000000	3.4568	8.1761	1.3305	0.0150	0.0674

Table C-9 Effect of changing K_x on the output model (Day 5)

Day 5 (2-Aug-04)					
K_x	X	Xr	tc	Xe	St
0.00001	4.1080	9.2856	0.4912	0.0320	0.0594
0.0001	4.1080	9.2856	0.4912	0.0320	0.0594
0.001	4.1080	9.2856	0.4912	0.0320	0.0594
0.01	4.1080	9.2856	0.4912	0.0320	0.0594
0.1	4.1080	9.2856	0.4912	0.0320	0.0594
1	4.1088	9.2847	0.4892	0.0307	0.0594
10	4.1129	9.2804	0.4798	0.0243	0.0594
50	4.1166	9.2763	0.4714	0.0183	0.0594
100	4.1175	9.2753	0.4694	0.0168	0.0594
500	4.1184	9.2744	0.4674	0.0154	0.0594
1000	4.1184	9.2744	0.4674	0.0154	0.0594
5000	4.1184	9.2744	0.4674	0.0154	0.0594
10000	4.1184	9.2744	0.4674	0.0154	0.0594
1000000	4.1186	9.2741	0.4669	0.0150	0.0594

Table C-10 Effect of changing K_x on the output model (Day 6)

Day 6 (3-Aug-04)					
K_x	X	Xr	tc	Xe	St
0.00001	3.9266	8.7778	0.4271	0.0439	0.0912
0.0001	3.9266	8.7778	0.4271	0.0439	0.0912
0.001	3.9266	8.7778	0.4271	0.0439	0.0912
0.01	3.9266	8.7778	0.4271	0.0439	0.0912
0.1	3.9268	8.7776	0.4268	0.4370	0.0912
1	3.9279	8.7776	0.4246	0.0418	0.0912
10	3.9342	8.7679	0.4124	0.0311	0.0912
50	3.9404	8.7599	0.4013	0.0208	0.0912
100	3.9419	8.7581	0.3986	0.0182	0.0911
500	3.9434	8.7561	0.3960	0.0157	0.0911
1000	3.9436	8.7558	0.3957	0.0153	0.0911
5000	3.9436	8.7558	0.3957	0.0153	0.0911
10000	3.9436	8.7558	0.3957	0.0153	0.0911
1000000	3.9438	8.7555	0.3953	0.0150	0.0911

Table C-15 Effect of changing K_x on the output model (Day 7)

Day 7 (4-Aug-04)					
K_x	X	Xr	tc	Xe	St
0.00001	4.5798	10.5961	0.7230	0.0189	0.1033
0.0001	4.5798	10.5961	0.7230	0.0189	0.1033
0.001	4.5798	10.5961	0.7230	0.0189	0.1033
0.01	4.5798	10.5961	0.7230	0.0189	0.1033
0.1	4.5798	10.5961	0.7230	0.0189	0.1033
1	4.5800	10.5959	0.7220	0.0187	0.1033
10	4.5810	10.5947	0.7174	0.0170	0.1033
50	4.5818	10.5937	0.7135	0.0160	0.1033
100	4.5820	10.5935	0.7126	0.0154	0.1033
500	4.5822	10.5933	0.7117	0.0151	0.1033
1000	4.5822	10.5933	0.7117	0.0151	0.1033
5000	4.5822	10.5933	0.7117	0.0151	0.1033
10000	4.5822	10.5933	0.7117	0.0151	0.1033
1000000	4.5822	10.5933	0.7115	0.0150	0.1033

Table C-16 Effect of changing K_x on the output model (Day 8)

Day 8 (5-Aug-04)					
K_x	X	Xr	tc	Xe	St
0.00001	5.9640	13.8377	0.7676	0.0475	0.0858
0.0001	5.9640	13.8377	0.7676	0.0475	0.0858
0.001	5.9640	13.8377	0.7676	0.0475	0.0858
0.01	5.9640	13.8377	0.7676	0.0475	0.0858
100	5.9804	13.8143	0.7000	0.0174	0.0858
500	5.9814	13.8129	0.6963	0.0155	0.0858
1000	5.9815	13.8127	0.6957	0.0152	0.0858
5000	5.9815	13.8127	0.6957	0.0152	0.0858
10000	5.9815	13.8127	0.6957	0.0152	0.0858
50000	5.9815	13.8127	0.6957	0.0152	0.0858
100000	5.9815	13.8127	0.6957	0.0152	0.0858
500000	5.9815	13.8127	0.6957	0.0152	0.0858
1000000	5.9817	13.8125	0.6952	0.0150	0.0858

Table C-17 Effect of changing a_p on the output model (Day 1)

Day 1 (29-Jul-04)					
a_p	X	Xr	tc	Xe	St
0.00001	3.0943	7.0132	0.5100	0.1610	0.0375
0.0001	3.0943	7.0132	0.5100	0.0375	0.0375
0.001	3.0943	7.0132	0.5100	0.0375	0.0375
0.01	3.0943	7.0132	0.5100	0.0375	0.0407
0.1	3.0935	7.0136	0.5123	0.0375	0.0696
1	3.0865	7.0174	0.5337	0.0375	0.3585
10	3.0178	7.0551	0.9201	0.0375	3.1954
20	2.9451	7.0957	4.7347	0.0375	6.2080
30	2.8745	7.1360	-1.4590	0.0375	9.1460
40	2.8067	7.1756	-0.6277	0.0375	11.9806
50	2.7408	7.2184	-0.3960	0.0375	14.7400

Table C-18 Effect of changing a_p on the output model (Day 2)

Day 2 (30-Jul-04)					
a_p	X	Xr	Tc	Xe	St
0.00001	3.5372	8.1157	0.6177	0.0155	0.0797
0.0001	3.5372	8.1157	0.6177	0.0155	0.0797
0.001	3.5372	8.1157	0.6177	0.0155	0.0797
0.01	3.5372	8.1157	0.6177	0.0155	0.0797
0.1	3.5363	8.1162	0.6209	0.0155	0.1151
1	3.5287	8.1204	0.6516	0.0155	0.4326
10	3.4533	8.1625	1.2982	0.0155	3.5563
20	3.3725	8.2084	-11.0250	0.0155	6.9183
30	3.2946	8.2537	-1.0379	0.0155	10.1699
40	3.2196	8.2981	-0.5412	0.0155	13.3149
50	3.1473	8.3418	-0.3646	0.0155	16.3573

Table C-19 Effect of changing a_p on the output model (Day 3)

Day 3 (31-Jul-04)					
a_p	X	Xr	tc	Xe	St
0.00001	3.1445	7.3117	0.8060	0.0153	0.0667
0.0001	3.1445	7.3117	0.8060	0.0153	0.0667
0.001	3.1445	7.3117	0.8060	0.0153	0.0671
0.01	3.1445	7.3117	0.8060	0.0153	0.0700
0.1	3.1437	7.3122	0.8117	0.0153	0.0990
1	3.1366	7.3159	0.8677	0.0153	0.3915
10	3.0670	7.3538	2.8329	0.0153	3.2621
20	2.9926	7.3952	-1.8287	0.0153	6.3445
30	2.9210	7.4357	-0.6857	0.0153	9.3186
40	2.8523	7.4755	-0.4199	0.0153	12.1885
50	2.7862	7.5146	-0.3017	0.0153	14.9587

Table C-11 Effect of changing a_p on the output model (Day 4)

Day 4 (1-Aug-04)					
a_p	X	Xr	tc	Xe	St
0.00001	3.4537	8.1764	1.3341	0.0157	0.0545
0.0001	3.4537	8.1764	1.3341	0.0157	0.0545
0.001	3.4537	8.1764	1.3341	0.0157	0.0545
0.01	3.4537	8.1764	1.3357	0.0157	0.0579
0.1	3.4559	8.1769	1.3498	0.0157	0.0892
1	3.4484	8.1813	1.5094	0.0157	0.4017
10	3.3752	8.2249	-7.9058	0.0157	3.4755
20	3.2967	8.2726	-0.9854	0.0157	6.7838
30	3.2210	8.3194	-0.5222	0.0157	9.9834
40	3.1482	8.3655	-0.3537	0.0157	13.0782
50	3.0779	8.4107	0.2667	0.0157	16.0719

Table C-21 Effect of changing a_p on the output model (Day 5)

Day 5 (2-Aug-04)					
a_p	X	Xr	tc	Xe	St
0.00001	4.1188	9.2742	0.4668	0.0154	0.0449
0.0001	4.1188	9.2742	0.4668	0.0154	0.0449
0.001	4.1188	9.2742	0.4668	0.0154	0.0449
0.01	4.1186	9.2742	0.4669	0.0154	0.0488
0.1	4.1178	9.2747	0.4685	0.0154	0.0840
1	4.1094	9.2795	0.4847	0.0154	0.4361
10	4.0262	9.3276	0.7431	0.0154	3.9048
20	3.9368	9.3802	1.8615	0.0154	7.6498
30	3.8504	9.4320	-3.5321	0.0154	11.2831
40	3.7668	9.4831	-0.8969	0.0154	14.8081
50	3.6860	9.5333	-0.5108	0.0154	18.2280

Table C-12 Effect of changing a_p on the output model (Day 6)

Day 6 (3-Aug-04)					
a_p	X	Xr	tc	Xe	St
0.00001	3.9437	8.7559	0.3956	0.0157	0.0770
0.0001	3.9437	8.7559	0.3956	0.0157	0.0770
0.001	3.9437	8.7559	0.3956	0.0157	0.0770
0.01	3.9437	8.7559	0.3956	0.0157	0.0770
0.1	3.9428	8.7565	0.3968	0.0157	0.1151
1	3.9349	8.7618	0.4084	0.0157	0.4570
10	3.8566	8.8145	0.5790	0.0157	3.8274
20	3.7724	8.8722	1.0933	0.0157	7.4665
30	3.6909	8.9288	11.0052	0.0157	10.9975
40	3.6122	8.9846	-1.3442	0.0157	14.4238
50	3.5361	9.0393	-0.6292	0.0157	17.7486

Table C-13 Effect of changing a_p on the output model (Day 7)

Day 7 (4-Aug-04)					
a_p	X	Xr	tc	Xe	St
0.00001	4.5826	10.5931	0.7103	0.0151	0.0877
0.0001	4.5826	10.5931	0.7103	0.0151	0.0877
0.001	4.5826	10.5931	0.7103	0.0151	0.0877
0.01	4.5826	10.5931	0.7103	0.0151	0.0877
0.1	4.5816	10.5937	0.7142	0.0151	0.1297
1	4.5726	10.5992	0.7518	0.0151	0.5071
10	4.4846	10.6535	8.0000	0.0151	4.2295
20	4.3896	10.7131	-5.8169	0.0151	8.2579
30	4.2976	10.7719	-1.2060	0.0151	12.1759
40	4.2084	10.8298	-0.5558	0.0151	15.9862
50	4.1219	10.8869	-0.3803	0.0151	19.6916

Table C-14 Effect of changing a_p on the output model (Day 8)

Day 8 (5-Aug-04)					
a_p	X	Xr	tc	Xe	St
0.00001	5.9818	13.8126	0.6950	0.0155	0.0675
0.0001	5.9818	13.8126	0.6950	0.0155	0.0675
0.001	5.9818	13.8126	0.6950	0.0155	0.0675
0.01	5.9817	13.8127	0.6953	0.0155	0.0724
0.1	5.9807	13.8134	0.6984	0.0155	0.1168
1	5.9705	13.8205	0.7306	0.0155	0.5602
10	5.8694	13.8912	1.3640	0.0155	4.9467
20	5.7598	13.9689	62.3205	0.0155	9.7199
30	5.6530	14.0458	-1.4041	0.0155	14.3888
40	5.5488	14.1218	-0.6889	0.0155	18.9548
50	5.4473	14.1969	-0.4542	0.0155	23.4197

Table C-25 Effect of changing a_x on the output model (Day 1)

Day 1 (29-Jul-04)					
a_x	X	Xr	tc	Xe	St
0.00001	3.1035	7.0038	0.4806	0.0016	0.0494
0.0001	3.1035	7.0038	0.4808	0.0016	0.0494
0.001	3.1029	7.0044	0.4826	0.0025	0.0494
0.01	3.0972	7.0102	0.5004	0.0112	0.0494
0.1	3.0404	7.0689	0.8040	0.0984	0.0494
0.2	2.9786	7.1378	2.7034	0.1950	0.0494
0.3	2.9184	7.2107	-1.8455	0.2916	0.0494
0.4	2.8599	7.2881	-0.6699	0.1950	0.0494
0.5	2.8032	7.3702	-0.4028	0.4842	0.0494

Table C-26 Effect of changing a_x on the output model (Day 2)

Day 2 (30-Jul-04)					
a_x	X	Xr	tc	Xe	St
0.00001	3.5463	8.1062	0.5801	0.0090	0.0928
0.0001	3.5463	8.1062	0.5803	0.0010	0.0928
0.001	3.5456	8.1068	0.5825	0.0019	0.0928
0.01	3.5400	8.1126	0.6053	0.0107	0.0928
0.1	3.4841	8.1722	1.0081	0.0982	0.0928
0.2	3.4231	8.2415	4.3153	0.1953	0.0928
0.3	3.3634	8.3143	-1.7944	0.2923	0.0928
0.4	3.3051	8.3910	-0.7269	0.3892	0.0928
0.5	3.2483	8.4717	-0.4497	0.4860	0.0928

Table C-27 Effect of changing a_x on the output model (Day 3)

Day 3 (31-Jul-04)					
a_x	X	Xr	tc	Xe	St
0.00001	3.1537	7.3024	0.7349	0.0008	0.0788
0.0001	3.1537	7.3024	0.7349	0.0009	0.0788
0.001	3.1538	7.3024	0.7349	0.0018	0.0788
0.01	3.1474	7.3087	0.7821	0.0105	0.0788
0.1	3.0906	7.3675	1.9099	0.0976	0.0788
0.2	3.0289	7.4363	-2.8591	0.1943	0.0788
0.3	2.9687	7.5091	-0.7935	0.2909	0.0788
0.4	2.9102	7.5863	-0.4528	0.3873	0.0788
0.5	2.8536	7.6680	-0.0313	0.4837	0.0788

Table C-28 Effect of changing a_x on the output model (Day 4)

Day 4 (1-Aug-04)					
a_x	X	Xr	tc	Xe	St
0.00001	3.4656	8.1663	1.1636	0.0012	0.0673
0.0001	3.4656	8.1663	1.1646	0.0012	0.0673
0.001	3.4649	8.1669	1.1738	0.0020	0.0673
0.01	3.4595	8.1731	1.2753	0.0108	0.0673
0.1	3.4050	8.2365	10.7209	0.0982	0.0673
0.2	3.3457	8.3102	-1.4248	0.1953	0.0673
0.3	3.2878	8.3876	-0.6551	0.2922	0.0673
0.4	3.2314	8.4690	-0.4200	0.3891	0.0673
0.5	3.1766	8.5547	-0.3062	0.4858	0.0673

Table C-29 Effect of changing a_x on the output model (Day 5)

Day 5 (2-Aug-04)					
a_x	X	Xr	tc	Xe	St
0.00001	4.1276	9.2645	0.4484	0.0007	0.0059
0.0001	4.1276	9.2645	0.4480	0.0008	0.0059
0.001	4.1269	9.2651	0.4496	0.0017	0.0059
0.01	4.1215	9.2710	0.4609	0.0105	0.0059
0.1	4.0667	9.3315	0.6186	0.0983	0.0059
0.2	4.0069	9.4015	1.0174	0.1959	0.0059
0.3	3.9481	9.4745	3.0444	0.2934	0.0059
0.4	3.8905	9.5506	-2.8814	0.3908	0.0059
0.5	3.8341	9.6303	-0.9580	0.4882	0.0059

Table 15 Effect of changing a_x on the output model (Day 6)

Day 6 (3-Aug-04)					
a_x	X	Xr	tc	Xe	St
0.00001	3.9522	8.7449	0.3818	0.0001	0.0911
0.0001	3.9520	8.7450	0.3819	0.0001	0.0911
0.001	3.9515	8.7456	0.3826	0.0200	0.0911
0.01	3.9463	8.7524	0.3912	0.0108	0.0911
0.1	3.8945	8.8206	0.5049	0.0986	0.0911
0.2	3.8380	8.8993	0.7571	0.1961	0.0911
0.3	3.7827	8.9815	1.5632	0.2934	0.0911
0.4	3.7287	9.0671	-12.9032	0.3907	0.0911
0.5	3.6761	9.1564	-1.2706	0.4879	0.0911

Table C-16 Effect of changing a_x on the output model (Day 7)

Day 7 (4-Aug-04)					
a_x	X	Xr	tc	Xe	St
0.00001	4.5910	10.5829	0.6723	0.0004	0.1032
0.0001	4.5909	10.5829	0.6726	0.0004	0.1032
0.001	4.5904	10.5829	0.6748	0.0014	0.1032
0.01	4.5851	10.5898	0.6981	0.0102	0.1032
0.1	4.5325	10.6537	1.0734	0.0983	0.1032
0.2	4.4749	10.7271	2.7787	0.1961	0.1032
0.3	4.4183	10.8034	-4.3845	0.2939	0.1032
0.4	4.3626	10.8825	-1.2013	0.3916	0.1032
0.5	4.3081	10.9647	-0.6881	0.4893	0.1032

Table C-17 Effect of changing a_x on the output model (Day 3)

Day 8 (5-Aug-04)					
a_x	X	Xr	tc	Xe	St
0.00001	5.9894	13.8015	0.6678	0.0007	0.0858
0.0001	5.9894	13.8015	0.6679	0.0008	0.0858
0.001	5.9989	13.8022	0.6696	0.0170	0.0858
0.01	5.9841	13.8091	0.6865	0.0106	0.0858
0.1	5.9361	13.8782	0.9213	0.0992	0.0858
0.2	5.8834	13.9570	1.5046	0.1976	0.0858
0.3	5.8313	14.0379	4.2530	0.2959	0.0858
0.4	5.7799	14.1211	-4.9239	0.3943	0.0858
0.5	5.7294	14.2065	-1.5382	0.4926	0.0858

Table C-18 Effect of changing K_g on the output model (Day 1)

Day 1 (29-Jul-04)					
K_g	X	Xr	tc	Xe	St
0.00001	3.0931	7.0138	0.5135	0.0160	0.4940
0.0001	3.0931	7.0138	0.5135	0.0160	0.4940
0.001	3.0931	7.0138	0.5135	0.0160	0.4940
0.01	3.0931	7.0138	0.5135	0.0160	0.4940
0.1	3.0931	7.0138	0.5135	0.0160	0.4940
1	3.0938	7.0134	0.5115	0.0160	0.4940
10	3.1005	7.0099	0.4929	0.0164	0.4940
50	3.1336	6.9925	0.4183	0.0177	0.4940
100	3.1855	6.9655	0.3402	0.0199	0.4940
300	3.7391	6.7092	0.1303	0.0380	0.4940
400	5.5714	5.9741	0.0603	0.0720	0.4940
420	7.5889	5.3491	0.0471	0.0898	0.0474
440	49.4318	-1.5657	0.0336	0.1230	0.0439
450	5.2491	-1.3838	0.0303	0.1321	0.0483
475	7.6068	-20.6900	0.0158	0.2435	0.0474

Table C-19 Effect of changing K_g on the output model (Day 2)

Day 2 (30-Jul-04)					
K_g	X	Xr	tc	Xe	St
0.00001	3.5359	8.1164	0.6226	0.0155	0.0928
0.0001	3.5359	8.1164	0.6226	0.0155	0.0928
0.001	3.5359	8.1164	0.6226	0.0155	0.0928
0.01	3.5359	8.1164	0.6226	0.0155	0.0928
0.1	3.5359	8.1164	0.6226	0.0155	0.0928
1	3.5367	8.1159	0.6196	0.0155	0.0928
10	3.5440	8.1120	0.5931	0.0158	0.0928
50	3.5807	8.0923	0.4900	0.0171	0.0928
100	3.6381	8.0618	0.3875	0.0164	0.0928
300	4.2359	7.7635	0.1375	0.0371	0.0899
400	6.3038	6.9277	0.0615	0.0716	0.0831
420	6.6748	6.7995	0.0579	0.0880	26.2800
440	236.0900	0.0000	0.0336	0.1246	55.7500
450	6.7843	0.0000	0.0336	0.1336	26.5000
475	8.4503	-21.1200	0.0166	0.2451	29.6600

Table C-35 Effect of changing K_g on the output model (Day 3)

Day 3 (31-Jul-04)					
K_g	X	Xr	tc	Xe	St
0.00001	3.1433	7.3124	0.8146	0.0153	0.0788
0.0001	3.1433	7.3124	0.8146	0.0153	0.0788
0.001	3.1433	7.3124	0.8146	0.0153	0.0788
0.01	3.1433	7.3124	0.8146	0.0153	0.0788
0.1	3.1433	7.3124	0.8146	0.0153	0.0788
1	3.1440	7.3120	0.8094	0.0153	0.0788
10	3.1505	7.3086	0.7650	0.0156	0.0788
50	3.1826	7.2918	0.6026	0.0169	0.0788
100	3.2330	7.2658	0.4556	0.0189	0.0788
300	3.7552	7.0125	0.1459	0.0366	0.0788
400	5.5422	6.3105	0.0633	0.0704	0.0072
420	7.4908	5.7125	0.0490	0.0879	0.0687
440	74.2146	0.0000	0.0336	0.1238	0.0672
450	3.4960	0.0000	0.0336	0.1201	0.0777
475	8.4268	-22.7300	0.0159	0.0243	0.0672

Table C-36 Effect of changing K_g on the output model (Day 4)

Day 4 (1-Aug-04)					
K_g	X	Xr	tc	Xe	St
0.00001	3.4554	8.1771	1.3583	0.0156	0.0674
0.0001	3.4554	8.1771	1.3583	0.0156	0.0674
0.001	3.4554	8.1771	1.3583	0.0156	0.0674
0.01	3.4554	8.1771	1.3583	0.0156	0.0674
0.1	3.4554	8.1771	1.3583	0.0156	0.0674
1	3.4562	8.1767	1.3435	0.0156	0.0674
10	3.4634	8.1725	1.2211	0.0159	0.0674
50	3.4991	8.1521	0.8437	0.1730	0.0674
100	3.5549	8.1205	0.5739	0.0194	0.0671
300	4.1348	7.8112	0.1519	0.0374	0.0659
400	6.1192	6.9464	0.0632	0.0718	0.0627
420	8.2505	6.1985	0.4870	0.0893	0.0601
440	69.6300	0.0000	0.0336	0.1238	0.0463
450	3.2936	-1.0433	0.0336	0.1217	0.0677
475	7.5586	-19.8840	0.0161	0.2409	0.0609

Table C-37 Effect of changing K_g on the output model (Day 5)

Day 5 (2-Aug-04)					
K_g	X	Xr	tc	Xe	St
0.00001	4.1173	9.2750	0.4696	0.0154	0.0594
0.0001	4.1173	9.2750	0.4696	0.0154	0.0594
0.001	4.1173	9.2750	0.4696	0.0154	0.0594
0.01	4.1173	9.2750	0.4696	0.0154	0.0594
0.1	4.1173	9.2750	0.4696	0.0154	0.0594
1	4.1182	9.2745	0.4679	0.0154	0.0594
10	4.1267	9.2697	0.4529	0.0154	0.0594
50	4.1688	9.2762	0.3913	0.0170	0.0594
100	4.2349	9.2096	0.3241	0.0191	0.0592
300	0.9259	8.8504	0.1296	0.0370	0.0584
400	7.3321	7.8293	0.0601	0.0718	0.0559
420	9.9508	6.9279	0.0472	0.0896	0.0539
440	52.5200	0.0001	0.0336	0.1233	0.0461
450	1.5200	0.1300	0.0349	0.0990	0.0639
475	8.5569	-23.7900	0.0157	0.2450	0.0549

Table C-38 Effect of changing K_g on the output model (Day 6)

Day 6 (3-Aug-04)					
K_g	X	Xr	tc	Xe	St
0.00001	3.9423	8.7568	0.3976	0.0157	0.0911
0.0001	3.9423	8.7568	0.3976	0.0157	0.0911
0.001	3.9423	8.7568	0.3976	0.0157	0.0911
0.01	3.9423	8.7568	0.3976	0.0157	0.0911
0.1	3.9423	8.7568	0.3976	0.0157	0.0911
1	3.9432	8.7562	0.3963	0.0157	0.0911
10	3.9512	8.7509	0.3854	0.0159	0.0911
50	3.9911	8.7249	0.3395	0.0173	0.0911
100	4.0535	8.6846	0.0874	0.0194	0.0911
300	4.7016	8.2873	0.1229	0.0376	0.0911
400	7.1300	7.4149	0.0589	0.0725	0.0809
420	8.6600	5.8272	0.0465	0.0898	0.0774
440	39.2600	0.0102	0.0336	0.1231	0.0549
450	1.2074	-0.0569	0.0329	0.0978	0.1055
475	6.1100	-15.4300	0.0165	0.0307	0.0837

Table C-39 Effect of changing K_g on the output model (Day 7)

Day 7 (4-Aug-04)					
K_g	X	Xr	tc	Xe	St
0.00001	4.5809	10.5941	0.7166	0.0150	0.1033
0.0001	4.5809	10.5941	0.7166	0.0150	0.1033
0.001	4.5809	10.5941	0.7166	0.0150	0.1033
0.01	4.5809	10.5941	0.7166	0.0150	0.1033
0.1	4.5809	10.5941	0.7166	0.0150	0.1033
1	4.5819	10.5935	0.7127	0.0150	0.1033
10	4.5911	1.5880	0.6784	0.0153	0.1033
50	4.6366	10.5608	0.5484	0.0167	0.1033
100	4.7078	10.5186	0.4245	0.0187	0.1027
300	5.4541	10.1023	0.1422	0.0365	0.0994
400	8.0432	8.9088	0.0618	0.0713	0.0902
420	10.8101	7.8459	0.0479	0.0892	0.0832
440	70.3149	-2.2272	0.0336	0.1236	0.0524
450	3.2560	0.0000	0.0336	0.1167	0.1104
475	8.5879	-23.2700	0.0158	0.2428	0.0886

Table 40 Effect of changing K_g on the output model (Day 8)

Day 8 (5-Aug-04)					
K_g	X	Xr	tc	Xe	St
0.00001	5.9797	13.8140	0.7011	0.0155	0.0858
0.0001	5.9797	13.8140	0.7011	0.0155	0.0858
0.001	5.9797	13.8140	0.7011	0.0155	0.0858
0.01	5.9797	13.8140	0.7011	0.0155	0.0858
0.1	5.9799	13.8139	0.7007	0.0155	0.0858
1	5.9811	13.8131	0.6972	0.0155	0.0858
10	5.9931	13.8049	0.6633	0.0158	0.0858
50	6.0528	13.7641	0.5351	0.0171	0.0858
100	6.1464	13.7008	0.4134	0.0192	0.0858
300	7.1294	13.0718	0.1376	0.0376	0.0858
400	10.5118	11.2159	0.0600	0.0733	0.0752
420	14.3877	9.8039	0.0467	0.0914	0.0696
440	43.3400	0.0108	0.0336	0.1233	0.0545
450	1.5200	0.0103	0.0337	0.1045	0.1059
475	8.4600	-23.8600	0.0156	0.2469	0.0793

Table C-41 Effect of changing K_{gp} on the output model (Day 1)

Day 1 (29-Jul-04)					
K_{gp}	X	Xr	tc	Xe	St
0.00001	3.0940	7.0134	0.5109	0.0161	0.0489
0.0001	3.0940	7.0134	0.5109	0.0161	0.0489
0.001	3.0940	7.0134	0.5109	0.0161	0.0489
0.01	3.0940	7.0134	0.5109	0.0161	0.0489
0.1	3.0940	7.0134	0.5109	0.0161	0.0489
1	3.0940	7.0134	0.5109	0.0161	0.0509
10	3.0940	7.0138	0.5132	0.0161	0.0823
20	3.0889	7.0161	0.5261	0.0161	0.2583
30	3.1009	7.0098	0.4925	0.0161	-0.2229
40	3.0971	7.0117	0.5021	0.0161	-0.0783
50	3.0960	7.0121	0.5042	0.0161	-0.0470

Table C-20 Effect of changing K_{gp} on the output model (Day 2)

Day 2 (30-Jul-04)					
K_{gp}	X	Xr	tc	Xe	St
0.00001	3.5369	8.1159	0.6188	0.0155	0.0918
0.0001	3.5369	8.1159	0.6188	0.0155	0.0918
0.001	3.5369	8.1159	0.6188	0.0155	0.0918
0.01	3.5369	8.1159	0.6188	0.0155	0.0918
0.1	3.5369	8.1159	0.6188	0.0155	0.0918
1	3.5368	8.1159	0.6191	0.0155	0.0961
10	3.5351	8.1159	0.6256	0.0155	0.1656
20	3.5192	8.1256	0.6939	0.0155	0.8227
30	3.5457	8.1110	0.5874	0.0155	-0.2705
40	3.5419	8.1131	0.6003	0.0155	-0.1170
50	3.5409	8.1136	0.6039	0.0155	-0.0746

Table C-43 Effect of changing K_{gp} on the output model (Day 3)

Day 3 (31-Jul-04)					
K_{gp}	X	Xr	tc	Xe	St
0.00001	3.1442	7.3118	0.8080	0.0153	0.0780
0.0001	3.1442	7.3118	0.8080	0.0153	0.0780
0.001	3.1442	7.3118	0.8080	0.0153	0.0780
0.01	3.1442	7.3118	0.8080	0.0153	0.0780
0.1	3.1442	7.3118	0.8080	0.0153	0.0780
1	3.1441	7.3119	0.8086	0.0153	0.0813
10	3.1428	7.3126	0.8177	0.0153	0.1323
20	3.1356	7.3165	0.8761	0.0153	0.4322
30	3.1542	7.3065	0.7415	0.0153	-0.3328
40	3.1490	7.3093	0.7743	0.0153	-0.1211
50	3.1479	7.3099	0.7820	0.0153	-0.0739

Table C-44 Effect of changing K_{gp} on the output model (Day 4)

Day 4 (1-Aug-04)					
K_{gp}	X	Xr	tc	Xe	St
0.00001	3.5464	8.1766	1.3396	0.1570	0.0666
0.0001	3.5464	8.1766	1.3396	0.1570	0.0666
0.001	3.5464	8.1766	1.3396	0.1570	0.0666
0.01	3.5464	8.1766	1.3396	0.1570	0.0666
0.1	3.5464	8.1766	1.3396	0.1570	0.0666
1	3.5464	8.1766	1.3409	0.1570	0.0697
10	3.4552	8.1773	1.3633	0.1570	0.1187
20	3.4453	8.1832	1.5897	0.1570	0.5349
30	3.4630	8.1727	1.2263	0.1570	-0.2096
40	3.4601	8.1744	1.2736	0.1570	-0.0881
50	3.4594	8.1748	1.2868	0.1570	-0.0557

Table C-45 Effect of changing K_{gp} on the output model (Day 5)

Day 5 (2-Aug-04)					
K_{gp}	X	Xr	tc	Xe	St
0.00001	4.1184	9.2743	0.4674	0.0154	0.0587
0.0001	4.1184	9.2743	0.4674	0.0154	0.0587
0.001	4.1184	9.2743	0.4674	0.0154	0.0587
0.01	4.1184	9.2743	0.4674	0.0154	0.0587
0.1	4.1184	9.2743	0.4674	0.0154	0.0587
1	4.1184	9.2743	0.4674	0.0154	0.0617
10	4.1171	9.2751	0.4699	0.0154	0.1158
20	4.2657	9.1913	0.3000	0.0154	-0.0572
30	4.1228	9.2718	0.4596	0.0154	-0.1219
40	4.1213	9.2727	0.4662	0.0154	-0.0600
50	4.1208	9.2729	0.4631	0.0154	-0.0399

Table C-46 Effect of changing K_{gp} on the output model (Day 6)

Day 6 (3-Aug-04)					
K_{gp}	X	Xr	tc	Xe	St
0.00001	3.9434	8.7561	0.3960	0.0157	0.0900
0.0001	3.9434	8.7561	0.3960	0.0157	0.0900
0.001	3.9434	8.7561	0.3960	0.0157	0.0900
0.01	3.9434	8.7561	0.3960	0.0157	0.0900
0.1	3.9434	8.7561	0.3960	0.0157	0.0900
1	3.9434	8.7561	0.3962	0.0157	0.0946
10	3.9415	8.7574	0.3987	0.0157	0.1730
20	3.9015	8.7842	0.4663	0.0157	1.8950
30	3.9502	8.7515	0.3866	0.0157	-0.2044
40	3.9478	8.7531	0.3899	0.0157	-0.0978
50	3.9470	8.7537	0.3910	0.0157	-0.0643

Table C-47 Effect of changing K_{gp} on the output model (Day 7)

Day 7 (4-Aug-04)					
K_{gp}	X	Xr	tc	Xe	St
0.00001	4.5822	10.5933	0.7116	0.0151	0.1019
0.0001	4.5822	10.5933	0.7116	0.0151	0.1019
0.001	4.5822	10.5933	0.7116	0.0151	0.1019
0.01	4.5822	10.5933	0.7116	0.0151	0.1019
0.1	4.5822	10.5933	0.7116	0.0151	0.1025
1	4.5821	10.5934	0.7121	0.0151	0.1076
10	4.4795	10.5949	0.7225	0.0151	0.2161
20	4.6232	10.5684	0.5805	0.0151	-1.6260
30	4.5887	10.5893	0.6867	0.0151	-0.1738
40	4.5868	10.5905	0.6939	0.0151	-0.0914
50	4.5861	10.5909	0.6965	0.0151	-0.0620

Table C-48 Effect of changing K_{gp} on the output model (Day 8)

Day 8 (5-Aug-04)					
K_{gp}	X	Xr	tc	Xe	St
0.00001	5.9814	13.8129	0.6962	0.1550	0.0845
0.0001	5.9814	13.8129	0.6962	0.1550	0.0845
0.001	5.9814	13.8129	0.6962	0.1550	0.0845
0.01	5.9814	13.8129	0.6962	0.1550	0.0845
0.1	5.9814	13.8129	0.6962	0.1550	0.0845
1	5.9813	13.8129	0.6965	0.1550	0.0900
10	5.9783	13.8151	0.7057	0.1550	0.2218
20	5.9915	13.8059	0.6674	0.1550	-0.3524
30	5.9857	13.8099	0.6838	0.1550	-0.0984
40	5.9847	13.8106	0.6866	0.1550	-0.0572
50	5.9843	13.8109	0.6877	0.1550	-0.0403

Appendix D

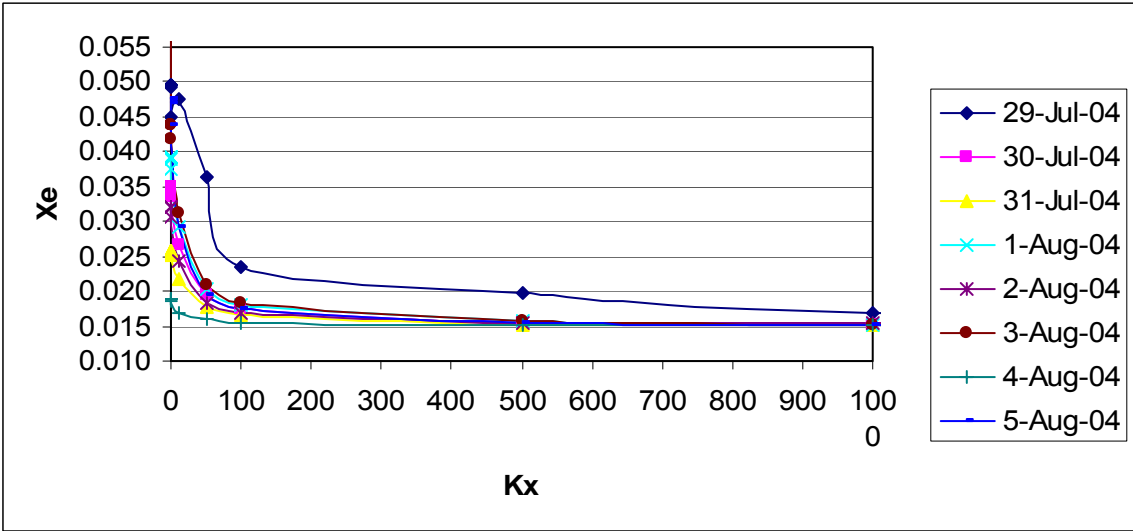


Figure D-4 Effect of perturbing Kx on Xe

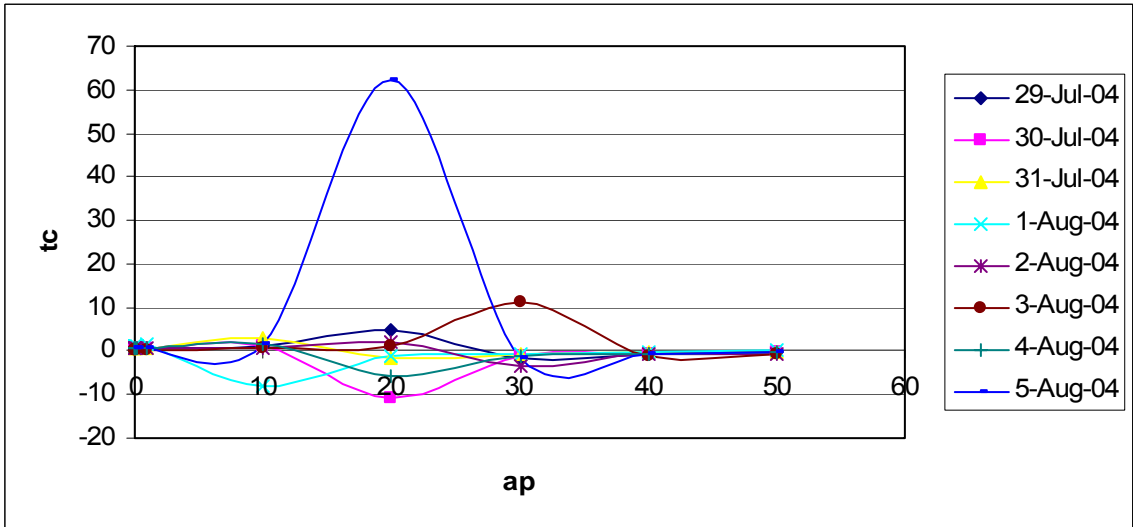


Figure D-5 Effect of perturbing ap on tc

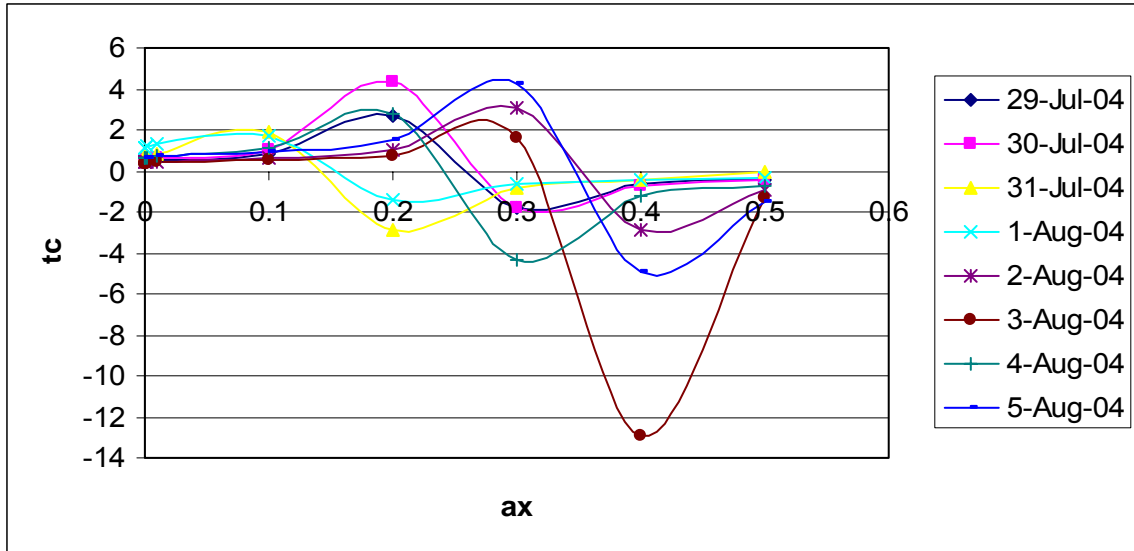


Figure D-6 Effect of changing ax on tc

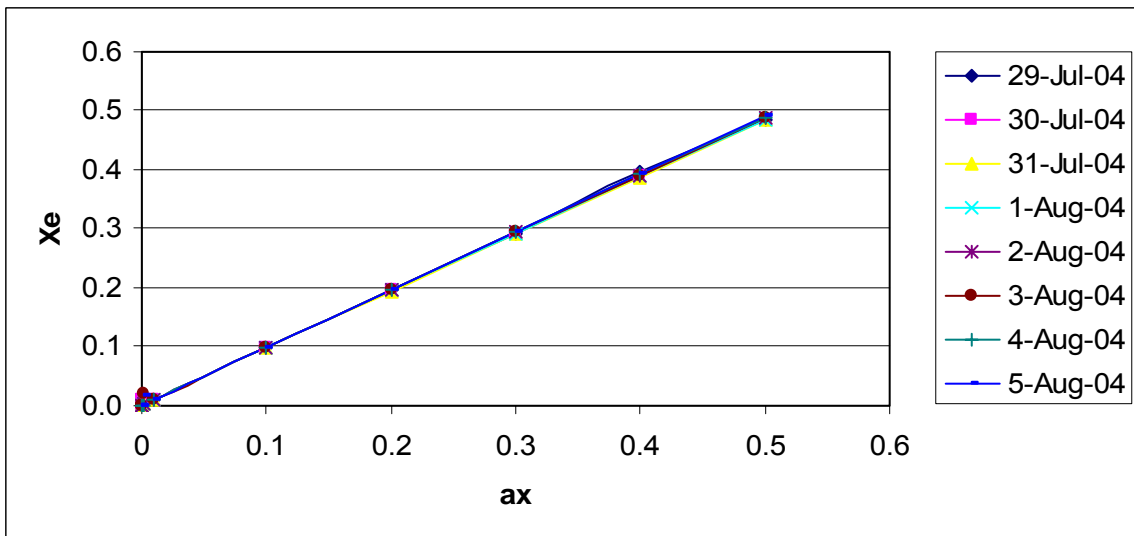


Figure D-7 Effect of perturbing ax on Xe

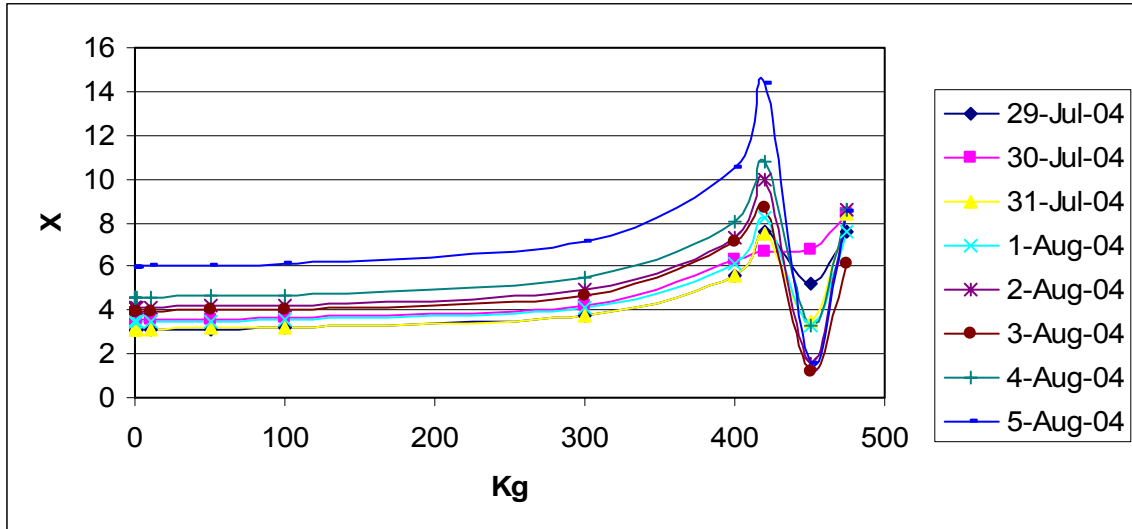


Figure D-8 Effect of perturbing Kg on X

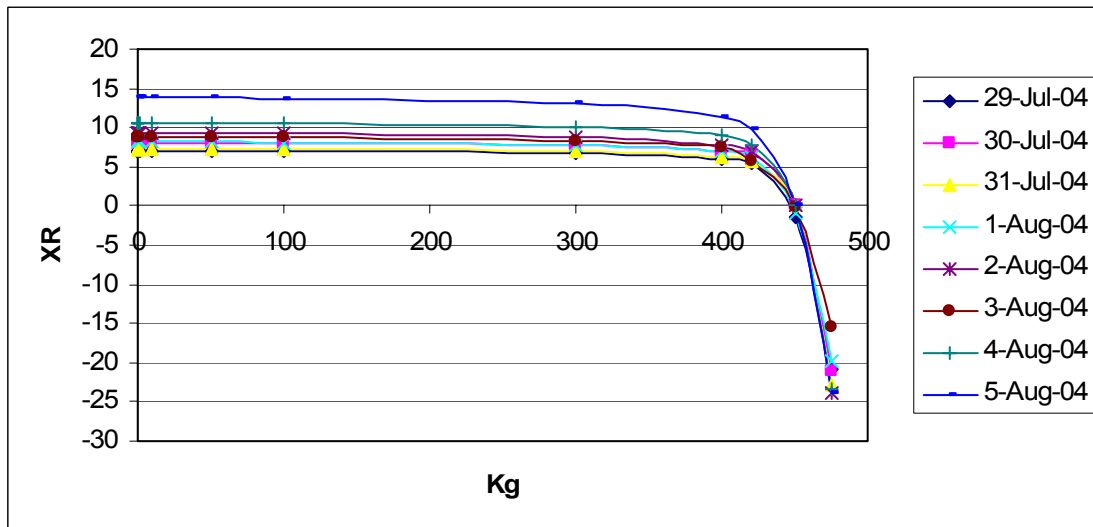


Figure D-9 Effect of perturbing Kg on XR

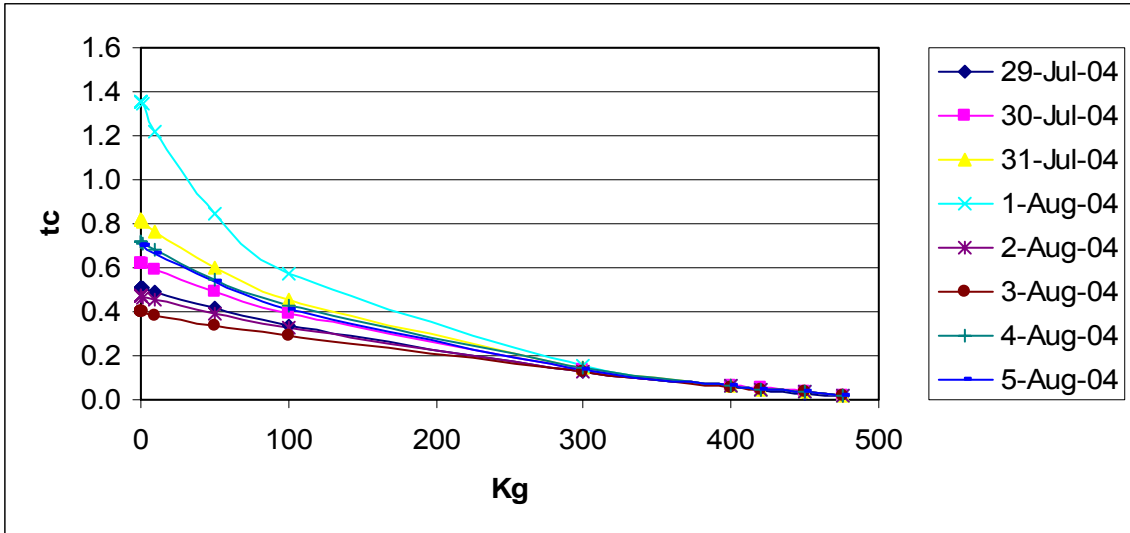


Figure D-10 Effect of perturbing Kg on tc

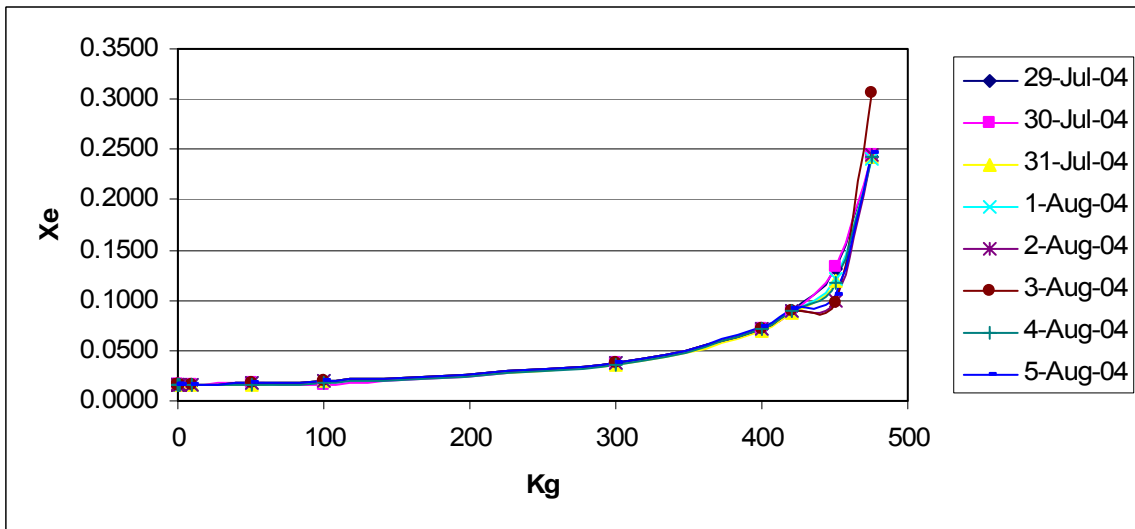


Figure D-11 Effect of perturbing Kg on Xe

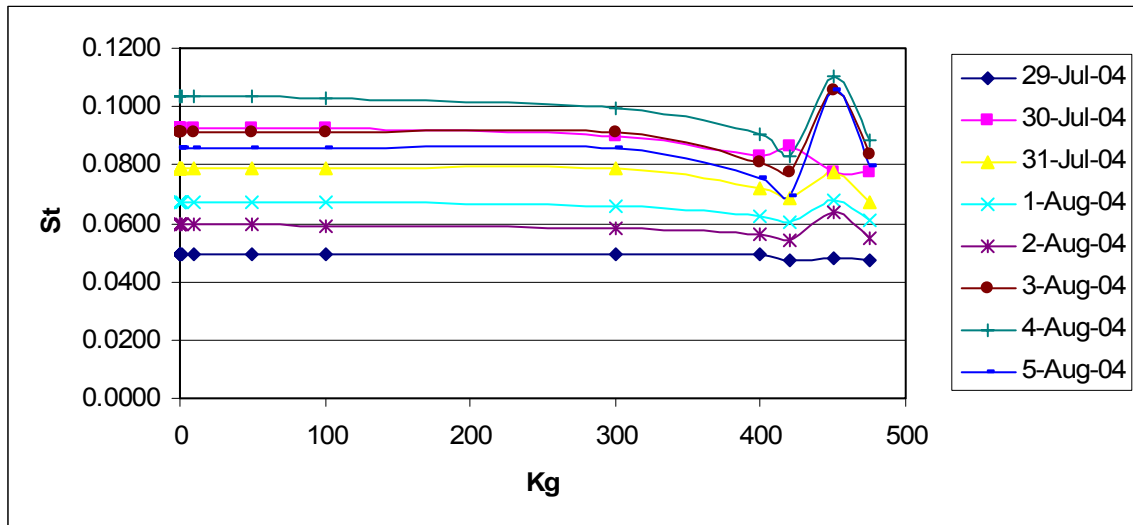


Figure D-12 Effect of perturbing Kg on St

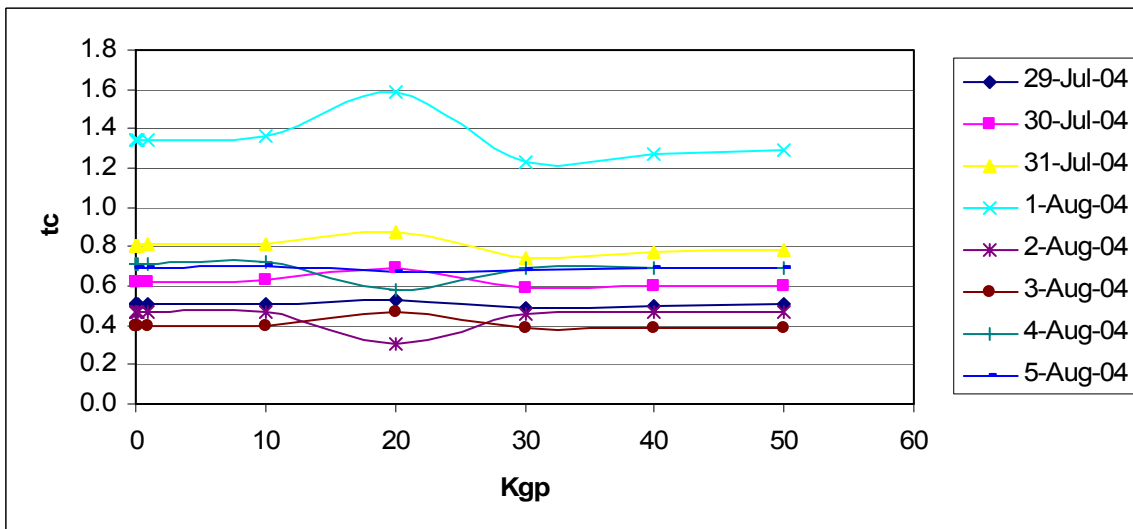


Figure D-13 Effect of perturbing Kgp on tc

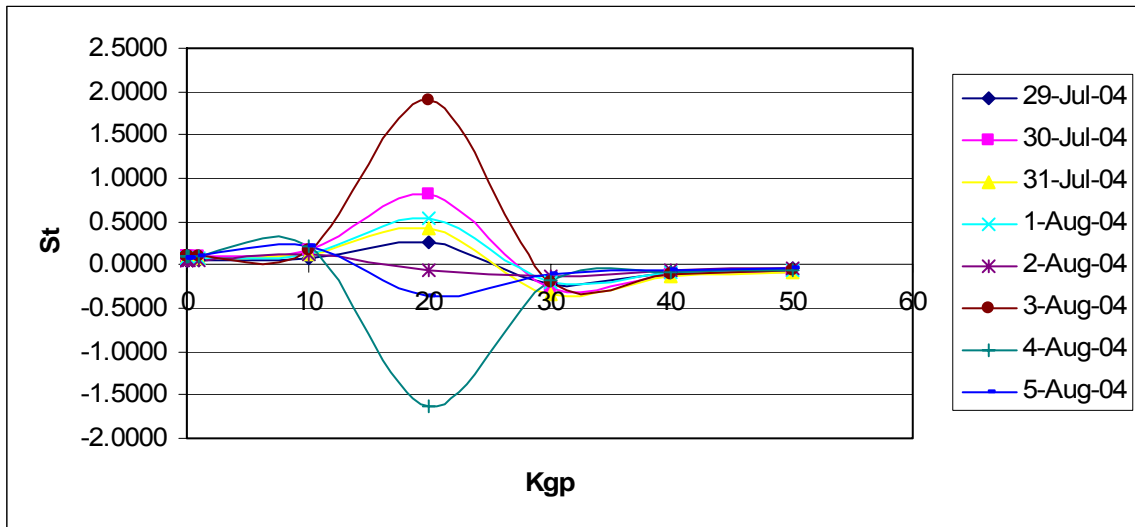


Figure D-14 Effect of altering Kgp on St

VITA

Ysabel Consuelo Viloría Bohórquez was born in Maracaibo, Venezuela, on January 14, 1976. In 1991, she graduated from High School in Sabana Libre. Later on, she graduated from Universidad del Zulia in March 2001, obtaining a degree of Bachelor of Sciences in Chemical Engineering. In fall 2005, she started at the University of New Orleans, pursuing a Master's of Science in Environmental Engineering.

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