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INVESTIGATION INTO THE PERFORMANCE
OF IDENTIFICATION TECHNIQUES
APPLIED TO UNCERTAIN DYNAMIC
SYSTEMS

by

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A thesis submitted for the degree of
Doctor of Philosophy

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DECLARATION

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ABSTRACT

Where the mathematical model is not a faithful representation of the real system, such as when, due to the lack of knowledge of the physical world "hidden uncertainties" in the system are not accounted for by the mathematical model, the use of the classical least squares approach to the estimation of constant unknown parameters of the model may not be adequate. The structural deficiencies of the model may be compensated for by the use of the smoothed least squares proposed by earlier workers who suggested that the identification of uncertain dynamic systems may be achieved by the joint solution of a parameter estimation problem to estimate constant model parameters and a smoothing problem to compensate for structural deficiencies.

These two approaches; the classical least squares and the smoothed least squares have been used to identify the models of a simulated mixing tank system and a pilot plant vaporiser system. The concept of "parameterisation" which evolved from further elaboration on the smoothed least squares technique whereby the proposed uncertainty is expressed as time-varying functions whose coefficients are estimated by the smoothing problem, has been implemented on the models of the two systems. Use was made of Chebychev polynomials and sine waves to approximate for the time-varying uncertainty.

The effects of the weightings of the errors between system and model responses and the time-varying uncertainty and its nominal trajectory on the performances of the two techniques have been evaluated.

Finally, critical evaluation of the performances of the classical least squares and the smoothed least squares techniques with regard to the estimated values of the constant model parameters has been made.

PRINCIPAL NOMENCLATURE

A	cross sectional area of the mixing tank (m^2)
A_V	cross sectional area of the vaporiser rig (m^2)
$B_{bm}(i)$	i^{th} value of the time varying uncertainty used in the model
C_d	freon valve discharge coefficient (SI units)
C	specific heat of water used in the mixing tank model $J/k_g^{\circ}K$
C_V	specific heat of hot water used in the vaporiser model $J/k_g^{\circ}K$
C_V	specific heat of freon liquid $J/k_g^{\circ}K$
D_V	diameter of vaporiser tube (m)
$\underline{f}$	expression for the model state differentials
h	height of water in the mixing tank (m)
$\underline{h}$	expression for the model observations
H_p	height of freon liquid in the vaporiser (m)
H_{tc}	heat transfer coefficient (SI units)
J_C	comparison index (objective function) used in conjunction with the classical least squares technique
J_S	comparison index (objective function) used in conjunction with the smoothed least squares technique

J_f	comparison index (objective function) used in conjunction with the filtered least squares technique
k_c	cold water valve constant (of the mixing tank system) (m^3/s)
k_h	hot water valve constant (of the mixing tank system) (m^3/s)
k_o	outlet water valve constant (of the mixing tank system) (m^3/s)
$K(t)$	time-dependent gain matrix associated with the filtered least squares technique
K_1	inlet pipe constant (in the vaporiser system) SI units
K_2	the freon valve constant (SI units)
K_G	outlet friction factor (in the vaporiser system)
L_A	heat losses to the atmosphere (J/S)
M_G	mass of vapour in the vaporiser (k_g)
M_{PB}	measured value of base pressure (N/m^2)
M_{PV}	measured value of vapour pressure (N/m^2)
M_{VH}	measured value of freon height (m)
$P(t)$	filter gain matrix trajectory associated with the filtered least squares technique
P_A	atmospheric pressure (N/m^2)

P_B	vaporiser base pressure (N/m^2)
P_I	freon valve inlet pressure (N/m^2)
P_S	vaporiser downstream pressure (N/m^2)
P_V	vapour pressure inside the vaporiser (N/m^2)
Q_B	volumetric freon boil off (m^3/s)
Q_C	cold water flow rate (in the mixing tank) (m^3/s)
Q_h	hot water flow rate (in the mixing tank) (m^3/s)
Q_L	volumetric freon inlet flow (m^3/s)
Q_O	outlet water flow rate (in the mixing tank) (m^3/s)
Q_V	volumetric freon vapour outlet flow (m^3/s)
Q_W	volumetric hot water flow (m^3/s)
r	radius (m)
$\underline{R}$	positive definite weighting matrix associated with uncertainty part of the objective function (V_S)
R_{Al}	relative aperture of the freon valve
S_{PICH}	setpoint for freon liquid height (m)
S_{PICP}	setpoint for vapour pressure (N/m^2)
T	observation time (seconds)

T_A	ambient temperature ($^{\circ}\text{K}$)
T_B	saturation temperature of freon liquid ($^{\circ}\text{K}$)
T_C	inlet cold water temperature (in the mixing tank) ($^{\circ}\text{K}$)
T_h	inlet hot water temperature (in the mixing tank) ($^{\circ}\text{K}$)
T_H	inlet hot water temperature (in the mixing tank system with introduced periodical variations)
T_i	freon liquid inlet temperature ($^{\circ}\text{K}$)
T_o	hot water inlet temperature in the vaporiser ($^{\circ}\text{K}$)
T_{raj}	nominal trajectory of the time-varying uncertainty
T_W	average temperature of hot water providing heat to freon ($^{\circ}\text{K}$)
$\underline{U}(t)$	m-vector of known input signals
V_{olv}	volume of vaporiser tube (m^3)
V_{P1}	freon valve normalised position
V_{P2}	hot water valve normalised position
W	positive definite weighting matrix associated with errors in system and model responses
$\underline{x}(t)$	n-vector of the states of the model
x_C	cold water valve position

x_h	hot water valve position
x_o	n-vector of known initial conditions
$\underline{y}(t)$	r-vector of model output responses
$z(t)$	real process observations
$\underline{z}$	height of freon liquid (m)
α	p-vector of constant model parameters
$\underline{\beta}(t)$	q-vector of time-varying model parameters
$\hat{\underline{\beta}}(t)$	nominal values of the time-varying model parameters
λ	latent heat of vaporisation of freon liquid (SI units)
ρ	water density (kg/m^3)
ρ_g	vapour density (kg/m^3)
ρ_L	freon liquid density (kg/m^3)
ρ_w	hot water density (kg/m^3)

Superscripts

+ or ' transpose of matrix or vector.

Conversion Factor

All parameters and variables listed above use the SI units except where a note has been made to the contrary. The conversion factor is then:

$$1 \text{ in w.g.} = 249.544 \text{ N/m}^2$$

Chapter 1

INTRODUCTION

The fact that modern technology has blossomed at an unprecedented rate within the last two decades is known to most people. Regardless of the accompanying social and political impact on society and international relations, this ascendance in human endeavour has resulted in a sharp inclination towards the use of computers directly or otherwise in almost every aspect of industrial life. A direct consequence of this has been the creation of complicated industrial structures which require enormous amounts of investments of natural resources and human efforts. Undoubtedly, this sophistication in industrial plants coupled with ever mounting costs of natural fuel have posed serious problems to the industrialists. This is due to the fact that with this degree of sophistication, a plant which has been developed to operate under certain conditions with certain goals in mind cannot easily be used for experimentation to test the feasibility of its use at new sets of operating conditions to serve new objectives. The human endeavour, which has always been in motion, being faced with this challenge, had to propose new practical ideas to overcome this problem, and thus the idea of modelling evolved.

According to Eykhoff (1977), a model is defined as "a representation of the essential aspects of an existing system (or a system to be constructed) which presents knowledge of that system in a usable form" where he defines a system as "a collection of objects arranged in an ordered form, which is, in some sense, purpose or goal directed".

However, although a model is built by close observation of the real system as reflected by system observation and measurements, problems arise with sophisticated systems, which are most common, where the exact nature of their behaviour is not readily noticeable. In such cases, a need arises for a systematic approach to specify the model so that it becomes able to predict system behaviour, giving rise to the concept of system identification. Zadeh (1962) defines identification as "the determination, on the basis of input/output, of a system within a specified class of systems, to which the system under test is equivalent".

Evidently, this definition of identification requires knowledge of the inputs to the system and the resulting observations made on the system due to these inputs. Moreover, although the definition may give the notion that preliminary knowledge of the system is not essential, in most engineering and biological processes, a priori knowledge based on at least partial understanding of the system operation is always available to the investigator. Further experimentation and application of identification process will result in modification or, at worst, abandonment of this a priori knowledge.

When dealing with dynamic systems, system identification becomes of prime importance. System identification arises when mathematical models for the process of interest cannot be completely specified and the model has to be "identified" using actual observation of the output and possibly the input. When the model is not a faithful representation of the system, discrepancies exist between system and model outputs. The identification process, thus, attempts to minimise such discrepancies to an arbitrarily accepted level by hypothesising the "area of difference" between system and model and implementing an appropriate technique to solve it. Such "area of

difference" may contain parameters in the mathematical model which represent physical quantities within the real system. The values of these parameters may not be known initially but may often be estimated by comparing observations of the real system with predictions obtained from the model. In the case where no unknown "area of difference" exists is assumed, that is, the mathematical model has no structural error, the classical least squares technique may be used to estimate the values of these parameters. According to Peckham (1969) "the problem of finding the parameters of a physical theory from experimental results, adjusting the parameters in a design to obtain the best possible performance or solving sets of non-linear simultaneous equations may frequently be reduced to the problem of finding the minimum of a sum of squares of non-linear functions". The classical least squares identification is useful for extracting information from noisy observations.

When the real system exhibits responses incompatible with those predicted by the model, for example, when hidden "uncertainties" exist in the real system the mathematical model will not be a faithful representation of the system unless these uncertainties are accounted for. Since the main objective is to obtain accurate estimates of the unknown constant parameters, accounting for these uncertainties makes the estimation problem insensitive to their existence, and hence more realistic estimates will result. Leal (1977) has proposed that these uncertainties in the system can be represented by additional time-varying parameters whose form is also estimated as part of the identification procedure.

This approach is based on an intuitive extension of the classical least squares technique. Georgantzis (1977) proposed and implemented "Parameterisation" as an approximate solution to the uncertainty problem proposed by Leal. Sines, cosines, Hermite polynomials, Laguerre functions, Chebychev polynomial and Fourier series approximation are examples of parameterisation. The overall problem can be seen to consist of a "parameter estimation" problem to estimate the value of the constant parameters of the model and a "smoothing problem" to estimate the form of the time varying parameters. Georgantzis who used this technique to identify the model of a chemical reactor managed to obtain improved results over the classical least squares technique.

In this research, the intention has been to apply these two techniques to the models of real and simulated systems in order to obtain accurate estimates of some parameters which cannot be measured directly. It is also intended to compare the performance of the two techniques and to assess their efficiency when applied to uncertain dynamic systems.

1.1 Contribution of the Thesis

Two identification techniques, the classical least squares and the smoothed least squares have been applied to the models of a simulated mixing tank system and a pilot-plant vaporiser system. The values of unknown constant parameters have been estimated using the above techniques. The classical least squares technique is concerned with the estimation of constant parameter values and the smoothed least squares concerned with compensation for model structural deficiencies.

The concept of "parameterisation" has been implemented to express compensation for time-dependent disturbances on the system responses, which suggest model structural errors, in terms of a time-varying entity whose parameters are estimated by the solution of the smoothing problem.

The model of the vaporiser system has been identified, under different operating conditions, where the values of the heat transfer coefficient (H_{tc}) are estimated and a sinewave or a Chebychev polynomial have been used to approximate for the "hidden" time varying uncertainty attached to the inlet hot water temperature.

In the tank system, a model of the simulated system in which simulated uncertainties were introduced, has been successfully identified in a similar way to that of the vaporiser identification.

In all the cases, the effects of compensation for model structural deficiencies on the parameter estimates have been evaluated and a comparison between the classical least squares and smoothed least squares techniques has, therefore, been achieved.

In addition, the effects of the weighting matrices on the performances of both techniques have been evaluated.

1.2 Layout of the Thesis

In Chapter 2 a general survey of available identification techniques is presented and evaluated with special emphasis on the classical least squares (C.L.S.) and smoothed least squares (S.L.S.) techniques.

In Chapter 3 a simulated mixing tank system based on a mixing rig which has been developed within the department is discussed and two mathematical models developed with intentionally introduced discrepancies between the "system" as simulated on the computer and its model.

Identification of these models using the classical least squares and the smoothed least squares technique is discussed in Chapter 4.

In Chapter 5 the vaporiser system which, again, has been developed within the department, is presented and a simplified model, based on previous work (Ellis, 1979) is employed. Open loop responses from both the real system and the model are given for different operating conditions.

Identification of the vaporiser model which includes estimation of constant parameters as well as compensation for structural deficiencies is discussed in Chapter 6.

The Appendices include mathematical background to the solution of the identification problem as well as the main Fortran programs which have been used to solve it.

Chapter 2

Identification Techniques

2.1 Introduction

The use of digital computers in engineering has promoted the use of mathematical models of systems, especially in the context of chemical, electrical and technological fields. Mathematical models are now commonly used in conjunction with process computers for process design, determination of operating conditions, control schemes and identification processes.

When developing a mathematical model of a system, a common problem encountered is determining numerical values of constant parameters in a non-linear system model. If real observations of the real system are available, the parameter values can be obtained by simulating the system and adjusting the constant parameters until the model and system responses agree according to a defined criteria. In this case, the model must be subjected to the same disturbance as that applied to the real system.

This process is often carried out by a digital computer which has been programmed to simulate the real system and to apply the appropriate identification procedure in order to estimate the unknown parameters. A measure of satisfaction with the estimated values of parameters usually takes the form of weighted least squares of errors, in which the identification algorithm manipulates the parameters to minimise the sum of squares of weighted errors between the model responses and system responses. This technique, known as the "model reference technique" and discussed by Noton (1972), assumes that the model is a faithful representation of the real system and does not allow for uncertainties in model structure.

Now, when uncertainties exist in either model structure, system inputs, model parameters or system observations, the nature of the identification problem changes and, hence, different and more specific approaches are needed for its solution.

For the particular case of stochastic uncertainties, Schweppe (1973) presented and discussed four approaches to deal with the identification of models besides the model reference approach. These are: state augmentation, maximum likelihood, correlation and instrument variables. In the state-augmentation approach the input and sensor disturbances are not white noise processes, but rather structured processes, that is, they are time-correlated. The states of these structured processes are augmented with the model states to give a larger state vector. Thus the assumption of sensor disturbance with no white noise component results in a mathematical model with perfect observations. This state augmentation approach can be extended easily to the case of time-varying system parameters which are modelled as stochastic or unknown-but-bounded processes.

The maximum likelihood approach is suitable for a stochastic process which is completely specified except for the values of the parameter vector. It is assumed here, that there are no structural errors i.e. there exists some unknown parameter value for which the model response corresponds exactly to the system observations. The maximum likelihood concept provides a viable, general and very powerful approach to estimating the numerical values of a linear system with Gaussian noise processes. The parameters to be estimated may specify the system's structure, the uncertainties or combinations thereof. If many observations are available, the Gaussian assumption is not crucial. However, the general equations are very complicated.

Correlation methods are suitable when the process is stationary and when there is no known input, and they do not need the Gaussian assumption. The basic idea underlying correlation methods is to choose the parameter value which reduces the error between the covariance matrix and correlation functions obtained using the hypothesised model and those using the system observations. A major disadvantage of correlation methods is that they do not provide a natural way to test the validity of system identification.

When the parameter estimate is found to suffer from the problem of bias, a straightforward solution may be achieved by the use of the Instrumental Variables method. Since the problem of bias arises due to observations which are contaminated with noise, it is assumed, when using this method, that there exists a matrix which is correlated with the system input but not with the noise. This matrix is used together with the system observations and the process output to calculate an asymptotically unbiased estimate.

Where the states of a stochastic linear system are not directly accessible for measurement (as in many practical situations) the Kalman Filter may be used for state estimation. The Kalman Filter is based on a model of the system states with a correction term depending upon the difference between the true output measurements and the estimated output measurements, and is a recursive estimation procedure.

The Extended Kalman Filter (Noton, 1972) which handles non-linear models by combining linearisation with the linear model theory, can be used for the approximate estimation of the states of non-linear systems and is discussed in many papers. The Extended Kalman Filter is

particularly suitable where process parameters drift or fluctuate and it is desirable to update them on-line. Parameter vector and state vector can be included in one augmented state equation and thus state estimation and parameter updating can be implemented simultaneously and recursively on line. This method requires the Gaussian assumption of the random variable involved to be made for its implementation, and a study of the error is necessary for the evaluation of possible biases in the estimates of the parameters. A major disadvantage of this method is the large computational programming required, especially when only the unknown parameters and not the states, are needed. The task of comparing the performances of some of the above mentioned and other identification techniques was taken by several researchers. Saridis (1974) compared the computational and convergence properties of six on-line identification algorithms, a modified discrete cross correlation, first and second order stochastic approximation, on-line maximum likelihood, maximum A-posteriori probability filter and the extended Kalman Filter tested on two fourth order discrete-time systems.

Isermann and others (1974) compared the performance, computation time and overall reliability of six recursive identification and parameter estimation methods; least squares, generalised least squares, instrumental variables, stochastic approximation, correlation analysis with least squares parameter estimation and Fourier analysis using three simulated processes. The authors of the paper cited the shortcomings of previous comparative studies in identification processes as: application purposes of the identified models were not regarded, processes of relatively low order with no more than four unknown parameters were used and that only linear processes were considered.

With these shortcomings in mind, the authors chose the ultimate goal of the identification process to be the design of a digital control algorithm where both the controller parameters and r.m.s. error of the closed loop controlled variable are compared for the identified and the exact model.

Isermann and his colleagues applied these six algorithms to three simulated processes; second order oscillating process, second-order nonminimum phase process and third-order low pass delay process.

Their results showed that for general linear processes correlation method had most advantages in comparison with the rest in terms of performance, computation time and overall reliability, as well as the apriori knowledge needed. The worst performance had been obtained with the least squares method though the method had good reliability.

The identification techniques mentioned have been tested and compared either on theoretical basis or on simulated systems, and unless such tests and comparisons are carried out on real physical systems, with their inevitable uncertainties and complications, no solid conclusion may be reached, with certain degree of confidence, on their applicability to real world.

However, successful attempts have been made to apply some of these techniques to industrial processes under different operating conditions. Sinha and Sin (1976) compared the performances of the method of least squares using the recursive pseudoinverse algorithm (Sen & Sinha, 1975), the stochastic approximation, the instrumental variables and

the algorithm combining pseudoinverse and stochastic approximation. The final estimates of the parameters obtained by each method was compared with values obtained using the time-series method due to Box and Jenkins (1970). The on-line identification of the parameters of the linearised model of a continuous stirred-tank process from the input-output data was considered. In this system, the linear model was considered a faithful representation of the real system, and the estimation of two parameters of the system transfer function was behind the identification process.

However, problems with these well founded identification techniques occur when the model is not a faithful representation of the real system, such as when the model structure is uncertain. An example of this is when a model which is found to give good agreement with a real system when the model parameters have been estimated using a particular input signal gives poor results when subjected to a different input signal. Overcoming this problem is important especially when, for economic, security or otherwise, the model is to be used for prediction of system behaviour under different conditions where it is not feasible to operate the system under the same range as the model. In such cases, if the model inadequacy has been correctly accounted for, operating the model under any range of interest will predict the exact behaviour of the real system. Whereas the model reference parameter technique is satisfactory in estimating parameter values of a "perfect model"; it may not be able to do the same when structural deficiencies exist in the model, This situation has led Roberts and Leal (1977) to classify uncertainties into three kinds:

i model structure:

uncertainties in model structure arise due to model simplification and inadequate knowledge of the real system. This means that in the real system, "hidden uncertainties" exist which can not easily be detected by the modelling process.

ii model parameters:

some of the model parameters which are thought to be constant and, hence, assigned "numerical" values may be in error and may change or drift with changes in the operating conditions.

iii real process observations:

output measurements obtained for the real process, assumed to be due to certain input signals only, may be in error due to instrumentation errors and other disturbances of which the investigator was unaware.

With this state of affairs in mind, Roberts and Leal (1977) attempted to devise an algorithm which overcomes model uncertainties. Further to the model constant parameters whose values are required to be determined by the normal parameter estimation procedure, they introduced time-varying parameters in the model equations for this purpose. Their elaboration on the classical least squares approach which assumes that all the uncertainties within the plant can be expressed as white noise on the observations, led them to the development of the "innovation approach" which requires the filtering of the observational data, and the "smoothed least squares" approach which requires smoothing of the observational data through an iterative process and has been found to be suitable for models which contain time-delays or are highly non-linear.

Their approach has, therefore, cited the identification problem of uncertain dynamic systems as consisting of parameter estimation problem to estimate the values of constant parameters and either smoothing problem or filtering problem to compensate for model structural deficiencies.

The solution of the parameter estimation problem has been achieved by the use of the classical least squares, the solution of the filtering problem by the use of the filtering equations based on Kalman Filter and the solution of the smoothing problem by the use of calculus of variations and the Riccatti techniques which results in complicated mathematical equations of considerable computational complexity particularly in determining and storing model derivatives. (See Appendix 1)

The performance of the parameter estimation techniques has been investigated using a digital computer simulation of the WINFRITH SGHWR nuclear plant (Roberts, 1980), and have proved fruitful in estimating accurately the values of the constant parameters of the plant.

Simplification of the complicated mathematical suite obtained by using the calculus of variations method was proposed and tested by Roberts and Georgantzis (1977) who found that these complications may be avoided by the use of parameterisation, where the uncertainty is expressed in terms of a time-varying function whose parameters (coefficients) need to be estimated. Thus, the infinite dimensional optimisation problem of determining the time-varying uncertainty is transformed into a finite dimensional optimisation problem of determining its coefficients and may be solved by using a standard numerical optimisation procedure.

Roberts and Georgantzis successfully applied this algorithm in a digital simulation study concerned with estimating five constant parameters in a non-linear dynamic model of an exothermic chemical reactor, using a single time-varying uncertainty with eight coefficients. Whilst the classical least squares techniques gave "inaccurate" estimates, the smoothing technique gave estimates close to the real values.

In this research, the intention has been to use Roberts and Leal's algorithm together with the parameterisation concept of Roberts and Georgegantzis to identify a simulated mixing-tank plant and a real vaporiser plant. In the former plant, the uncertainty in model structure has been intentionally introduced whilst in the latter, the limited knowledge of the physical world, which overshadows existing uncertainties in the model structure, accounts for the discrepancies between the model and the real plant.

In the next few sections Robert and Leal's three techniques namely, classical least squares, smoothed least squares and filtered least squares, will be presented and discussed.

The classical least squares and smoothed least squares have been applied to the simulated and real systems and their respective performances compared.

2.2 Model Structure

The structure of the mathematical model of the industrial plant is considered to consist of a set of first-order non-linear differential equations and a set of algebraic equations, as it is usually the case when applying conservational relationship such as mass and heat balance principles. These equations usually contain a set of constant parameters whose values are to be estimated by a certain technique by comparison of model and system observations, in addition to process state variables, input signals and measurement signals. A typical structure of a dynamic mathematical model with n -first order differential equations, r -algebraic relationships defining the output measurement signals, m -input signals, and p -parameters whose values are unknown is

$$\dot{\underline{x}} = \underline{f}(\underline{x}, \underline{u}, \underline{\alpha}), \quad \underline{x}(0) = \underline{x}_0 \quad 2.1$$

$$\underline{y} = \underline{h}(\underline{x}) \quad 2.2$$

where $\underline{x}$ = a n -state vector

$\underline{u}$ = m -vector of known input signals

$\underline{\alpha}$ = p -vector of constant model parameters

$\underline{y}$ = r -vector of model output responses

$\underline{x}_0$ = n -vector of known initial conditions

$\underline{f}$ and $\underline{h}$ define non-linear relationships.

If there are no structural deficiencies in the model, then estimated values of the constant parameter vector $\underline{\alpha}$ obtained by using a particular parameter ^{estimation} procedure which compares model and process observations at a particular type and range of input signals $\underline{u}$ will also be valid at any other type and range of input signals. But due to the nature of the modelling process which often makes simplifications, assumptions and approximations the model is, usually, not a faithful representation of the real system and, hence, parameter estimates $\underline{\alpha}$ may depend upon the range and type of input signals and consequent outputs employed in the estimation procedure.

To counter the inevitable uncertainties of the mathematical model, the model structure is modified to take account of these uncertainties, thus:

$$\dot{\underline{x}} = \underline{f}(\underline{x}, \underline{u}, \underline{\beta}(t), \underline{\alpha}), \underline{x}(0) = \underline{x}_0 \quad 2.3$$

$$\underline{y} = \underline{h}(\underline{x}) \quad 2.4$$

where $\underline{\beta}(t)$ is a q-vector of additional time-varying model parameters introduced to compensate for "hidden" uncertainties.

This is a simplified structure of the mathematical model considered by Roberts and Leal, since their model structure contains parameter-dependant initial conditions and time delays.

In the following discussion of the identification techniques it will be assumed that model and system observations have been obtained when both the model and the system are excited with the same input signals $\underline{u}(t)$. It is also assumed that the time-varying uncertainties have known nominal values $\hat{\underline{\beta}}(t)$ which may be constant.

2.3 Classical Least Squares

This technique assumes that all the uncertainties within the plant can be expressed as white noise on the observations. Thus it takes no account of the time-varying uncertainties $\underline{\beta}(t)$, which are set at their nominal values, i.e.

$$\underline{\beta}(t) = \hat{\underline{\beta}}(t) \quad 2.5$$

The method attempts to estimate the values of the unknown constant parameters $\underline{\alpha}$ which cause the model observations $\underline{y}(t)$ to match the corresponding real process observations $\underline{z}(t)$, according to a certain comparison index (objective function) ($J_c(\underline{\alpha})$) regarding the error between the model and corresponding system outputs, where

$$J_c(\underline{\alpha}) = \int_0^T \left\{ (\underline{y}(t) - \underline{z}(t))^+ \cdot W(\underline{y}(t) - \underline{z}(t)) \right\} dt \quad 2.6$$

where T = observation time

W = positive definite weighting matrix, whose elements are chosen to weight the relative importance of the square errors

$$(\underline{y}_i(t) - \underline{z}_i(t))^2, \quad i = 1, 2, \dots, r$$

The parameter estimation process may be defined as attempting to solve the minimisation problem

$$\min_{\underline{\alpha}} \left\{ J_c = \int_0^T \left[(\underline{y}(t) - \underline{z}(t))^+ \cdot W(\underline{y}(t) - \underline{z}(t)) \right] dt \right\}$$

where

$$\begin{aligned} \underline{y}(t) &= \underline{h}(\underline{x}) \\ \underline{x} &= \underline{f}(\underline{x}, \underline{u}, \hat{\underline{\beta}}(t), \underline{\alpha}), \quad \underline{x}(0) = \underline{x}_0 \end{aligned}$$

which may be solved using standard computer algorithms (Roberts, 1977)

2.4 Smoothed Least Squares Technique

In many practical cases, the inadequacy of the mathematical model cannot be attributed to the existence of noise on the observational data where the classical least squares approach gives satisfactory results. In such cases, the inadequate performance of the model may be due to the existence of hidden variations or "uncertainties" attached to one or more of the state variables or parameters which have not been detected by the model. Discovering such hidden forms of uncertainty is not an easy task and, indeed, only close observation of the behaviour of sensitive state variables or parameters may lead to some knowledge about their nature. Once the uncertainty is specified in mathematical form, a nominal trajectory or probabilities to departures from the nominal trajectory may be assigned to them. Since such uncertainties are normally time varying entities, their deviation from the nominal trajectory may be considered as an objective function which is adjoined to the classical least squares objective function.

Thus, the smoothed least squares approach is an extension of the classical least squares technique to take account of time-dependant uncertainties $\underline{\beta}(t)$. The objective function becomes smoothed out to include the possible variation of the uncertainty from its nominal value, and is written as:

$$J_s(\underline{\beta}(t), \underline{\alpha}) = \int_0^T \left\{ \left[(\underline{y}(t) - \underline{z}(t))^+ \cdot W \cdot (\underline{y}(t) - \underline{z}(t)) \right] + \left[(\underline{\beta}(t) - \hat{\underline{\beta}}(t))^+ \cdot R \cdot (\underline{\beta}(t) - \hat{\underline{\beta}}(t)) \right] \right\} dt \quad 2.7$$

Following from intuitive arguments (Schweppe 1973) a model reference least squares approach to the estimation problem is to determine the values of $\underline{\beta}(t)$ and $\underline{\alpha}$ to solve the two stage minimisation problem.

$$\min_{\underline{\alpha}} \min_{\underline{\beta}(t)} J_s(\underline{\beta}(t), \underline{\alpha})$$

subject to equations (3), (4) and (7)

Minimisation of the objective function with respect to $\underline{\beta}(t)$ constitutes a smoothing problem and minimisation with respect to $\underline{\alpha}$ constitutes the parameter estimation problem. Return to the classical least squares is obtained by setting the time-varying uncertainty $\underline{\beta}(t)$ at its nominal value $\hat{\underline{\beta}}(t)$.

Two methods have been devised to solve the smoothing problem (Roberts, Leal and Georgantzis 1977). The first method employs calculus of variations to solve the problem in an optimal control formulation. This requires the calculation and storing of model derivatives at each estimate of the smoothing parameters in a lengthy iterative procedure. See Appendix 1

The second method attempts to avoid this lengthy procedure by obtaining an approximate solution of the smoothing problem by the use of parameterisation. The two methods result in iterative procedures which have been implemented in terms of computer programmes (Leal and Roberts 1977a, Georgantzis 1977)

2.5 Filtered Least Squares

The formulation of the overall parameter estimation problem as a solution of the smoothing problem has similarities to the Kalman Filter (Kalman and Bucy 1961).

The basis of the filtered least squares is to determine the constant model parameters $\underline{\alpha}$ which solve the minimisation problem

$$\min_{\underline{\alpha}} \left\{ J_f = \int_0^T (\tilde{\underline{y}}(t) - \underline{z}(t))^+ \cdot \underline{W} \cdot (\tilde{\underline{y}}(t) - \underline{z}(t)) dt \right\} \quad 2.8$$

where

$$\begin{aligned} \tilde{\underline{y}}(t) &= \underline{h}(\tilde{\underline{x}}) \\ \dot{\tilde{\underline{x}}} &= \underline{f}(\tilde{\underline{x}}, \underline{u}, \hat{\underline{\beta}}(t), \underline{\alpha}) + K(t) \{ \underline{z}(t) - \tilde{\underline{y}}(t) \}, \\ \tilde{\underline{x}}(0) &= \underline{x}_0 \end{aligned} \quad 2.9$$

where $\tilde{\underline{x}}(t)$ and $\tilde{\underline{y}}(t)$ are regarded as model derived filtered estimates of the process state and output signals, respectively. The filtered estimates are obtained from the model equations, with the uncertain parameters $\underline{\beta}(t)$ set at their nominal values $\hat{\underline{\beta}}(t)$, and with an additional term depending upon the error between the filtered output variables $\tilde{\underline{y}}(t)$ and their corresponding real process observations $\underline{z}(t)$. $K(t)$ is a time-dependent gain matrix which is determined by solving the following equation:

$$K(t) = 2P(t) \underline{h}'_{\underline{x}} W \quad 2.11$$

$$\dot{P} = \underline{f}_{\underline{x}} P + P \underline{f}'_{\underline{x}} + 0.5 \underline{f}_{\underline{\beta}} R^{-1} \underline{f}'_{\underline{\beta}} - 2 \underline{P} \underline{h}'_{\underline{x}} W \underline{h}_{\underline{x}} P \quad 2.12$$

where $\underline{f}_{\underline{x}}$, $\underline{f}_{\underline{\beta}}$ and $\underline{h}_{\underline{x}}$ are matrices of first order partial derivatives evaluated along the non-linear functions $\underline{f}$ and $\underline{h}$.

The comparison index within equation (8) contains a modified time-dependent weighting matrix defined as

$$\tilde{W} = [W^{-1} + 2 \underline{h}_{\underline{x}} P(t) \underline{h}'_{\underline{x}}]^{-1} \quad 2.13$$

Thus, the filtered least squares approach to determining the constant model parameters $\underline{\alpha}$ involves minimising an integral time-weighted square error between the real observations and corresponding model-derived filtered output signals, with a time-dependent weighting function. The solution requires an iterative technique to solve equations 12 and 13 which requires the evaluation of sensitivity relationships along estimates of the filtered states and model output signals.

In this work the classical least squares and the smoothed least squares techniques have been applied to a mixing tank simulated system and a vaporiser pilot plant. Chapters 4 and 6 discuss the identification of the mixing tank system and the vaporiser system respectively where these two techniques are implemented whilst chapters 3 and 5 deal with the development of the mathematical models as well as obtaining system responses.

Chapter 3

MIXING TANK SYSTEM

3.1 Introduction

Mixing processes are very common in industrial life especially in the chemical field where mixing of materials is carried out to produce new components, new concentrations and new properties. Proper control of the liquids involved in the case of liquid mixing is essential if the correct product is to result from the mixing process. Usually, mass, momentum and heat balance principles are adopted to model these processes for accurate predictions.

The pilot scale mixing rig which had been devised in the department to allow the testing of different multivariable control schemes went through several stages of development.

Furlong (1972) attempted to apply computer control to the mixing rig using a Ferranti Argus - 500 computer by implementing two multivariable controllers; one intended for complete non-interaction, and the other based on Inverse Nyquist Array method (Rosenbrock 1970). Inaccuracies in estimation of system parameters prevented the complete elimination of interaction.

Korolis (1973) attempted to use Furlong's controllers together with an optimal controller but using level and heat content (instead of level and temperature) as his state variables. He did not succeed in implementing non-interacting and optimal controllers because of their sensitivity to model inaccuracies, difficulty in implementing the resulting controllers or solving the optimal equations.

Bogdanovic (1974) used Korolis's model with Inverse Nyquist Optimal control and Pole Assignment methods. Only the Inverse Nyquist method yielded significant improvement over the other techniques.

Makarenko (1975) managed to design and implement a multivariable control algorithm using the Inverse Nyquist Array technique. Thus, liquid level and temperature in the tank which mixes hot and cold water inflow streams were controlled adequately under a variety of conditions.

However, in this research, which is concerned with the application of identification techniques, open loop responses of the mixing rig are needed. The control algorithms mentioned will not be referred to in this thesis. Furthermore, the real observations needed for the identification process have been obtained from the simulated mixing tank system and not from real experimentation. This serves two purposes; the first is that the simulated discrepancies between the system and the model are accurately known and can be changed as desired to affect the simulation of different kinds of "hidden uncertainties". The other purpose is to give a means of evaluating the performances of the techniques since the correct values of the parameters to be estimated are known.

3.2 Plant Description

The rig is basically a mixing tank into which streams of hot and cold water are fed. A conventional pneumatic diaphragm valve is used in each stream to control the flow. The outflow from the tank passes through a fixed restriction valve so that the flow is only affected by the pressure at the bottom of the tank, and hence by the liquid level. A diagram of the rig is given in Fig. 3.1.

A small stirrer is fitted to the tank to ensure homogeneity of its contents. The temperature of the water leaving the tank is measured by a thermocouple fitted to the outflow pipe close to the tank itself. The level is measured by a strain-gauge pressure transducer in a conventional bridge circuit, the transducer being mounted near the bottom of the tank. The outputs from the thermocouple and the transducer are in the range 0-10mv.

The plant is controlled by means of a Ferranti Argus-500 computer (which is being replaced by a KRATOS computer system). This computer installation incorporates a number of interface channels for analog inputs and outputs of which four are used to interface the mixing rig and four for the vaporiser rig.

The control valves receive appropriate signals from the analog output system of the computer. The signals, in the standard 4-20mA range, are transduced by Elliot-Automation Current-to-Air converters into pneumatic signals fed to the valve positioners in the usual way.

3.3 Mathematical Modelling

At the outset of any modelling process, when using a direct formulation, the purposes for which the model is to be used must be clearly laid down. These purposes influence the degree of complexity of the resulting model. All models, even the most sophisticated ones, must possess some simplifying assumptions about the nature of the system. A model, even with rather severe simplifications (resulting from these assumptions) may still prove to be adequate for the purposes laid down.

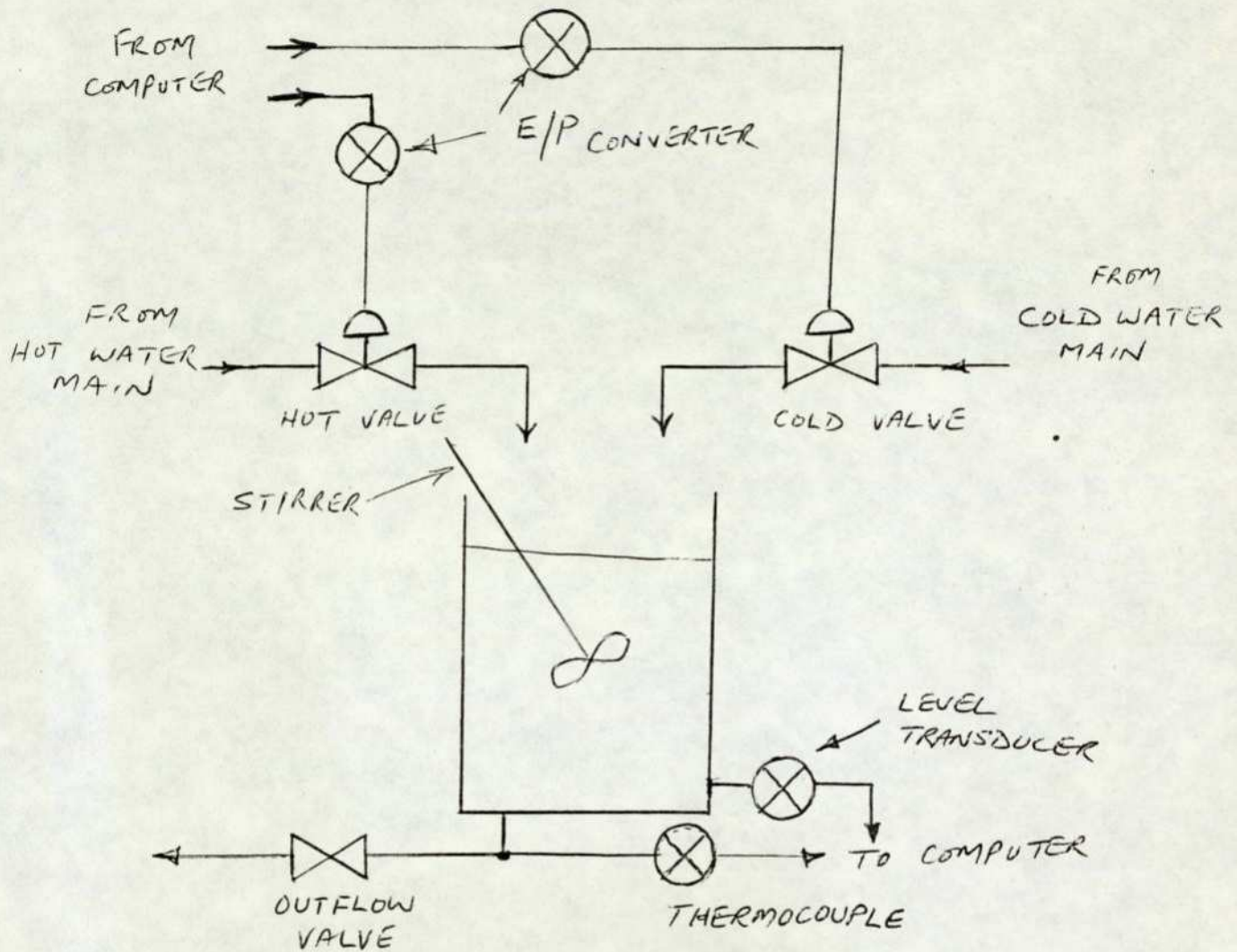


Fig. 3.1: The structure of the mixing tank system

3.3.1 System with no Heat Losses

In modelling the mixing tank system, the following assumptions have been made:

- 1) Continuous supplies of hot and cold water are available and at constant pressure;
- 2) Perfect mixing takes place within the tank, i.e. temperature in the tank is uniform, and so is the outflow temperature;
- 3) Density and specific heat of water remain constant over the temperature range involved;
- 4) Heat losses to the surroundings are negligible (this assumption will be dropped later).

Now, the mathematical model is obtained by the application of the laws of conservation of mass and heat onto the contents of the tank.

Mass Balance

Rate of change of the mass^{of} water in tank =

mass flow rate of inlet cold water +
mass flow rate of inlet hot water -
mass flow rate of outlet mixed water

$$\frac{d}{dt} (A.h.\rho) = Q_c.\rho + Q_h.\rho - Q_o.\rho$$

where

A = cross sectional area of tank (m^2)

h = height of water in tank (m)

ρ = density of water (kg/m^3)

Q_c = volumetric flow rate of inlet cold water (m^3/s)

Q_h = volumetric flow rate of inlet hot water (m^3/s)

Q_o = volumetric flow rate of outlet mixed water (m^3/s)

assuming constant density,

$$\frac{dh}{dt} = \frac{1}{A} (Q_c + Q_h - Q_o) \quad 3.1$$

Heat Balance

Rate of change of heat content in the tank =
rate of heat flow in
- rate of heat flow out

$$\therefore \frac{d}{dt} (A.h.\ell.c.T_o) = Q_c.\ell.c.T_c + Q_h.\ell.c.T_h - Q_o.\ell.c.T_o \quad 3.2$$

where

c = specific heat of water $J/kg^{\circ}K$
 T_o = mixed water temperature $(^{\circ}K)$
 Q_c = cold water flow rate (m^3/s)
 Q_h = hot water flow rate (m^3/s)
 Q_o = mixed water (outlet) flow rate (m^3/s)
 T_c = cold water temperature $(^{\circ}K)$
 T_h = hot water temperature $(^{\circ}K)$
 T_o = mixed water temperature $(^{\circ}K)$

assuming ℓ and c remain constant, hence they cancel out,
and substituting Eqn. 3.1 into 3.2

$$\therefore Ah \frac{dT_o}{dt} + T_o (Q_c + Q_h - T_o) = Q_c T_c + Q_h T_h - Q_o T_o$$

$$\therefore \frac{dT_o}{dt} = \frac{1}{Ah} [Q_h \cdot (T_h - T_o) + Q_c \cdot (T_c - T_o)] \quad 3.3$$

Now in the real mixing tank system, there is a non-linear relationship between the position of the valves and the fluid flow passing through them. However, for model simplification, it is assumed here that a linear relationship exists between fluid flow and the position of the two valves. Furthermore the position of each valve is normalised to be in the range 0-1 and the following equations are used to calculate the volumetric flows:

$$Q_h = k_h \cdot x_h$$

$$Q_c = k_c \cdot x_c$$

$$Q_o = k_o \cdot \sqrt{h}$$

where

k_h = hot water valve constant

k_c = cold water valve constant

k_o = outlet water valve constant

x_h = hot water valve position

x_c = cold water valve position

Design Calculations

Since the application of identification techniques requires observations obtained by operating the simulated system in an open loop mode starting from steady state conditions, the mixing tank model has been designed to achieve this purpose. Thus, a steady state value of h of 0.1m, $Q_h = 3 \times 10^{-6} \text{ m}^3/\text{s}$, $Q_c = 2 \times 10^{-6} \text{ m}^3/\text{s}$, the hot and cold water valves half opened, i.e. $x_h = x_c = 0.5$, $T_h = 343^\circ\text{K}$ and $T_c = 278^\circ\text{K}$, the following design variables have been obtained -

$$\begin{aligned} k_h &= 6 \times 10^{-6} \text{ m}^3/\text{s} \\ k_c &= 4 \times 10^{-6} \text{ m}^3/\text{s} \\ k_o &= 1.58 \times 10^{-6} \text{ m}^{5/2}/\text{s} \end{aligned}$$

Also, the steady state value of T_o is 317°K .

Using the steady state values of the two state variables (h and T_o) and the design values of the valve constants and other variables, the tank has been simulated on the CDC 7600 computer, tested in the steady state, and under a step change in one of the valves and used to investigate the performance of the identification techniques discussed in Chapter 2.

3.3.2 Computer Simulation

A computer program "EXAMPLE" was constructed to simulate the dynamic behaviour of the system. The program reads data, writes required information and sets the required parameters for the integration subroutine. Subroutine MODEL calculates the derivatives of the state variables (h & T_o) using information passed to it from the main program.

To validate the model structure, steady state values of the state variables (h & T_o) and design values of other constants and variables were fed in and output responses for h and T_o were obtained using the NAG integration subroutine DO2AJF (NAGLIB; 1387/O:MK5:FEB.76). This subroutine integrates a system of first order differential equations over a range, using a divided difference formulation of Gear's method for stiff system of equations. Although this subroutine is more suitable for a stiff system of equations it has been used in the mixing tank model for convenience. (See Appendix 2).

3.3.3 Step Response

To investigate the dynamic behaviour of the tank model, a step change can be applied to one of the two manipulable variables (the valve positions x_h and x_c).

a) Step change applied to cold water valve:

If a 50% change is applied to cold water valve i.e.

$$\begin{aligned}x_c &= 0.75, \text{ then } Q_c = 3 \times 10^{-6} \text{ m}^3/\text{s}, \\Q_o &= 6 \times 10^{-6} \text{ m}^3/\text{s} \\T_o &= 310.5^\circ\text{K}, \\h &= 0.144\text{m}\end{aligned}$$

For this step change, the computer simulation gives the open loop responses for h and T_o shown in Figs. (3.2) and (3.3).

Knowing the new steady state values of h and T_o as calculated above, the effective time constants of h and T_o may be evaluated using the dynamic part of responses. This can be done by projecting the tangent to the response at its starting point until it meets the ultimate steady state value. The time corresponding to the point of intersection is the time constant. From Figs 3.2 and 3.3, the time constants of the height and mixed water temperature are 475 and 220 seconds respectively.

b) Step change applied to hot water valve:

If a 50% step change is applied to x_h so that x_h changes from 0.5 to 0.75, then

$$\begin{aligned} Q_h &= 4.5 \times 10^{-6} \text{ m}^3/\text{s} & Q_o &= 6.5 \times 10^{-6} \text{ m}^3/\text{s} \\ T_o &= 323^\circ\text{K} & , \quad h &= 0.169 \text{ m} \end{aligned}$$

For this step change, the responses obtained for h and T_o are shown in Figs. 3.4 and 3.5.

From the graphs, the time constants of h and T_o are 470 and 220 seconds respectively. This difference in the two values of the time constant of the height response is inevitable due to drawing errors.

JACOBIAN MATRIX

In order to obtain theoretical values of the time constants of height and temperature responses of the tank the eigen values must be calculated at a particular operating condition. The state variable equations are:

$$\dot{h} = \frac{1}{A} (Q_h + Q_c - Q_o)$$

$$\dot{T}_o = \frac{1}{Ah} \left[Q_h (T_h - T_o) - Q_c (T_o - T_c) \right]$$

Since $Q_o = K_o \sqrt{h}$, these equations can be rewritten as:

$$\dot{h} = \frac{1}{A} \left[(Q_h + Q_c) - \frac{K_o \sqrt{h}}{A} \right] \quad 3.4$$

$$\dot{T} = \frac{1}{Ah} \left[Q_h T_h + Q_c T_c - (Q_h + Q_c) T_o \right] \quad 3.5$$

It can be seen that Eqns. 3.4 and 3.5 are non-linear, hence linearisation is necessary especially for control system design.

If the steady state values of the variables in the above equations are obtained, then a system disturbance will result in a small variation about the steady state.

This variation may be evaluated using the Jacobian matrix. Consider a system of the form:

$$\dot{\underline{z}} = \underline{f}(\underline{z}, \underline{w}) \quad 3.5$$

where $\underline{z}$ is a n-state vector and $\underline{w}$ is an m-control vector.

Let $\bar{\underline{w}}$ be the corresponding value of $\underline{w}$ obtained by solving $\underline{f}(\underline{z}, \underline{w}) = 0$ for $\bar{\underline{w}}$, and define the small variations as $\underline{x} = \underline{z} - \bar{\underline{z}}$, $\underline{u} = \underline{w} - \bar{\underline{w}}$. Then a Taylor series expansion linearises equation (5) to

$$\dot{\underline{x}} = \underline{A} \underline{x} + \underline{B} \underline{u}$$

If f_1 denotes $\dot{h}$ and f_2 denotes $\dot{T}_o$ then:

$$A = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \dots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \dots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \dots & \frac{\partial f_n}{\partial x_n} \end{bmatrix}$$

$$B = \begin{bmatrix} \frac{\partial f_1}{\partial w_1} & \frac{\partial f_1}{\partial w_2} & \dots & \frac{\partial f_1}{\partial w_n} \\ \frac{\partial f_2}{\partial w_1} & \frac{\partial f_2}{\partial w_2} & \dots & \frac{\partial f_2}{\partial w_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial w_1} & \frac{\partial f_n}{\partial w_2} & \dots & \frac{\partial f_n}{\partial w_n} \end{bmatrix}$$

Since the aim is to find the time constants matrix B is not needed.

Thus, for the mixing tank model, the two state variables are h and T_o and the two inputs are x_c and x_h . But for convenience Q_c and Q_h will be considered as the two inputs since (for linear values) they are directly related to the valve positions (x_c and x_h) through the valve constants.

$$\therefore f_1 = \frac{1}{A} (Q_h + Q_c - K_o \sqrt{h})$$

$$f_2 = \frac{1}{Ah} [Q_h (T_h - T_o) - Q_c (T_o - T_c)]$$

$$\frac{\partial f_1}{\partial h} = -\frac{k_o}{2A \sqrt{h}}$$

$$\frac{\partial f_1}{\partial T_o} = 0$$

$$\frac{\partial f_2}{\partial h} = -\frac{1}{Ah^2} [Q_h (T_h - T_o) - Q_c (T_o - T_c)]$$

$$\frac{\partial f_2}{\partial T_o} = \frac{-1}{A \cdot h} [Q_h + Q_c]$$

$$\frac{\partial f_1}{\partial Q_h} = \frac{1}{A} \quad \frac{\partial f_1}{\partial Q_c} = \frac{1}{A}$$

$$\frac{\partial f_2}{\partial Q_h} = \frac{1}{Ah} \cdot (T_h - T_o), \quad \frac{\partial f_2}{\partial Q_c} = \frac{-1}{Ah} \cdot (T_o - T_c)$$

In matrix form

$$\begin{bmatrix} \dot{h} \\ \dot{T_o} \end{bmatrix} = \begin{bmatrix} -\frac{k_o}{2A \sqrt{h}} \\ \frac{-1}{Ah^2} [Q_h (T_h - T_o) - Q_c (T_o - T_c)] \\ \frac{1}{A} \\ \frac{1}{Ah} (T_h - T_o) \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{-(Q_h + Q_c)}{Ah} \\ \frac{1}{A} \\ \frac{-1}{Ah} (T_o - T_c) \end{bmatrix} \cdot \begin{bmatrix} h \\ T_o \\ Q_h \\ Q_c \end{bmatrix} \quad 3.6$$

At the steady state values of $h = 0.1$ and $T_o = 317^\circ K$ as the operating point, evaluation of the upper matrix will give:

$$\begin{bmatrix} \dot{h} \\ \dot{T} \end{bmatrix} = \begin{bmatrix} 0.00221 & 0 \\ 0 & 0.00442 \end{bmatrix} \cdot \begin{bmatrix} h \\ T \end{bmatrix} + \begin{bmatrix} 88.5 & 88.5 \\ 2.3 \times 10^4 & -3.45 \times 10^4 \end{bmatrix} \cdot \begin{bmatrix} Q_h \\ Q_c \end{bmatrix}$$

The eigen values of the A-matrix are obtained by solving the equation $|SI - \underline{A}| = 0$.

$$\therefore (S_1 - 0.00221) (S_2 - 0.00442) = 0$$

$$\therefore S_1 = 0.00221 \quad S_2 = 0.00442$$

The time constant is the inverse of eigen value

$$\therefore T_1 = 452 \text{ seconds} \quad T_2 = 226 \text{ seconds}$$

where T_1 is the time constant of height response and T_2 is that of the mixed water temperature response.

The corresponding values obtained from the actual responses are 467 and 220 seconds when the step change was applied to the hot water value and 475 and 220 seconds when the step change was applied to the cold water value. Allowing for errors when drawing the tangents to the graph, the two sets of values agree with each other to within 5%.

It can also be seen that the two values of time constants of height and those of temperature are the same, indicating that the time constant remains constant for both positive and negative disturbances.

The model used so far assumes that there are no heat losses from the mixing tank to the surrounding i.e. the tank is perfectly insulated. To be more realistic, heat losses must be included in the system, an improvement which will be discussed in the following subsection.

3.3.4 SYSTEM WITH HEAT LOSSES:

The addition of a heat losses term to the system model will serve two purposes. First, the system will become more realistic, since a perfectly insulated system is hard to achieve. Secondly, for the purpose of system identification - to be dealt with later - the addition of this heat losses term will be treated as uncertain variations in the system which the identification process has to deal with.

The addition of a heat losses term will not affect the mass balance of the system but will affect the heat balance. Thus, the new heat balance will be as follows:

$$\frac{d}{dt} (A.h.\ell.\hat{c}.T_o) = Q_h.\ell.\hat{c}.T_h + Q_c.\ell.\hat{c}.T_c - Q_o.\ell.\hat{c}.T_o - 2\pi.r.h.H_{tc}.(T_o - T_a)$$

where

r = radius of the tank (m)

H_{tc} = heat transfer coefficient of the tank wall SI units

T_a = ambient temperature ($^{\circ}k$)

The height h used in the heat losses term in the above equation should be the total height of the vessel since the whole outer surface of the vessel is exposed to the surroundings.

$$\begin{aligned} \therefore A \cdot \ell \cdot \hat{c} \left(h \frac{dT_O}{dt} + T_O \frac{dh}{dt} \right) &= Q_h \cdot \ell \cdot \hat{c} \cdot T_h + Q_c \cdot \ell \cdot \hat{c} \cdot T_c - \\ &\quad Q_O \cdot \ell \cdot \hat{c} \cdot T_O - 2 \pi \cdot r \cdot H_{tc} (T_O - T_a) \\ \therefore \frac{dT_O}{dt} &= \frac{1}{A \cdot \ell \cdot \hat{c} \cdot h} \left[Q_h \cdot \ell \cdot \hat{c} \cdot T_h + Q_c \cdot \ell \cdot \hat{c} \cdot T_c - Q_O \cdot \ell \cdot \hat{c} \cdot T_O - \right. \\ &\quad \left. 2 \pi \cdot r \cdot H_{tc} \cdot (T_O - T_a) - A \cdot \ell \cdot \hat{c} \cdot T_O \frac{1}{A} (Q_c + Q_h - Q_O) \right] \\ &= \frac{1}{A \cdot h} \left[Q_h \cdot (T_h - T_O) - Q_c (T_O - T_c) \right] - \frac{2 \cdot H_{tc}}{\ell \cdot \hat{c} \cdot r} (T_O - T_a) \end{aligned} \quad 3.7$$

Now, in the steady state, the values of all the variables will remain as before except T_O , which depends on the value of the heat transfer coefficient H_{tc} . Graph (3.6) shows how the steady state value of T_O varies with H_{tc} . If H_{tc} is too high, the losses to the surroundings will be unrealistically high. Similarly, if H_{tc} is too small the losses become too low that the system will behave as an insulated one. As a trade off between the two extremes a value of $H_{tc} = 100$ is accepted. This will give a steady state mixed water temperature $T_O = 313.34^\circ \text{K}$.

3.3.5 STEP RESPONSE

If a 50% step change is applied to the cold water valve position so that $x_c = 0.75$, the final steady state values of the state variables will be

$$h = 0.144 \text{ m and } T_O = 307.76^\circ \text{K}$$

These values were calculated in the same way as those calculated earlier.

To approximate further to a real uncertain dynamic system, a sinewave variation is attached to the hot water input temperature (T_h), thus,

$$T_H = T_h (1.0 + 0.01 \times \sin(\omega t)) \quad (\text{See Fig 3.7})$$

This sinusoidal variation on T_h will have a direct effect on T_o and will appear on the response as will be seen later in the identification chapter.

Application of identification techniques discussed in Chapter 2 to this uncertain dynamic system will be discussed in the next Chapter.

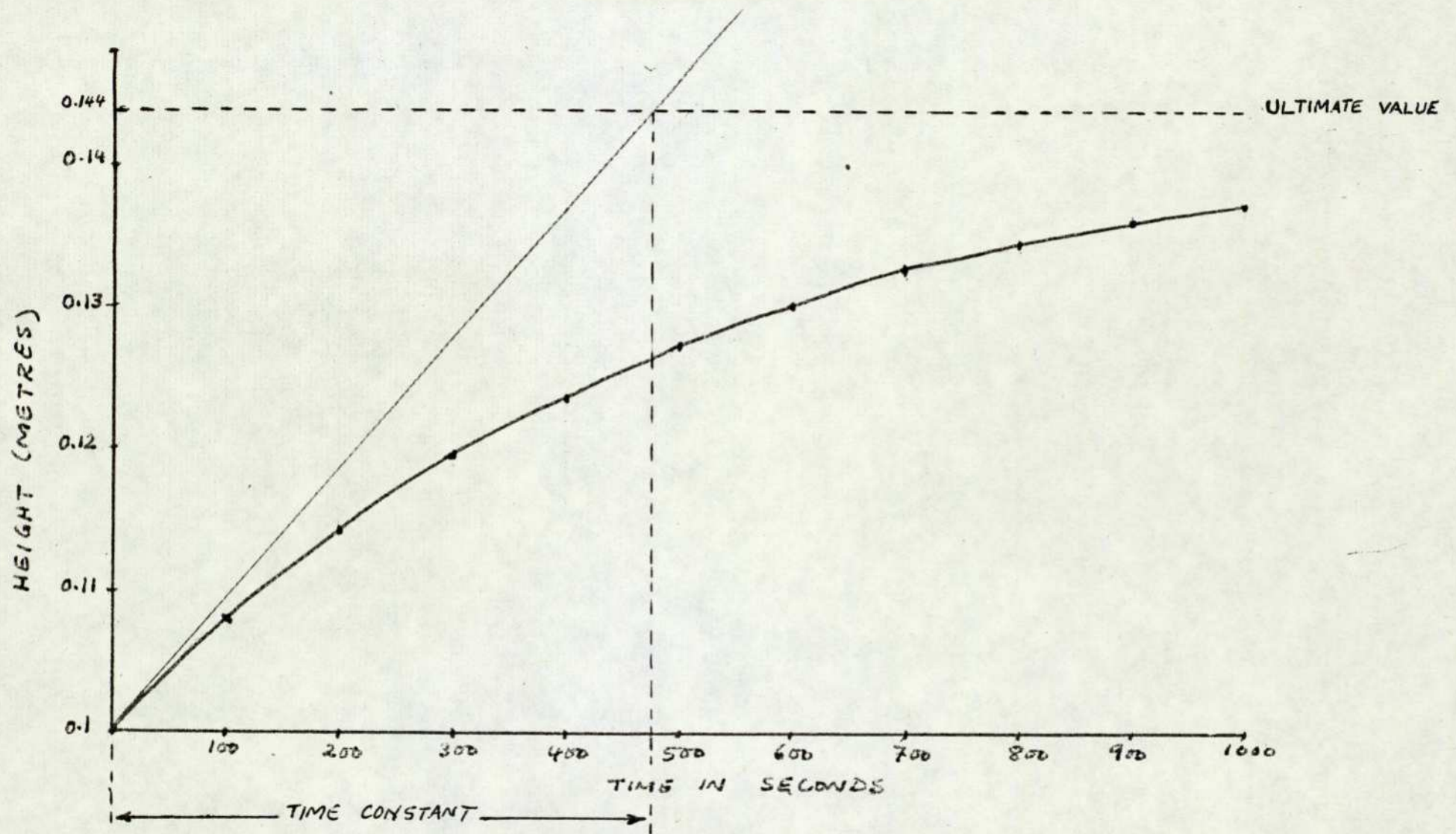


Fig.3.2. Height Response due to a 50% Step Change, in x_c .

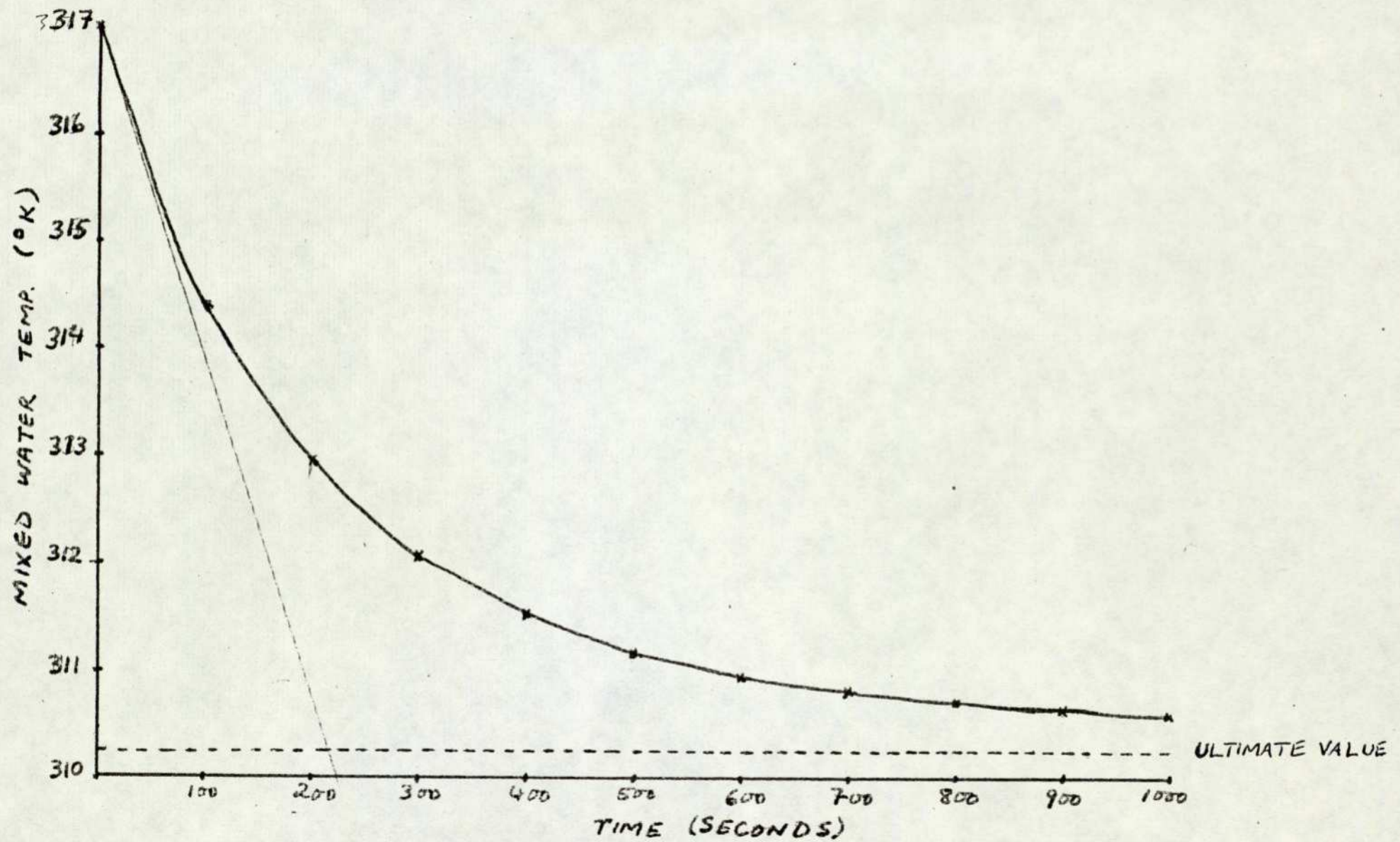


Fig.3.3. Mixed Water Temperature Response to a 5% Step Change in x_c .

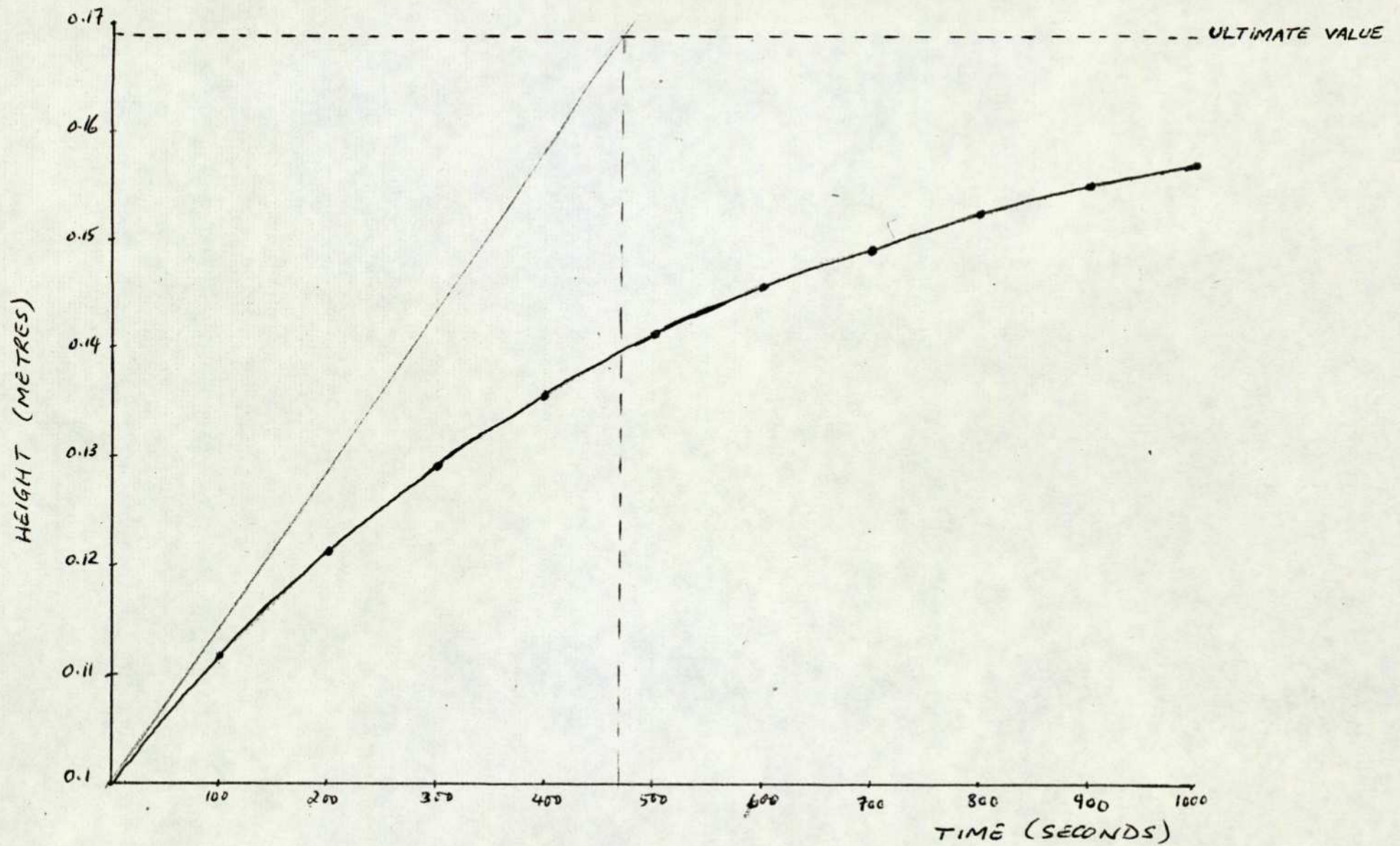


Fig.3.4. Height Response to a 50% Step Change in x_n .

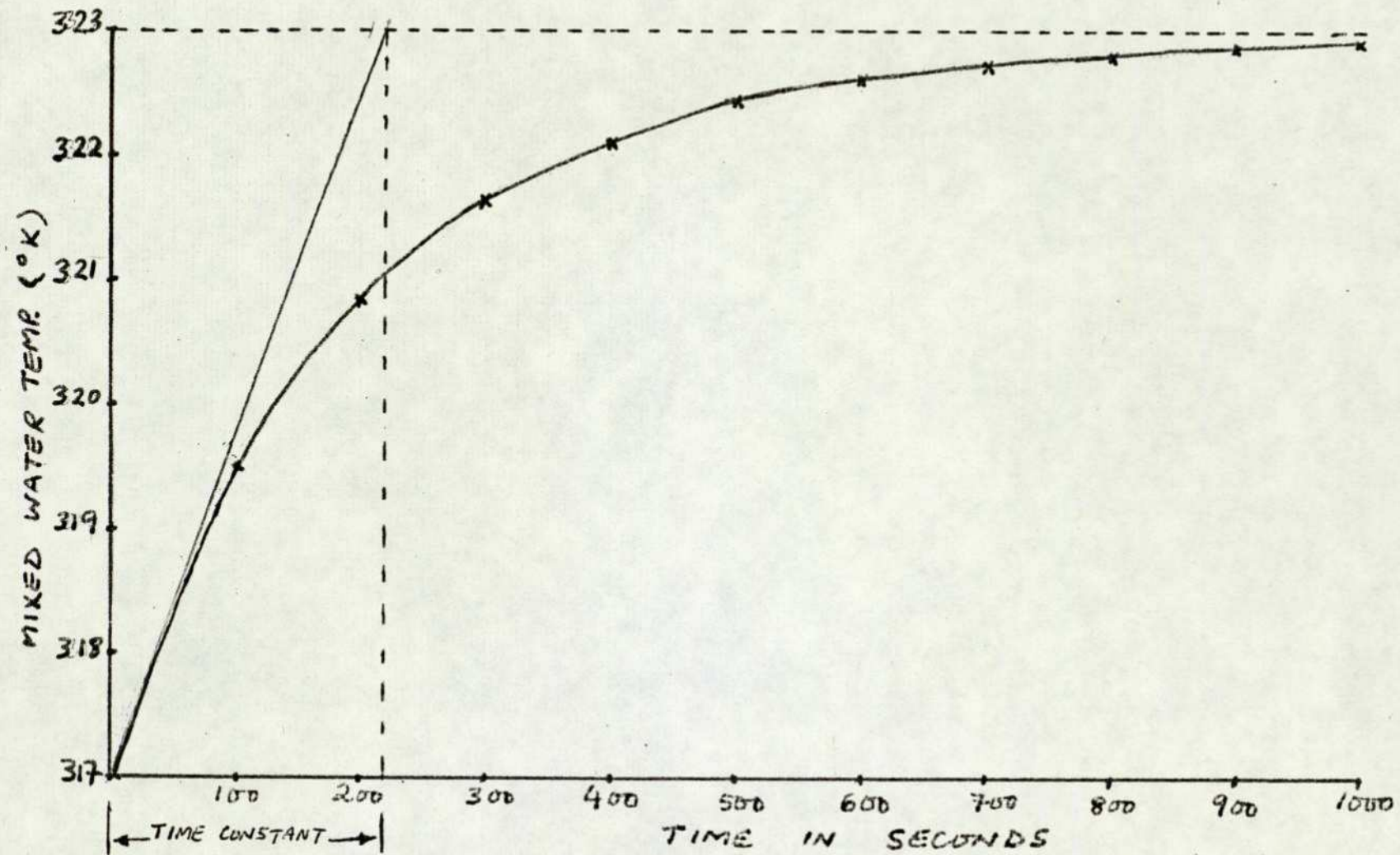


Fig. 3.5: Mixed water temperature response to a 50% step change in x_h

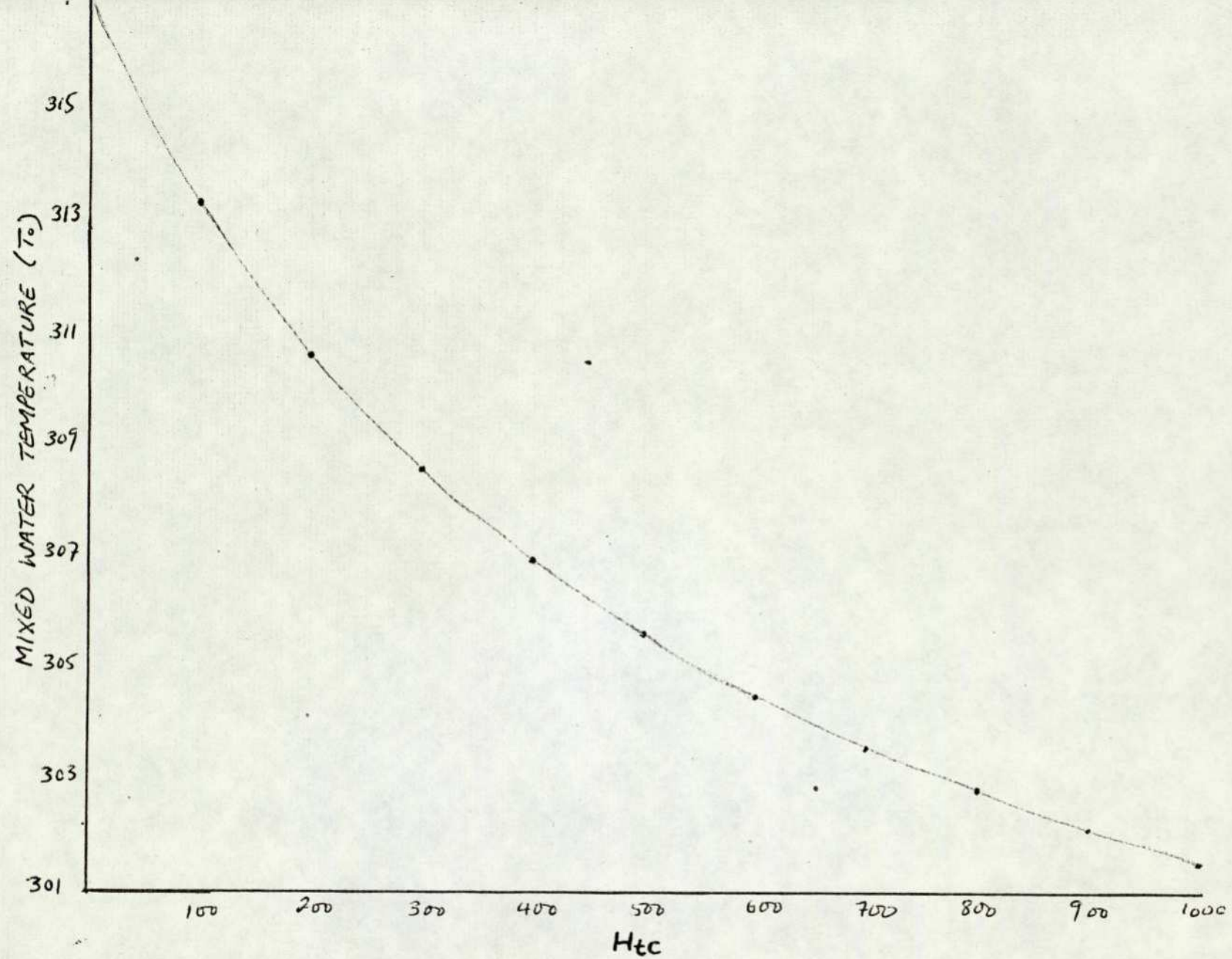


Fig. 3.6: The effect of H_{tc} value on the steady state value of mixed water temp.

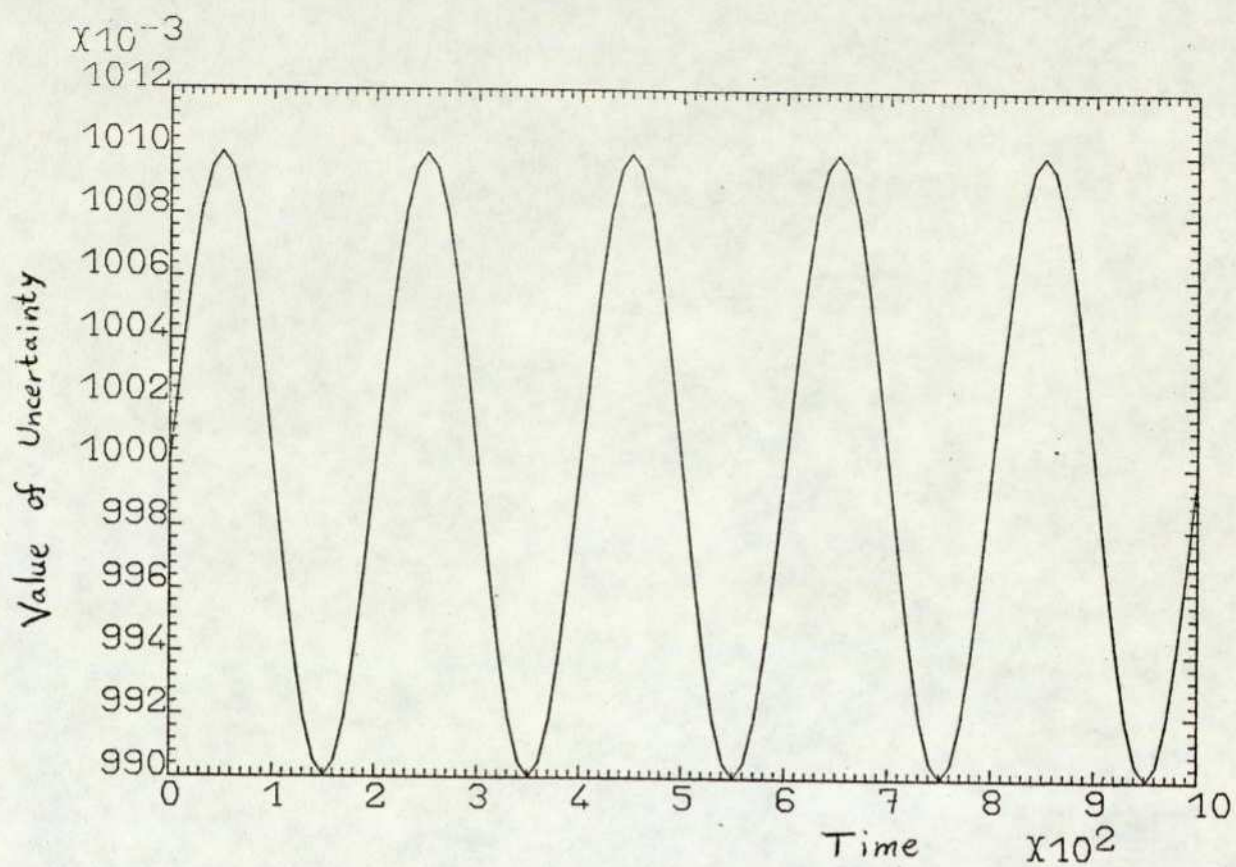


Fig. 3.7 The Time-varying Uncertainty Attached to T_h where $T_H = T_h \times \left[1.0 + 0.01 * \sin\left(\frac{\omega t}{100}\right) \right]$

CHAPTER 4

IDENTIFICATION OF THE MIXING TANK SYSTEM

4.1 Introduction

The model of the mixing tank system developed in Chapter 3 is a simplified one due to the assumptions made of the system. If these assumptions had not been made the model structure would have been much more sophisticated. Since processes such as identification and optimisation are of an iterative nature the computation procedures needed for execution of these processes become very costly indeed giving rise to the tendency towards severe model simplification to a degree determined by the purposes of modelling. Models resulting from this simplification will reflect the general behaviour of the system ignoring finite details which require lengthy and cumbersome differential equations. Although any simplified model will reflect some aspects of the real world, a trade off must be made between the purposes of the model and its degree of sophistication.

In this chapter the problem of identification of the mixing tank system is presented and discussed. The system simulation discussed in Chapter 3 is taken as the real system for this purpose. Two different situations have been considered in this simulation. In the first situation, the assumption that there is no heat losses to the surroundings is made and a sinusoidal variation on the inlet hot water temperature is introduced. In the second

situation, heat losses to the surroundings are considered in the real system together with the sinusoidal variation on the inlet hot water temperature. When modelling the first system the "uncertainty" in the outlet temperature response (caused by the sinusoidal variation in the inlet hot water temperature), assuming its real cause is not known, is accounted for by introducing time-varying uncertainty to the hot water temperature. The estimation of parameters of this time-varying uncertainty constitutes the smoothing problem. When modelling the second system, the uncertainty caused by the introduction of the heat losses term into the real system as well as the sinusoidal variation in the inlet hot water temperature is accounted for by the introduction of time varying uncertainties to the inlet hot water temperature and to the derivative of the outlet temperature.

In both situations, the estimation problem is concerned with finding the best estimate of the value of the outlet valve restriction constant (k_o). Its real value is that used in the simulation of the real system.

The overall problem is formulated such that the estimation problem and smoothing problem are dealt with separately and iteratively until convergence is achieved when a convergence criteria has been fulfilled. A comparison between the performance of the classical least squares and the smoothed least squares techniques is obtained by starting the identification process with the time-varying uncertainty set at its nominal value. The first solution of the estimation problem in this case is that of the classical least squares technique whilst subsequent solutions of the two problems are the smoothed least squares solutions.

In the forthcoming sections the formulation and the functions of essential computer programs and subroutines will be presented and discussed whilst the Fortran program suites are contained in Appendix 3.

4.2 Program EXAMPLE

The identification process is carried out by this program which had been written, compiled and run on the CDC 7600 computer. It reads the design values of the system as well as the initial values of the state variables (h and T_0) and sets the integration parameters and the parameters needed for the identification process at appropriate values. An integration procedure then follows, producing "observational data" for the two state variables (h and T_0) which are stored in a 2×100 matrix (YA.) The integration process used is the NAG subroutine DO2AJF which is suitable for a stiff set of differential equations and is being employed here purely for convenience. The derivatives of the system state variables required by this integration subroutine are obtained using subroutine SYSTEM. Having obtained the "real" system observations, the program proceeds with the identification process. This is accomplished by calling subroutine OPTIM, which coordinates the solutions of the two problems. Finally, the system and the identified model responses are plotted by subroutine PLOT.

4.2.1. Subroutine SYSTEM:

This subroutine is assumed to be a faithful representation of the mixing tank rig. In this subroutine, the two state variables (h and T_0) are set to their previous values and the inlet hot and cold water and the outlet flows calculated. A sinusoidal variation of amplitude equal to 1% of the nominal value of T_h and frequency of $\pi/100$ rads/S is superimposed on T_h , thus:

$$T_H = T_h \times (A + B \times \sin(\omega t))$$

where

$$A = 1.0, B = 0.01 \text{ and } \omega = \frac{\pi}{100} \text{ rads/sec}$$

The derivatives of the two state variables are then calculated according to Eqns 3.4 and 3.5

The value of k_o (outlet valve restriction constant) used to calculate Q_o is that obtained in the design calculation in Chapter 3. It is this value which the parameter estimation problem has to find in the process of model identification, and is normalised to 1.0.

4.2.2. Subroutine OPTIM

This subroutine coordinates the solution of the joint problem of parameter estimation and smoothing. It starts by computing the initial responses of the mixing tank and then proceeds to the solution of the iterative process of identification. On exit from the DO loop which contains the solution of the two problems after the convergence criterion have been fulfilled, the final responses of the mixing tank are computed and returned to the main program (EXAMPLE).

4.2.2.1. Parameter Estimation Problem

This problem is concerned with finding an estimate of the constant unknown parameter k_o (the outlet valve restriction constant) using NAG subroutine EØ4ABF. This NAG subroutine finds the minimum in a given finite interval of a continuous function of a single variable

This minimum value is that which reduces the difference between the system and model responses to a minimum, where

$$\underline{V}_c = \sum_{i=1}^n [\underline{Z}(i) - \underline{h}(x(i))]^T \cdot W \cdot [\underline{Z}(i) - \underline{h}(x(i))]$$

where $\underline{Z}(i)$ and $\underline{h}(x(i))$ are the i^{th} system and model output vectors respectively, W is the weighting matrix and $\underline{V}_c$ is the classical least squares objective function. This procedure is a straightforward classical least squares process. The NAG subroutine EØ4ABF requires a subroutine (FUNCTI) to compute the model responses and hence the objective function at each iteration. It also requires specifying the range within which the parameter to be estimated is likely to lie in order to avoid unnecessary searches outside this range.

4.2.2.2. Smoothing Problem

The estimate obtained for the constant parameter k_o in the parameter estimation problem is kept constant when solving the smoothing problem by the NAG subroutine EØ4FAF. This subroutine

"finds the least squares solution of M-non linear equations in N variables by a method due to Peckham"(28). The variables to be manipulated here are the parameters of the time varying uncertainty whose optimum values are those which minimise the objective function

$$V_s = \sum_{i=1}^n \left\{ \left[\underline{z}(i) - \underline{h}(\underline{x}(i)) \right]^T \cdot W \cdot \left[\underline{z}(i) - \underline{h}(\underline{x}(i)) \right] + \left[\text{Traj} - B_{bm}(i) \right]^T \cdot R \cdot \left[\text{Traj} - B_{bm}(i) \right] \right\} \quad 4.2.1$$

where

- Traj = nominal trajectory of the uncertainty
- $B_{bm}(i)$ = i^{th} value of the time-varying uncertainty
- R = positive definite weighting matrix.

Thus the two problems are dealt with separately and iteratively.

However, the separation of the identification problem into two separate problems; parameter estimation and smoothing does not mean that smoothing parameters have no effect on the classical least squares part of the objective function because the time varying uncertainty affects $\left(\frac{dT_o}{dt}\right)$ and hence affects the model responses used for the classical least squares estimation.

The NAG subroutine E04FAF requires a subroutine (FUNCT) to calculate the value of the objective function for each set of estimates of the smoothing parameters.

The overall iterative process continues between the two problems until a convergence criterion is satisfied.

4.2.2.3. Convergence Criterion

The convergence criterion used in the identification of the tank system is that the objective function remains unchanged over an overall iteration, i.e. if the value of the objective function on entry to the parameter estimation problem is S_1 , and on exit S_2 and on entry to the smoothing problem S_2 and on exit S_3 , then the criteria is satisfied only when $|S_1 - S_3| < \epsilon$, where ϵ is an arbitrarily small number, otherwise the iterative process continues.

A better and more accurate criterion which could have been used is that which requires parameter estimates to be unchanged over two iterations. This is because even if the objective function remains unchanged over two iterations, the parameter may change in such a way that the collective effect of this change has no effect on the objective function (see Fig 4.2.2). In this case, the objective function has a flat minimum as illustrated below.

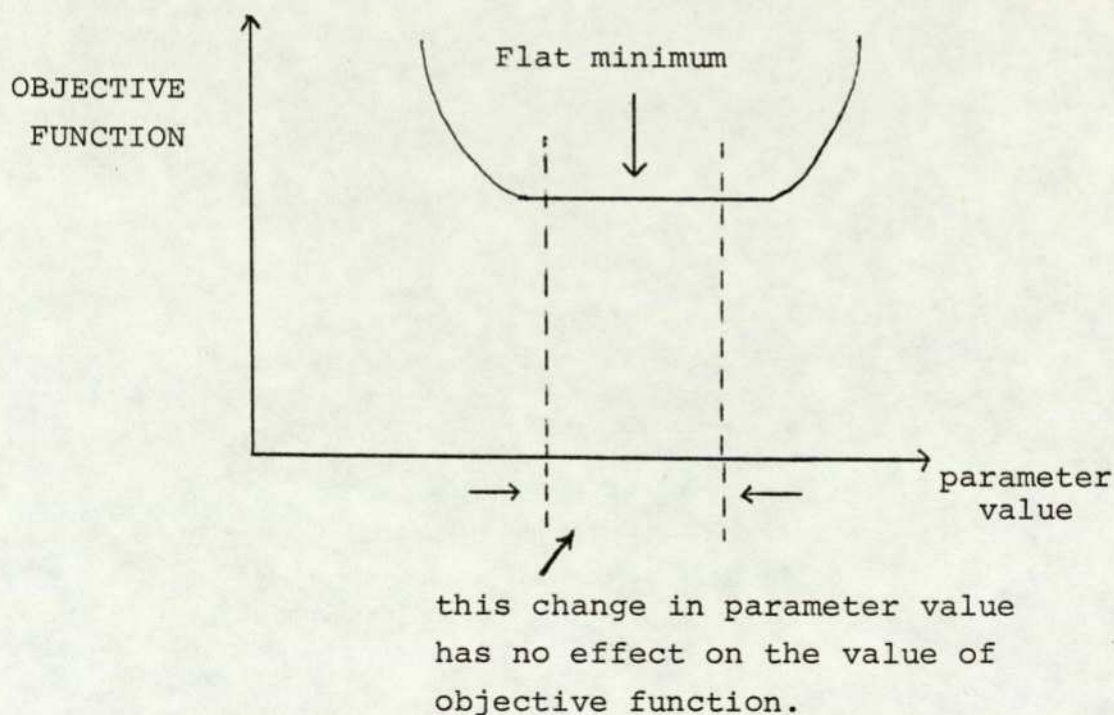


Fig. 4.2.2. Possible behaviour of the objective function with respect to parameter value.

However, in order to economise on computing time, this convergence criteria has not been used here but has only been used in the identification of the vaporiser system (Chapter 6).

4.2.3. Subroutine FUNCT (& FUNCT1)

The estimation problem is concerned with finding the estimate of only one parameter whilst the smoothing problem is concerned with finding the estimates of more than one parameter.

For this reason, the two NAG subroutines E04ABF and E04FAF have been used. Subroutine E04ABF requires subroutine FUNCT1 whilst subroutine E04FAF requires subroutine FUNCT to calculate the objective function and compute responses. The two subroutines (FUNCT1 and FUNCT) are essentially the same, the difference being in their arguments which are specified by E04ABF and E04FAF.

Each of the two subroutines computes the model responses of the mixing tank system to a step change in one of the hot or cold water control variables (valve positions). From these responses and the real system observations, the objective function is calculated using Eqn 4.2.1.

The integration procedure is done using the NAG subroutine D02AJF which is suitable for integrating a set of stiff differential equations. Although the differential equations of the mixing tank system are not stiff, this subroutine had been used due to the familiarity with its use in the vaporiser model to be discussed in the forthcoming chapters. The integration process is carried out over the range 0 - 100 seconds with samples obtained at 10 seconds intervals. These results $[\underline{h}(\underline{x}(t))]$ (for height and mixed water temperature) are compared with those obtained similarly for the system simulation $[\underline{z}(t)]$. The differences between the system and model observations are multiplied by the weighting matrix $\underline{W}$ which is a positive definite matrix.

The smoothing part of the objective function is concerned with the departure of the uncertainty from its nominal value and is calculated as follows:

- (a) if the uncertainty is approximated to by a sinewave then:

$$\beta(t) = P(1) + P(2) \cdot \sin [P(3) \cdot t + P(4)]$$

where $P(1)$, $P(2)$, $P(3)$ and $P(4)$ are the parameters of the time varying uncertainty whose form is to be found by the identification process. The value of $\beta(t)$ is compared with its nominal trajectory and the difference is multiplied by the weighting matrix $\underline{R}$ which is a positive definite matrix, and is chosen to give proper weighting for $\beta(t)$.

- (b) if the uncertainty is approximated to by a Chebychev polynomial, then its value is calculated as:

$$\beta(t) = P(1) \cdot T_0 + P(2) \cdot T_1 + P(3) \cdot T_2 + \dots$$

where T_0 , T_1 , T_2 ... are Chebychev polynomials and $P(1)$, $P(2)$, $P(3)$, ... etc are the coefficients of these polynomials. These coefficients are the parameters which are manipulated by the identification procedure when dealing with the smoothing problem.

The classical least squares solution is obtained by starting the identification process with the time-varying uncertainty set to its nominal value. The overall objective function (Eqn 4.2.1) thus reduces to that of the classical least squares. It must be noted that subsequent solutions of the problem where the $\beta(t)$ has values different from its nominal value are smoothed least squares solutions.

4.3 RESULTS

The identification program of the mixing tank system was run under two different conditions where:

- i) the identification process is concerned with identifying a well insulated uncertain dynamic system, and
- ii) the identification process is concerned with identifying a system which loses heat to the environment at a rate depending on the value of a heat transfer coefficient (H_{tc}).

Under the first condition, the variations on the system responses are accounted for by incorporating a time-varying uncertainty in the model. This uncertainty was approximated to by two forms:

- a) a sinewave attached to T_h
- b) a Chebychev polynomial attached to T_h

Under the second condition, the variations on the system responses were approximated to by a sinewave and Chebychev polynomial attached to T_h and $\frac{dT_o}{dt}$ respectively.

4.3.1 SYSTEM WITH NO HEAT LOSSES

The results obtained for different values of the weighting matrices $\underline{W}$ and $\underline{R}$ are summarised in Tables 4.3.1, 4.3.7, 4.3.12, 4.3.14, 4.3.18 and 4.3.22. The Tables give a summary of the overall picture of the results in a column-row form as follows:

- Column 1 - the case number (for convenience)
- Column 2 - the weighting matrix for the particular case
- Column 3 - the classical least squares solution of the estimation parameter (k_o)
- Column 4 - smoothed least squares solution of the estimation parameter (k_o)

Columns 5 - 10 - the converged values of the smoothing parameters i.e. the parameters of the time varying uncertainty contained in the array PRB(6)

Column 11 - the number of overall iterations, where an overall iteration consists of the solution of the parameter estimation problem followed by the solution of smoothing problem

Column 12 - the central processor time used by the identification process

The weighting matrices $\underline{W}$ and $\underline{R}$ are positive matrices chosen either by engineering judgement or in such a way as to normalise the errors to 1.0. This can be achieved by taking the inverse of the normal value of the sample thus: $\underline{W} = \frac{1}{\underline{y}}$ and $\underline{R} = \frac{1}{T_{raj}}$

where $\underline{y}$ = normal value of height or temperature.

The following values of the weighting matrices have been obtained by calculations based on the above concept, thus

$$W(1) = 10.0, W(2) = 0.5 \text{ and } R = 10.0$$

where $W(1)$ = the weighting matrix of the squares of the errors in the height response,

$W(2)$ = the weighting matrix of the squares of the errors in the mixed water temperature response

and R = the weighting matrix of the squares of the deviations of the time-varying uncertainty from its nominal value.

In each of the three tables in sections 4.3.1a and 4.3.1b two of these three weighting matrices are kept constant whilst the third is varied as shown.

Thus, in table 4.3.1 W(2) and R are kept at 0.5 and 10.0 whilst W (1) is varied from 0.1 to 100.0. In table 4.3.7 W(1) and R are kept at 10.0 and 10.0 whilst W(2) is varied from 0.1 to 5.0. In table 4.3.12 W(1) and W(2) are kept at 10.0 and 0.5 whilst R is varied from 1.0 to 1000.0. In this manner an insight is obtained into the behaviour of the model as the weightings on the responses and uncertainty are varied.

4.3.1a Chebychev-form uncertainty

The results obtained for various values of weighting matrices implementing Chebychev-form uncertainty attached to the hot water temperature T_h are summarised in Tables 4.3.1, 4.3.7 and 4.3.12. In most cases there is marked improvement due to the smoothed least squares technique over the parameter estimate obtained by the classical least squares technique. The true value used in the system simulation is normalised to 1.0.

Table 4.3.1 shows the effect of varying W (1) from 0.1 to 100.0. It is evident that as W(1) is increased the classical least squares technique yields results (for k_o) nearer to the true value, and thus, the need for smoothing becomes less. However, over this range, the smoothing has resulted in slightly improved estimates of k_o ranging from 0.0035% in Case 5 to 0.55% in Case 1. This minimal improvement has been achieved at a high cost of computing time.

The classical least squares and the smoothed least squares estimates of k_o have been plotted against the log of W(1) as in Fig. 4.3.2.

The effect of the weighting matrix $W(1)$ on the parameter estimate k_0 is understandable on the basis that $W(1)$ is the weighting of the errors between system and model height responses, and that the height value is related to k_0 by the equation:

$$Q_0 = k_0 \sqrt{h}$$

Thus increasing the weighting will put more emphasis on this part of the objective function which will become dominant with inclination towards finding the correct value. This explains the less accurate estimate obtained by the classical least squares technique when $W(1) = 0.1$ for example.

The water height and the mixed water temperature responses which correspond to Case 3 in Table 4.3.1 (and also to Case 2 in Table 4.3.7 and Case 3 in Table 4.3.12) are shown in Figs. 4.3.3 and 4.3.4 respectively. Since the parameter estimate (k_0) obtained by the identification process is almost the same as the true value used in the system simulation (1.0) the height responses of the system and the model are indistinguishable.

The mixed water temperature response obtained by the identified model follows the general trend of the system response but not its periodical variations. The solution of the smoothing problem has yielded parameters which give the time-varying uncertainty - Chebychev polynomial form - shown in Fig. 4.3.25a. Clearly the shape of the uncertainty differs from the real one shown in Fig. 3.7, but has certainly contributed towards the compensation for model structural deficiencies resulting in a better value of parameter estimates. In fact, in all the cases where Chebychev

polynomials have been used in the model to approximate for the time-varying uncertainties in the simulated system, the exact shapes of the real uncertainty have not been predicted.

The model and simulated system mixed water temperature responses corresponding to Case 5, in which much emphasis has been put onto the errors in the height responses, as reflected by the large value of the weighting matrix $W(1)$, are shown in Fig. 4.3.5. The responses reflect little noticeable difference from those of Fig. 4.3.4. The height responses for the same case have not been shown here because, again, they look exactly the same as those of Fig. 4.3.3.

Table 4.3.7 shows the effects of varying $W(2)$ on the parameter estimates yielded by the classical least squares and the smoothed least squares techniques. As $W(2)$ is increased, the parameter estimate k_0 becomes less accurate and the need for smoothing becomes more acute. This result can be appreciated by reference to Fig. 4.3.8 in which k_0 is plotted against $W(2)$, with other weightings kept at constant values. The improvement on the value obtained by the classical least squares technique due to the smoothed least squares technique ranges from 0.007% in Case 1 to about 2.1% in Case 6. However at its best improvement (in Case 6) the smoothed least squares could not yield the true value of k_0 (1.0) and hence the system and model height responses do not have good agreement. Fig. 4.3.9 shows, for this case, the discrepancy between simulated system and identified model height responses due to inaccurate estimate of the parameter (k_0). Similar responses were obtained for Case 1 in Table 4.3.1. The mixed water temperature response for this case (Case 6, Table 4.3.7) is shown in Fig. 4.3.10. This is very similar to those shown in Figs. 4.3.4. and 4.3.5. in which the average trend of the system response was followed but its periodical variations could not be predicted by the identification process. For Case 4 in Table 4.3.7 the mixed water temperature responses are shown in Fig. 4.3.11. Although the identified model, could not follow the variations on the system response, it is nearer to it than the previous responses. The height responses are indistinguishable from each other (similar to Fig. 4.3.3) due to the accurate estimate of k_0 , and have, thus, not been presented here to avoid repetition.

Table 4.3.12 shows the effects of varying R (the weighting matrix associated with the errors between the uncertainty and its nominal value) on the classical least squares and the smoothed least squares estimates of k_0 . The classical least squares technique is insensitive to R due to the fact that the classical least squares solution is obtained by setting the uncertainty at its nominal value thereby setting the contribution of the uncertainty to the overall objective function to zero. However, the smoothing which gives the uncertainty values other than its nominal trajectory, results in improved parameter estimates of k_0 for lower values of R , whilst for larger values, no improvement is achieved, as can be seen in Fig. 4.3.6. This may be due to the idea that with larger values of R , the product of the weighting and the errors between the time-varying uncertainty and its nominal value becomes so large that only keeping the uncertainty at its nominal trajectory or near to it will result in reduction of the objective function. This means that the smoothing results in no-change in model structure and the results will be the same as or very near to the classical least squares solution.

CASE	W (1)	PRA(k _o) C.L.S.	PRA(k _o) S.L.S.	PRB(1)	PRB(2)	PRB(3)	PRB(4)	PRB(5)	PRB(6)	NO. OF OVERALL ITERS.	CP TIME SECONDS
1	0.1	0.9503	0.9555	1.000035	-0.417798	0.163557	0.325213	-0.314972	0.000005	6	60
2	1.0	0.9563	0.9616	1.000038	0.075223	0.017005	-0.01576	0.142853	0.000036	3	27
3	10.0	0.9964	1.00058	1.000701	-0.002792	0.001136	-0.002548	0.0008	-0.001471	5	14
4	20.0	0.99903	0.9995	1.000112	-0.462724	0.862462	0.24245	0.21172	0.00006	11	86
5	100.0	0.99989	0.999925	1.00028	0.133447	0.4365	-0.278794	0.29219	-0.000148	12	120

Table 4.3.1 Results Obtained for Varying Values of W(1) with W(2) = 0.5 and R = 20.0

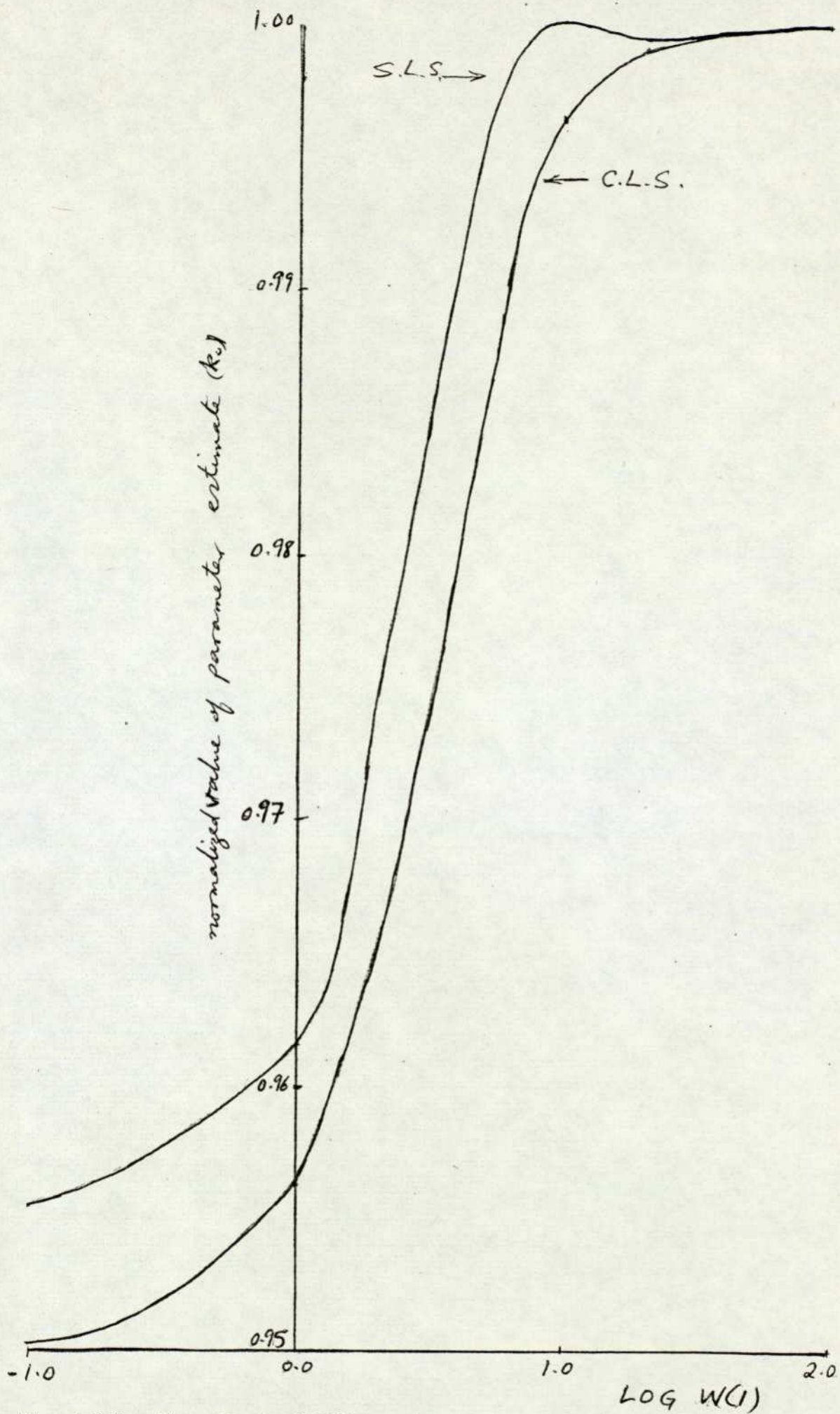


Fig.4.3.2. The effect of $W(1)$ on the parameter estimate k_0 (for Chebychev case).

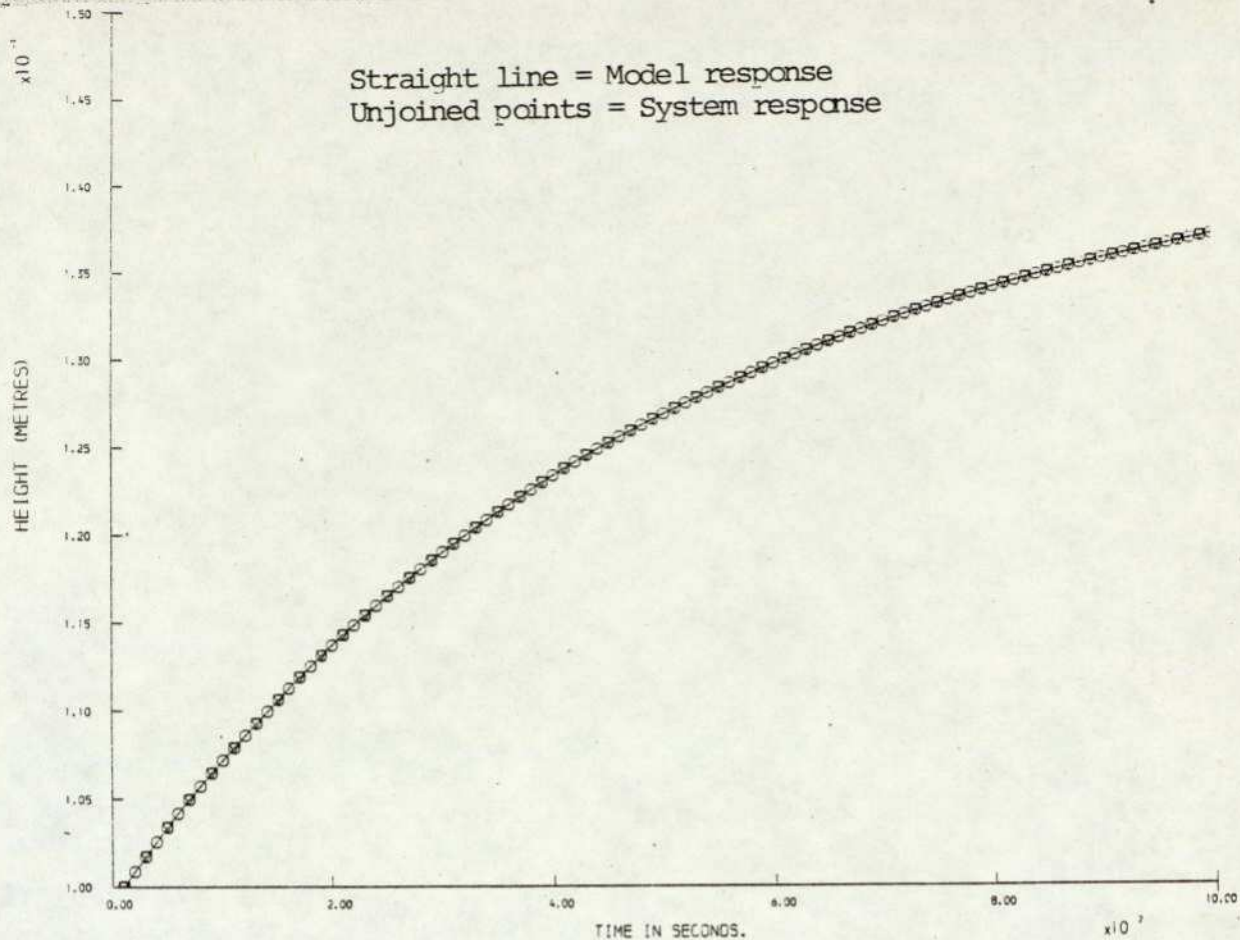


Fig.4.3.3. Open Loop Height Responses of Simulated System and Identified Model of the Mixing Tank for the Case where $W(1) = 10.0$, $W(2) = 0.5$ and $R = 20.0$.

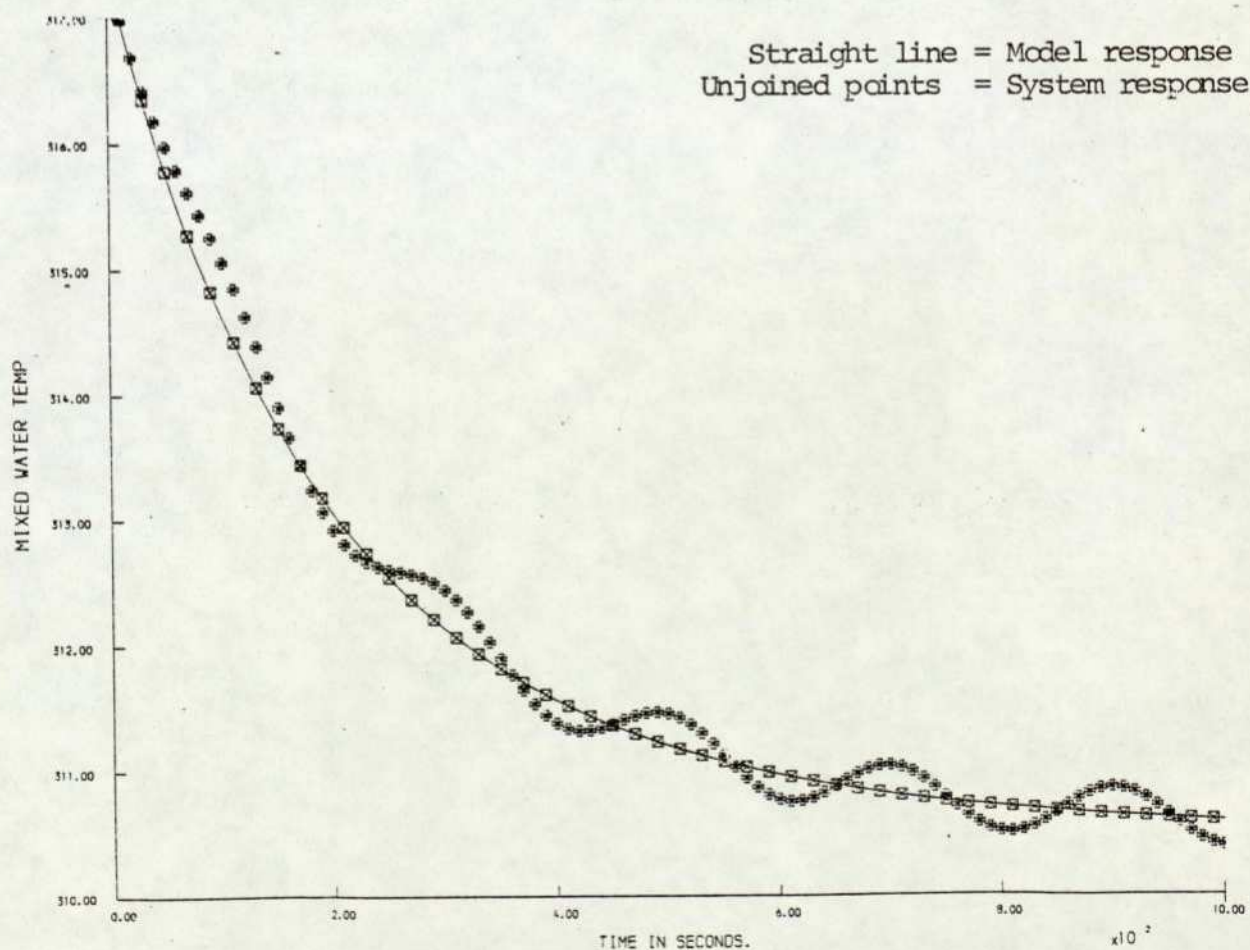


Fig.4.3.4. Open Loop Mixed Water Temperature Responses of Simulated System and Identified Model of mixing tank for the case where $W(1) = 10.0$, $W(2) = 0.5$ and $R = 20$.

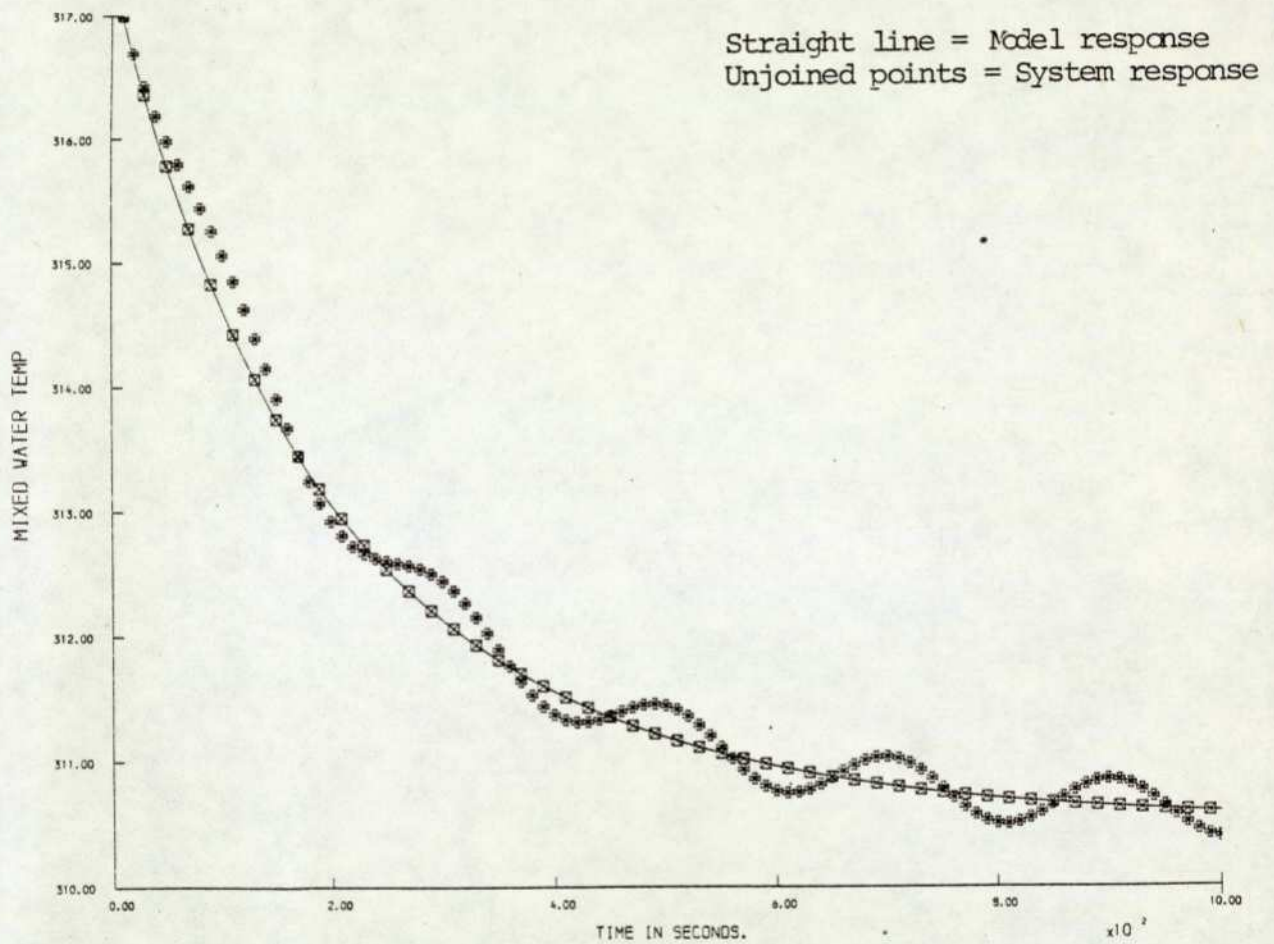


Fig.4.3.5. Open Loop Mixed Water Temperature Responses of Simulated System and Identified Model of the Mixing Tank for the case where $W(1) = 100.0$, $W(2) = 0.5$ and $R = 20$.

CASE	W (2)	PRA(k_o) CLASSICAL LEAST SQ. SOLUTION	PRA(k_o) SMOOTHED LEAST SQ. SOLUTION	PRB(1)	PRB(2)	PRB(3)	PRB(4)	PRB(5)	PRB(6)	NO. OF OVERALL ITERS.	C.P. TIME SECS.
1	0.1	0.99978	0.99985	1.00014	-0.20665	-0.014006	0.222378	0.395018	0.000048	3	26
2	0.5	0.9964	1.000058	1.000701	-0.002792	0.001136	-0.002548	0.0008	-0.001471	5	14
3	0.75	0.9927	0.9996	1.000107	-0.003804	0.000132	-0.003238	0.000168	-0.00191	4	12
4	1.0	0.9883	0.9988	1.000182	-0.004418	0.000363	-0.003799	0.000648	-0.002464	4	12
5	2.0	0.9748	0.9898	1.000196	0.938473	0.415723	-0.506618	-0.446638	0.000347	9	111
6	5.0	0.9572	0.9773	1.000007	0.253418	-0.383442	0.237888	0.378242	0.000396	12	144

Table 4.3.7. Results Obtained for Varying Values of W(2) with W(1) = 10.0 and R = 20.0.

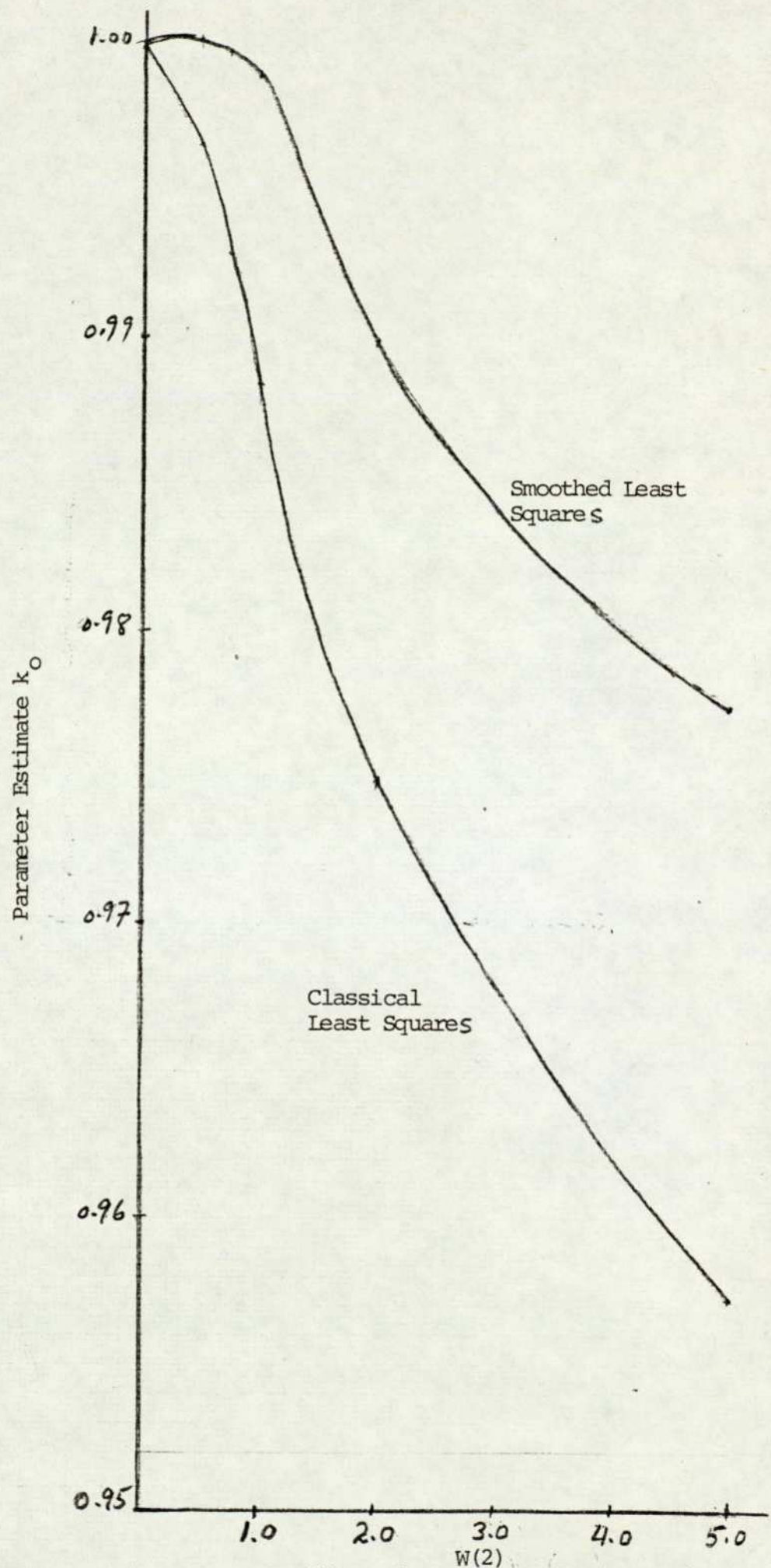


Fig.4.3.8. The effect of the value of $W(2)$ on the Parameter Estimate Obtained by C.L.S. and S.L.S. techniques for Chebychev-form Uncertainty.

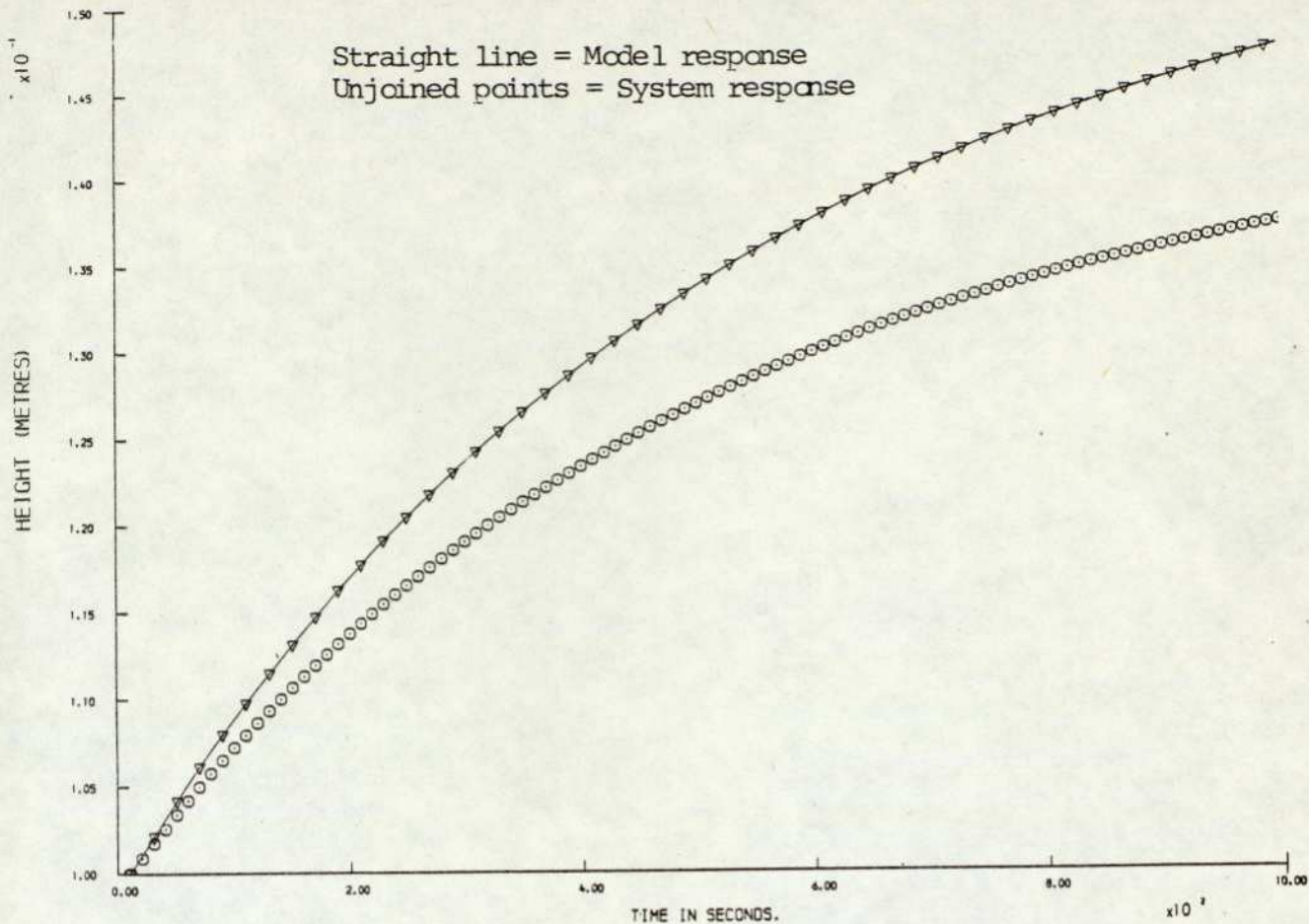


Fig.4.3.9 Open Loop Height Responses of Simulated System and Identified Model of the Mixing Tank System for the case where $W(1) = 10$, $W(2) = 5.0$ and $R = 20.0$.

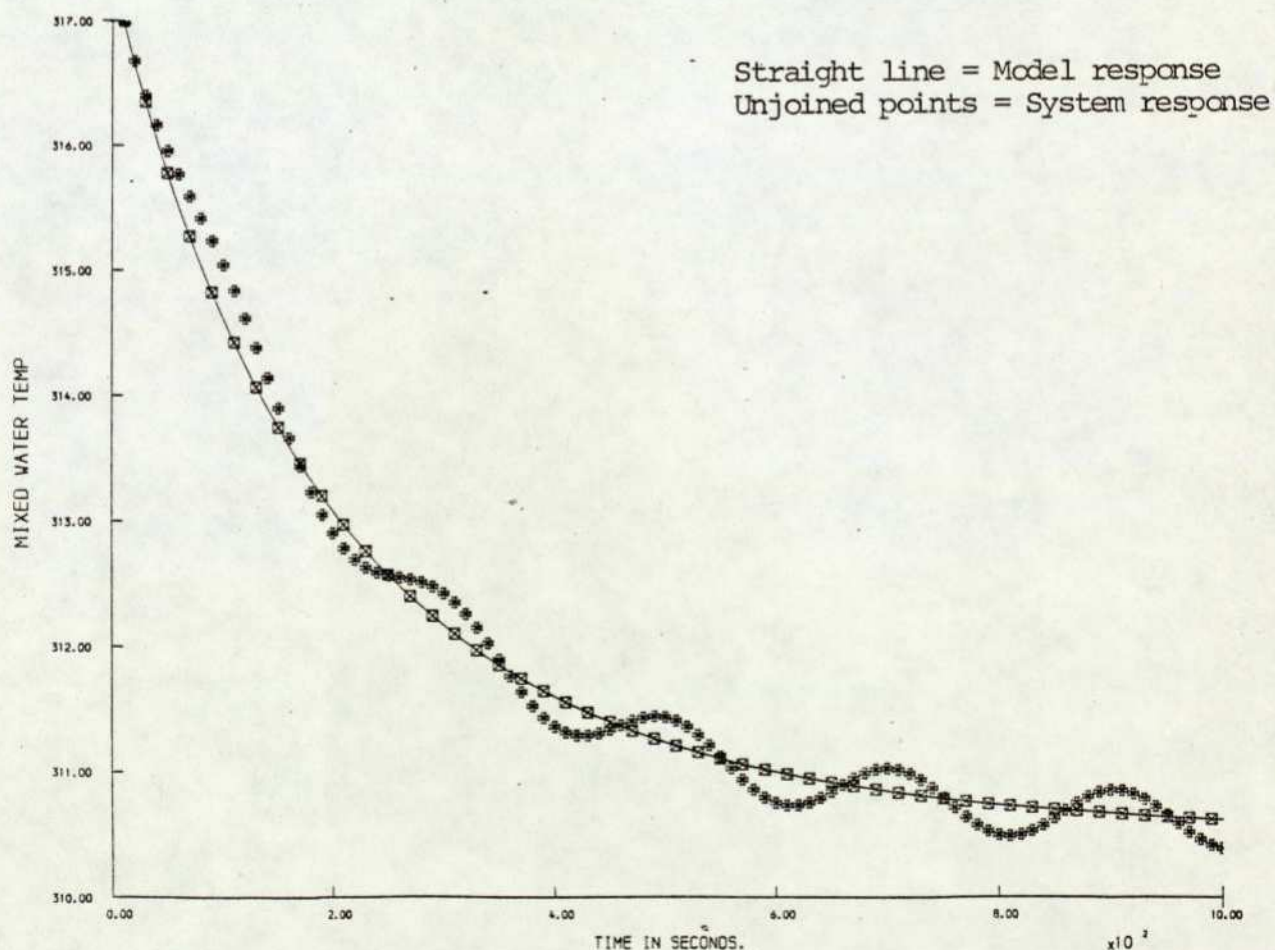


Fig.4.3.10 Open Loop Mixed Water Temperature Responses Simulated System and Identified Model of the Mixing Tank System for the Case where $W(1) = 10.0$, $W(2) = 5.0$ and $R = 20.0$.

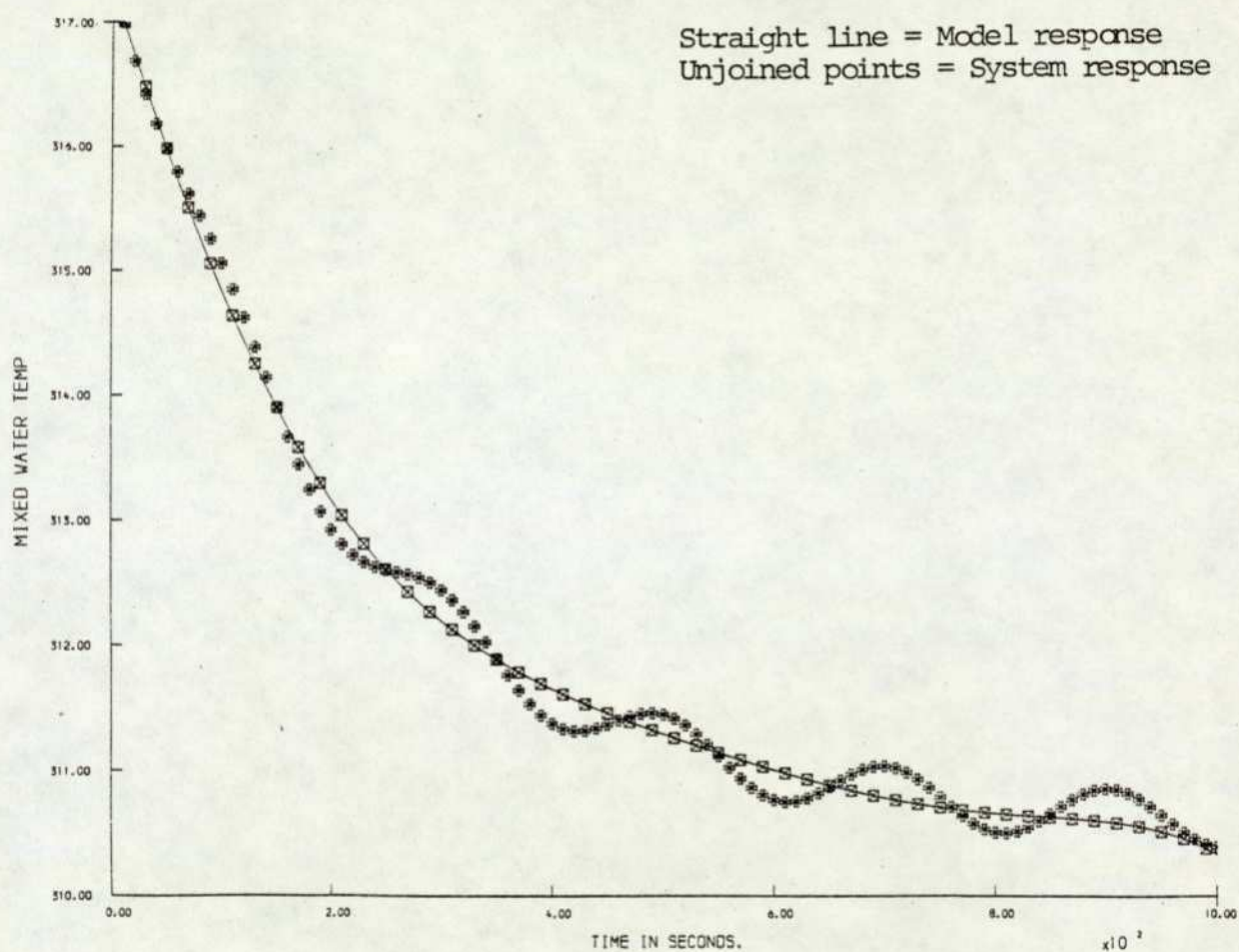


Fig. 4.3.11. Open Loop Mixed Water Temperature Responses of Simulated System and Identified Model of the Mixing Tank System where $W(1) = 10$, $W(2) = 1.0$ and $R = 20.0$

CASE	R	PRA (k_o) C.L.S.	PRA (k_o) SMLS	PRB (1)	PRB (2)	PRB (3)	PRB (4)	PRB (5)	PRB (6)	NO.OF OVERALL ITERS.	CP TIME SECS
1	1.0	0.9965	0.99994	1.000253	0.050834	-0.05518	-0.27194	0.335478	0.000371	4	48
2	10	0.9964	1.000058	1.000701	-0.002792	0.001136	-0.002548	0.0008	-0.001471	5	14
3	20	0.9965	0.999	1.000231	0.349457	-0.549379	0.746591	-0.144905	0.000315	6	73
4	100	0.9965	0.9965	1.000003	0.042942	-0.16252	0.011015	0.242383	0.000002	2	22
5	1000	0.9965	0.9965	1.0	0.0	0.0	0.0	0.0	0.0	2	26

Fig.4.3.12. Results Obtained for Varying Values of R with $W(1) = 10.0$ and $W(2) = 0.5$ using Chebychev-form Uncertainty.

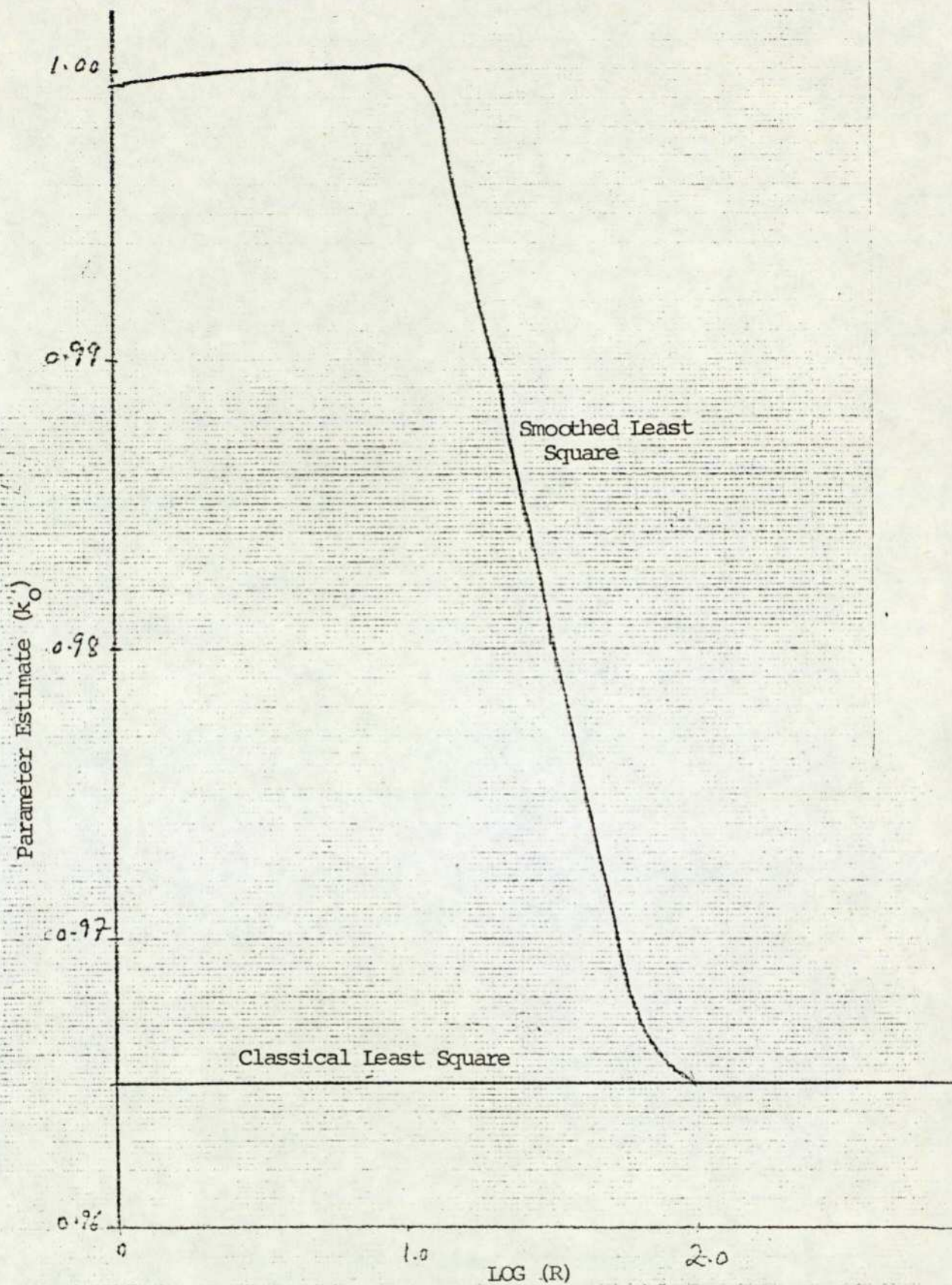


Fig.4.3.13. The Effect of R on the Parameter System k_0 obtained by C.L.S. and S.L.S. techniques for Chebychev form Uncertainty.

4.3.1b. Sinewave form uncertainty

When the time varying uncertainty is approximated to by a sinewave, thus

$$T_H = T_h \times (A+B \sin (CxT+D))$$

where A,B,C and D are the smoothing parameters whose values are estimated by the smoothing problem using the variations on the system observations, the results obtained are summarised in Table 4.3.14 for varying values of W(1) Table 4.3.18 for varying values of W(2) and Table 4.3.22 for varying values of R.

In all these cases the classical least squares solutions are the same as those obtained in the previous section for Chebychev form uncertainty. This can be explained on the basis that regardless of the form of the uncertainty, the classical least squares solution which is obtained by setting the uncertainty at its nominal value will always result in the same values for the same system since no modification or compensation for structural deficiencies has been made.

Figs. 4.3.15 and 4.3.16 show the height and the mixed water temperature responses obtained for Case 3 in Table 4.3.14. The system and model height responses are indistinguishable since the correct value of k_o has been achieved by the identification process. However the identified model hot water temperature response does not follow the variations on the corresponding system response but passes through its average trend. When the weighting

matrix associated with the errors in the height response is increased to 100 (Case 5) in Table 4.3.14, the correct value of k_o has been achieved as well as the variations on the mixed water temperature response. Fig. 4.3.17 reflects the model ability to predict these variations although the height of these sinusoidal variations is not the same as that of the system variations.

Now the mixed water temperature responses corresponding to Case 4 in Table 4.3.18 are shown in Fig. 4.3.19. The remarkable achievement of the smoothed least squares technique is reflected by the full agreement between the simulated system and the identified model responses. The height responses which are not shown here, since they are similar to those of Fig. 4.3.15, are also indistinguishable because the correct value of k_o has been achieved by the smoothed least squares technique.

On the contrary, for Case 6 where $W(2)$ has been increased to 5.0, inaccurate estimate of k_o has resulted in clear disagreement between the simulated system and identified model height responses shown in Fig. 4.3.20. For the same case, the mixed water temperature responses are shown in Fig. 4.3.21. Although some variations have been predicted by the smoothed least squares technique, their frequency and amplitude differ from those of the system.

From this it can be said that weighting matrices have a crucial effect on the outcome of the identification process.

Table 4.3.22 shows the effects of the variation of R (the weighting matrix associated with the errors between the value of the time-dependent uncertainty and its nominal trajectory) on the parameter estimates obtained by the classical least squares and the smoothed least squares technique. Again, at low values of R , the smoothed least squares technique has yielded improvements in the values of the parameter estimates obtained by the classical least squares technique, whilst at high values of R (100, 500 and 1000) no improvement has been obtained. As has been said in the Chebychev-form uncertainty case, this may be explained on the basis that at very high values of R , reduction in the value of the uncertainty part of the objective function can be achieved by keeping the value of the time-dependent uncertainty as close as possible to its nominal value, thus the weighted squares of errors are very close to zero.

Generally it can be said that with the sinewave form uncertainty the smoothed least squares technique results in slight improvements over the classical least squares solutions for the parameter estimate of k_0 . These improvements are of the same magnitude as those obtained using Chebychev-form uncertainty. The results obtained for varying values of $W(1)$, $W(2)$ and R are almost identical to those already discussed in Section 4.3.1a).

An important difference is the computing time required by the identification process in the two cases. The Tables show that, generally, the sinewave type of uncertainty requires a larger computing time to converge than does the Chebychev-type.

CASE	W (1)	PRA (k_o) C.L.S.	PRA (k_o) S.L.S.	PRB (1)	PRB (2)	PRB (3)	PRB (4)	NO. OF OVERALL ITERS.	C.P. TIME SECS.
1	0.1	0.9503	0.9543	1.00	-0.00067	0.000244	0.000437	3	51
2	1.0	0.9563	1.00043	1.000127	0.004362	0.031312	0.074486	16	255
3	10	0.9965	0.999	1.000245	0.000966	0.625273	0.066669	6	197
4	20	0.999	0.99994	1.008877	0.009193	-0.001218	-0.873279	16	240
5	100	0.99989	0.99997	1.000143	-0.00468	-0.031304	-0.72504	5	122

Table 4.3.14 Results Obtained for Varying Values of W(1) with W(2) = 0.5 and R = 20
for the Sinewave-form Uncertainty.

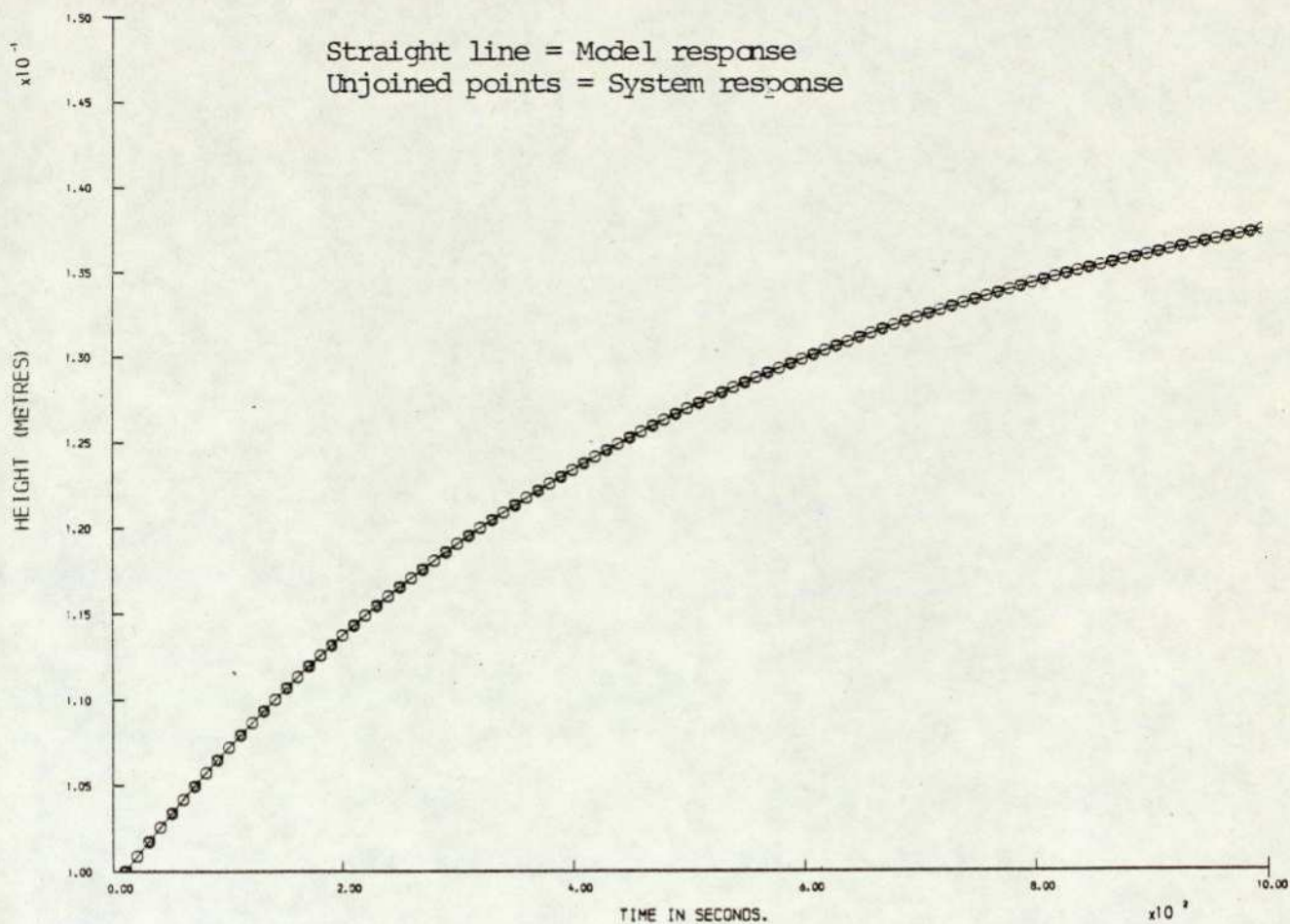


Fig.4.3.15 Open Loop Height Responses of Simulated System and Identified Model of the Mixing Tank for the case where $W(1) = 10.0$, $W(2) = 0.5$ and $R = 20.0$

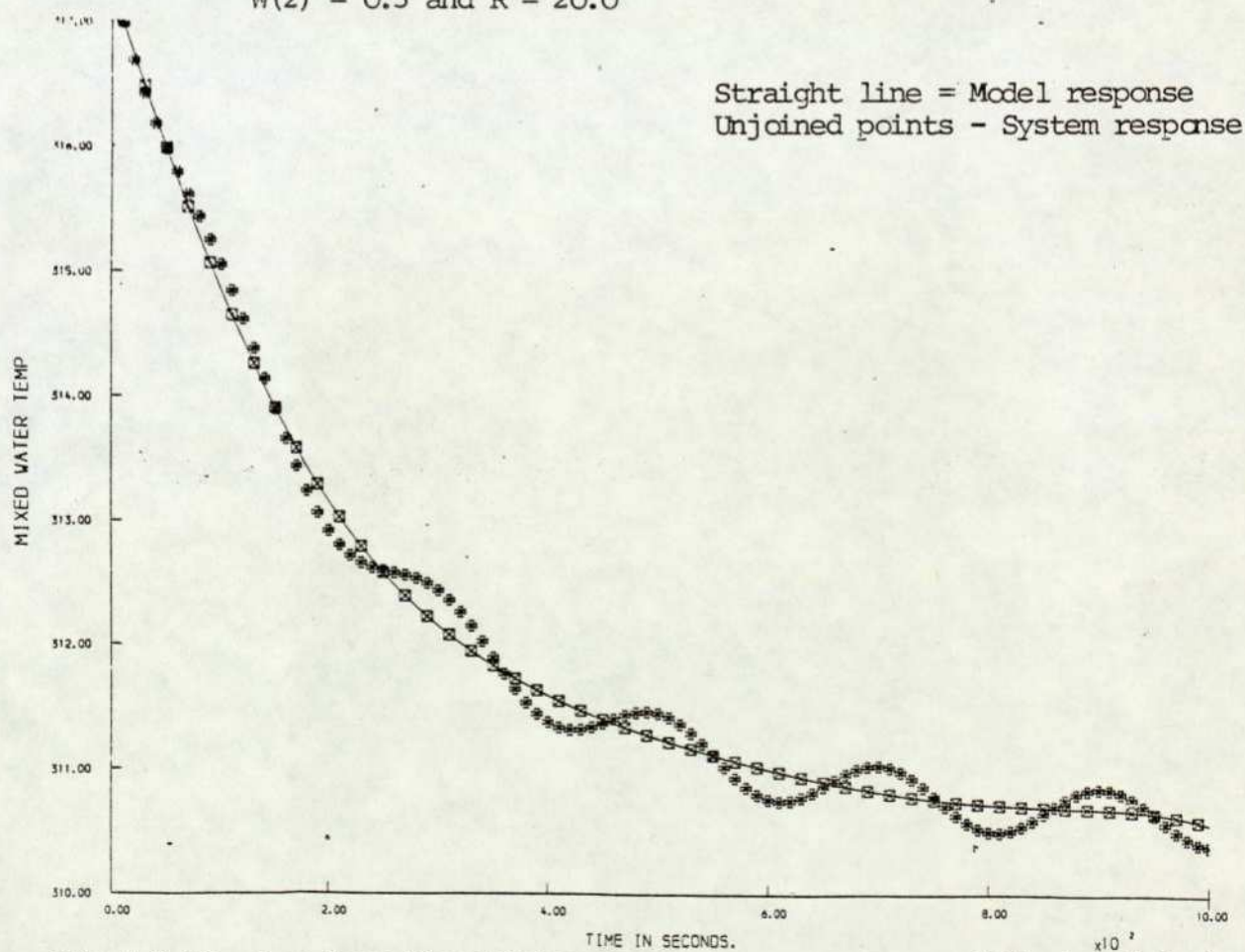


Fig.4.3.16. Open Loop Mixed Water Temperature responses of Simulated System and Identified Model of Mixing Tank for the case where $W(1)=10.0$, $W(2) = 0.5$ and $R = 20.0$.

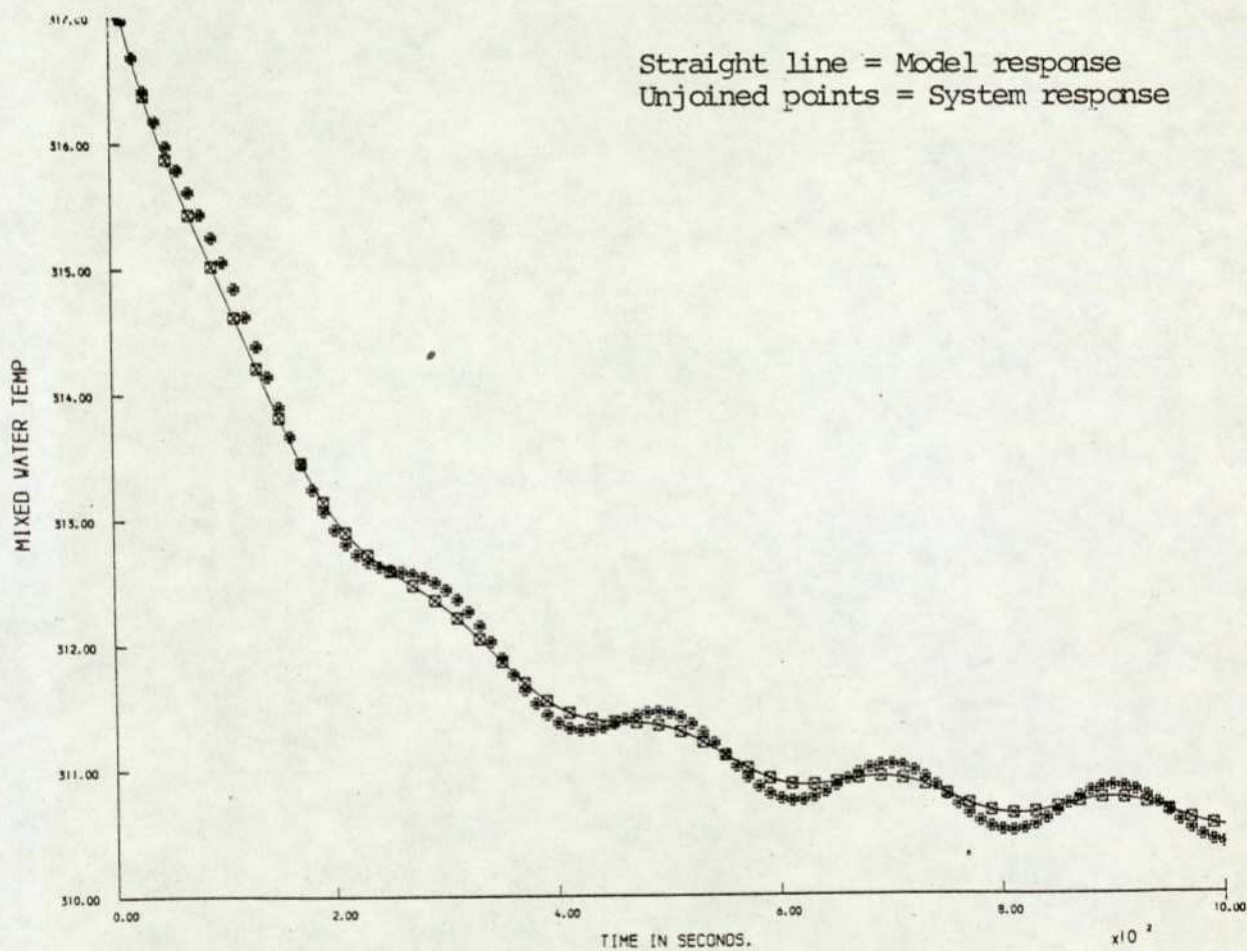


Fig.4.3.17. Open Loop Mixed Water Temperature Responses of Simulated System and Identified Model of the Mixing Tank for the case where $W(1) = 100$, $W(2) = 0.5$ and $R = 20$.

CASE	W (2)	PRA(k_o) C.L.S.	PRA(k_o) S.L.S.	PRB(1)	PRB(2)	PRB(3)	PRB(4)	NO. OF OVERALL ITERS.	C.P. TIME SECS.
1	0.1	0.999784	0.999784	1.0	0.0	0.0	0.0	2	28
2	0.5	0.996	0.999	1.000245	0.000966	0.625273	0.066669	6	197
3	0.75	0.9928	0.9996	1.000136	-0.000118	-0.298335	0.196652	6	89
4	1.0	0.9887	1.0008	1.000057	-0.007744	-0.031394	-0.042036	4	97
5	2.0	0.9738	1.0022	1.000035	-0.009231	-0.031405	-0.01309	8	228
6	5.0	0.9568	0.9648	1.000023	0.005753	0.08992	-0.122755	10	840

Table 4.3.18 Results Obtained for Varying Values of W(2) with W(1) = 10.0 and R = 20.0
for Sinewave-form Uncertainty

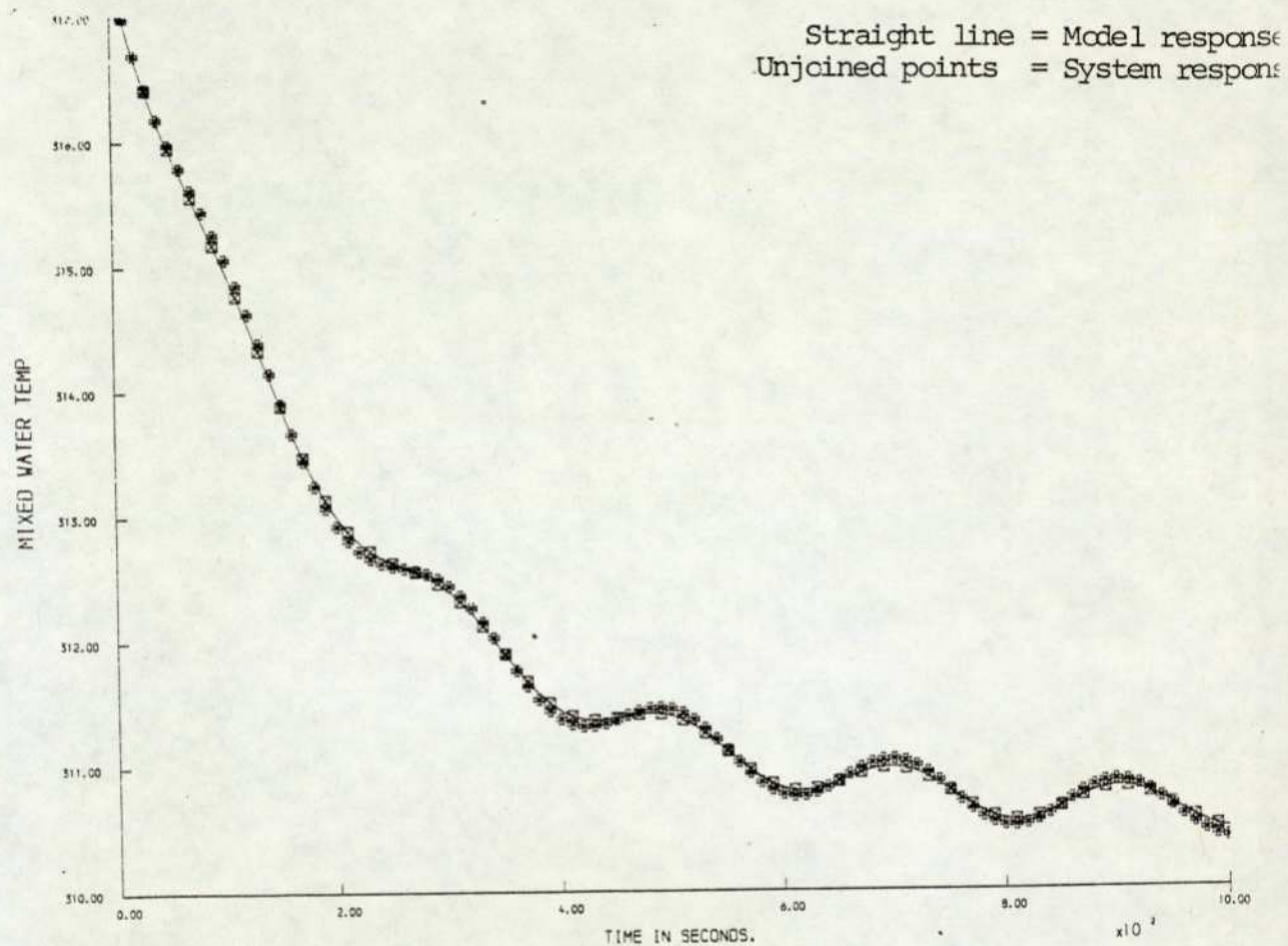


Fig. 4.3.19. Open Loop Temperature Responses of Simulated System and Identified Model of Mixing Tank for the case where $W(1) = 10.0$, $W(2) = 1.0$ and $R = 20.0$.

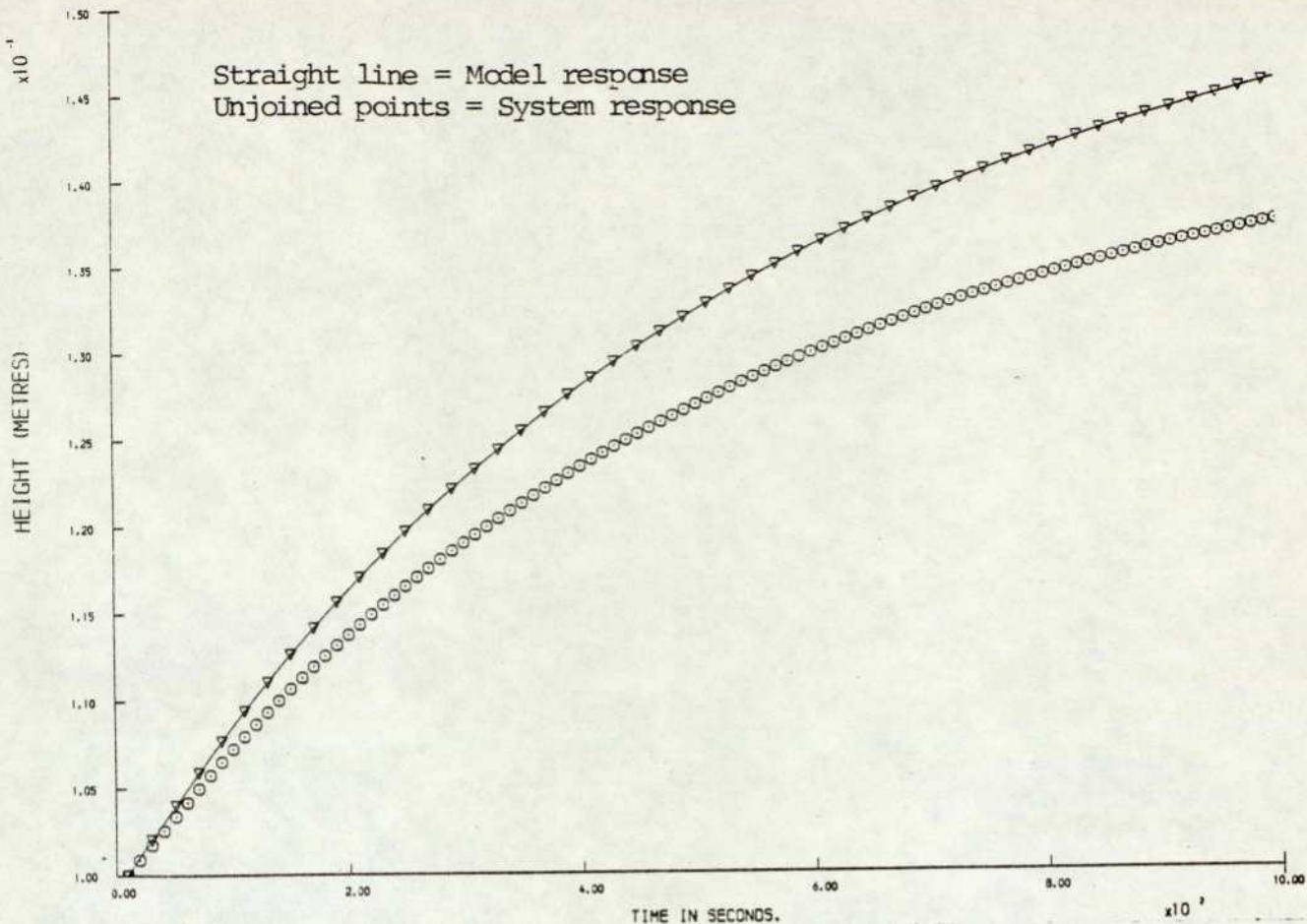


Fig.4.3.20. Open Loop Height Responses of Simulated System and Identified Model of Mixing Tank for the Case where $W(1) = 10.0$, $W(2) = 5.0$, and $R = 20.0$.

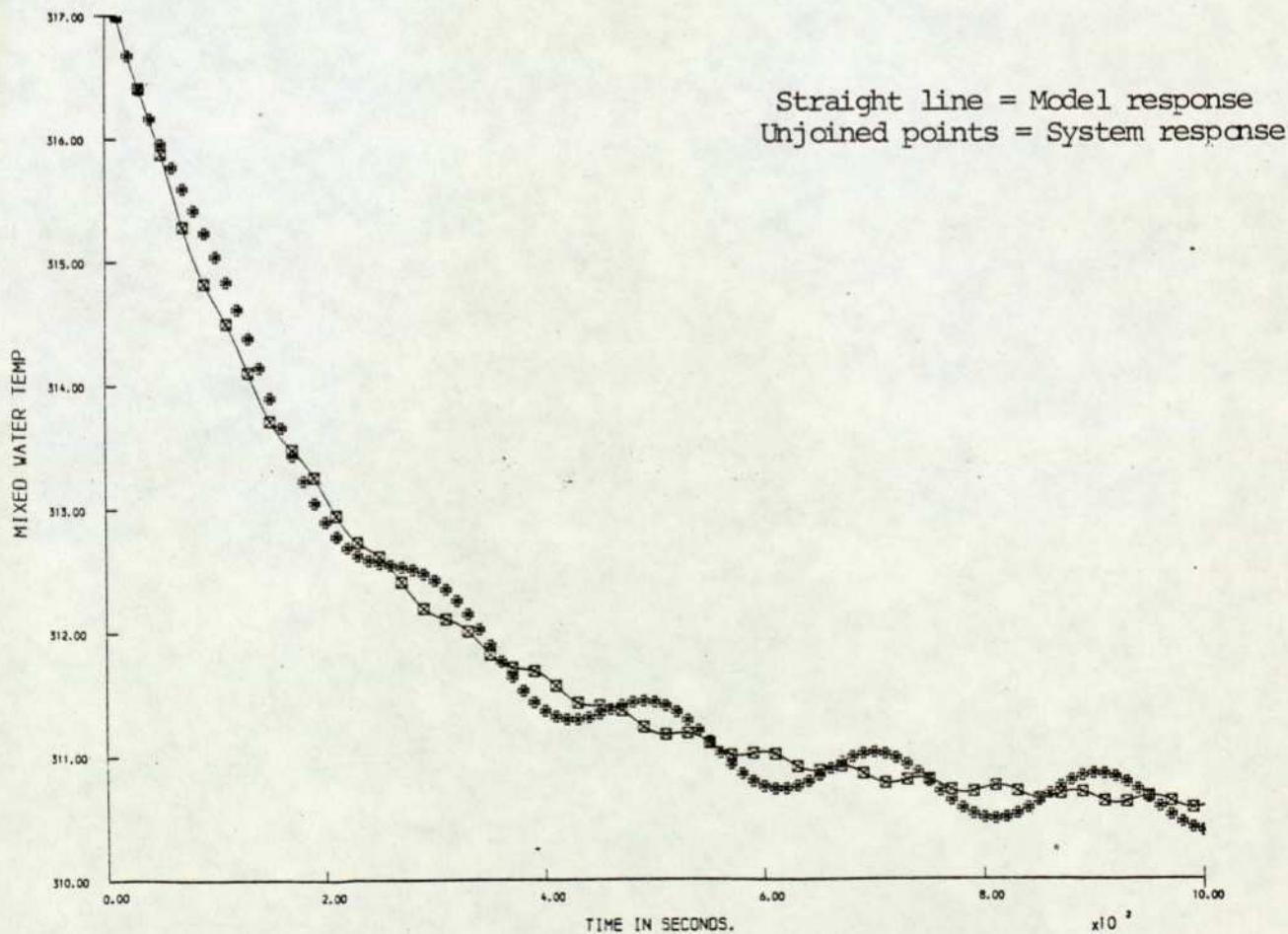


Fig.4.3.21. Open Loop Mixed Water Temperature Responses Simulated System and Identified Model of the Mixing Tank for the case where $W(1)=10.0$, $W(2) = 5.0$ and $R = 20.0$.

CASE	R	PRA (k_o) C.L.S.	PRA (k_o) S.L.S.	PRB (1)	PRB (2)	PRB (3)	PRB (4)	NO. OF OVERALL ITERS	C.P. TIME SECS
1	1.0	0.9966	0.9992	1.00021	-0.0005789	-0.103009	0.15303	4	102
2	10	0.996	0.999	1.000245	0.000966	0.625273	0.066669	6	177
3	20	0.996	0.9996	1.000181	-0.001755	-0.031263	-0.109485	5	150
4	100	0.996	0.996	1.0	0.0	0.0	0.0	2	40
5	500	0.996	0.996	1.0	0.0	0.0	0.0	2	25
6	1000	0.996	0.996	1.0	0.0	0.0	0.0	2	29

Table 4.3.22 Results Obtained for Varying Values of R with $W(1) = 10.0$, $W(2) = 0.5$ for
sinewave-form Uncertainty.

Another important difference is the ability of the smoothed least squares technique to produce accurate estimates of the unknown parameter (k_o) as well as accurate estimates of the smoothing parameters given the proper form of the uncertainty and the proper weighting matrices.

Comparison between the two techniques

A comparison between the classical least squares solution which takes place in one overall iteration, and the smoothed least squares solution which comprises of several overall iterations can be made with reference to Figs. 4.3.24, 4.3.26, 4.3.28, 4.3.30 and 4.3.32. In all these graphs, the values of the parameter estimate k_o (PRA) and the objective function after each overall iteration (an overall iteration is one which comprises of the solution parameter estimation problem followed by the solution of the smoothing problem) are plotted against the number of overall iterations for the two cases of sinewave form and Chebychev form uncertainties. Each graph represents a set of weighting matrices.

Fig 4.3.24 which is for the nominal weightings, that is, $W(1) = 10.0$, $W(2) = 0.5$ and $R = 20.0$, shows that most of the work of reducing the objective function has been carried out by the classical least squares and that further iterations whilst slightly modifying the parameter estimate resulted in only slight reduction in the objective function. The graph also shows that with small numbers of overall iterations, the use of Chebychev polynomial resulted in a better parameter estimate and lower value of objective function.

The resulting time dependent uncertainties are shown in Fig. 4.3.25. Neither of the two forms of the uncertainty is similar to the real sinusoidal variations shown in Fig. 3.7.

For small value of $W(1)$ Fig. 4.3.26 shows the performances of the classical least squares and the smoothed least squares techniques. In this case although the sinewave form uncertainty required many overall iterations and thus more computing time, the results obtained by the smoothed least squares technique were remarkably better than those yielded by the same technique but with Chebychev type uncertainty. The smoothed least squares solution using sinewave form uncertainty has improved significantly both on the parameter estimate (k_0) bringing its classical least squares estimate of approximately 0.9555 up to approximately the true value of 1.0 and on the objective function.

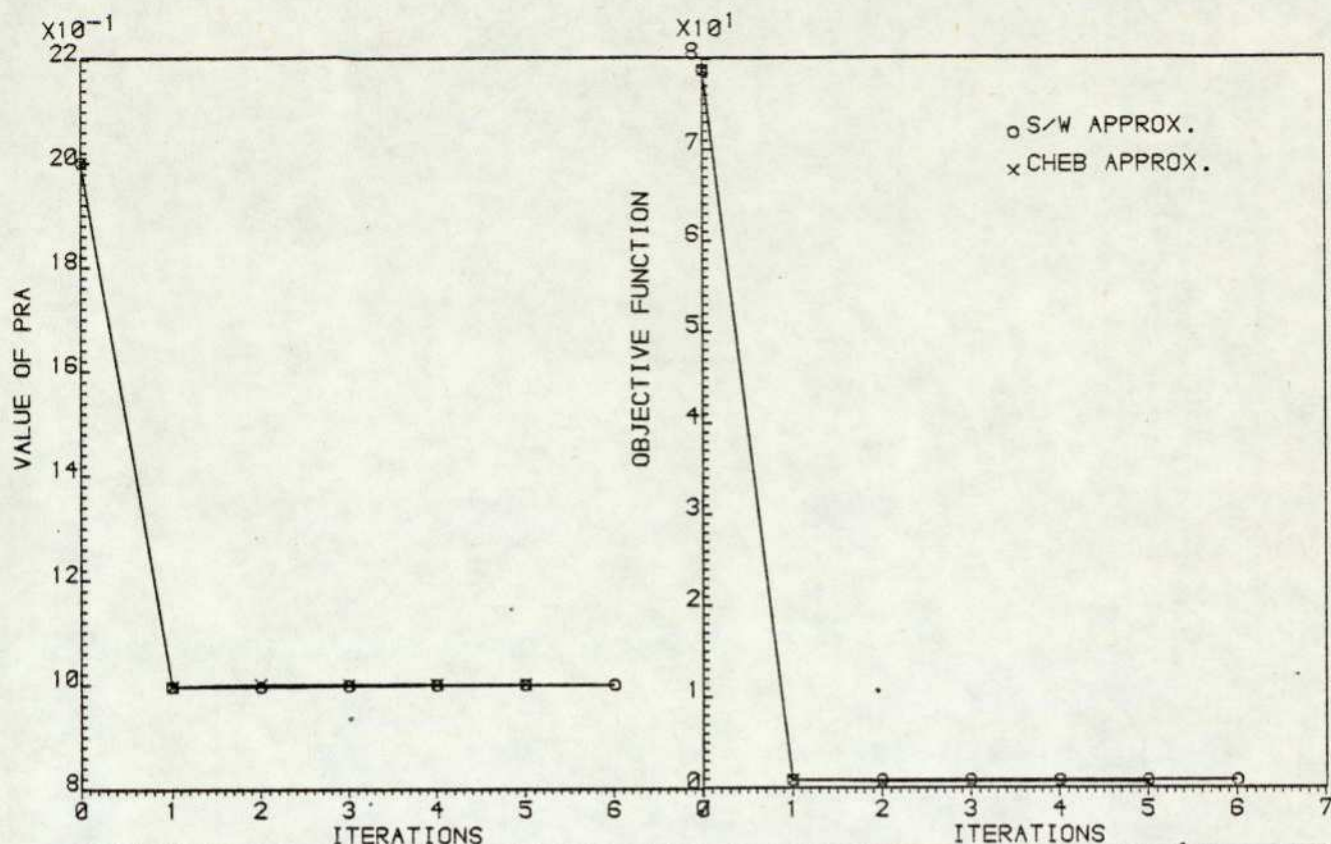
In fact, the exact form of the uncertainty has been produced by the smoothed least squares though its amplitude is lower than the real value. On the other hand, the use of Chebychev form uncertainty could not yield the accurate form of the uncertainty.

For large value of $W(1)$, Fig. 4.3.28 shows the performance of the classical least squares and the smoothed least squares techniques. As mentioned before, the classical least squares yielded almost the accurate solution leaving no work to be done by the smoothed least squares technique which went through 14 overall iterations (for the case of sinewave form uncertainty). With only five overall iterations, the use of Chebychev form uncertainty resulted in slightly better parameter estimate and objective function.

However although the improvement produced by the smoothed least squares technique (in the case of Chebychev form) on the value of k_0 has been slight (due to the fact that the classical least squares technique has already produced estimates close to the accurate value leaving no room for much improvement) good estimates have been obtained for the coefficients of the sinewave form uncertainty giving the time varying uncertainty in Fig.4.3.29b. The use of Chebychev form uncertainty has contributed to the improvement on the estimate of k_0 but could not predict the correct form of the uncertainty.

Now when $W(2)$ is increased to 5.0, that is, the weighting of the errors between the mixed water temperature system and model responses, the behaviour of the two techniques is given by Fig.4.3.30. The classical least squares estimate is not accurate, and thus the smoothed least squares technique has gone through several overall iterations (for both forms of uncertainty) resulting in slightly improved estimates, but not the accurate ones. The use of sinewave form uncertainty has yielded better estimate and thus lower value of objective function. The lengthy attempts of the smoothed least squares to enhance on the value of k_0 (in both forms of uncertainty) have resulted in estimates of the smoothing parameters which have produced the time-varying uncertainties shown in Fig. 4.3.31. Again, the use of the sinewave-form of uncertainty has resulted in sinusoidal variations similar to those of the system but of different values of amplitude and frequency. A better value of $W(2)$ which has resulted in accurate parameter estimates as well as of uncertainty is 1.0. Fig.4.3.32 shows the behaviour of the two techniques using both forms of uncertainty. The smoothed least squares technique has improved on the classical least squares estimate in

both cases with a corresponding reduction in the objective function. The use of sinewave form uncertainty has resulted in better parameter estimate and more accurate form of uncertainty as shown in Fig. 4.3.33. Again the use of Chebychev form uncertainty has resulted in accurate parameter estimate but could not produce the accurate form of the uncertainty.



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE

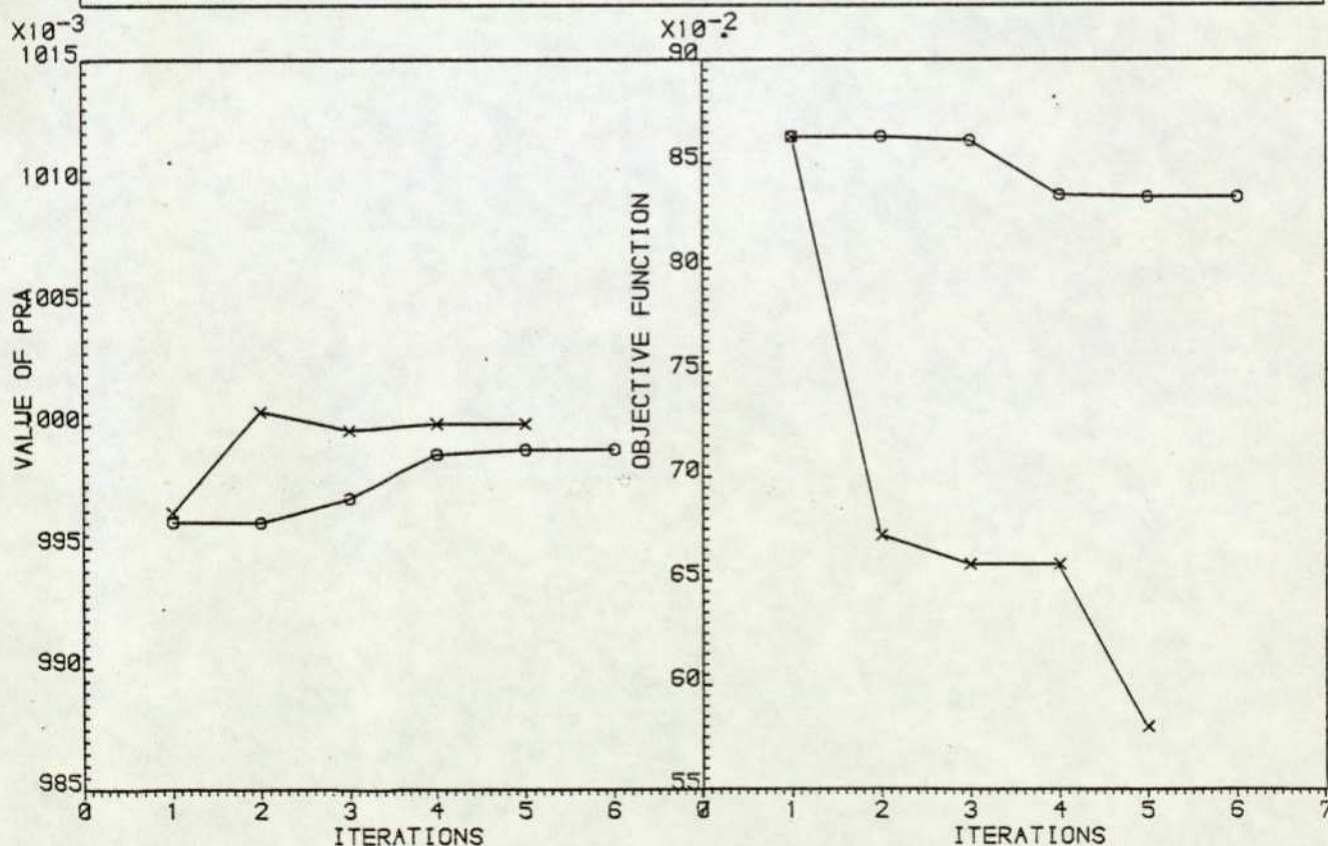
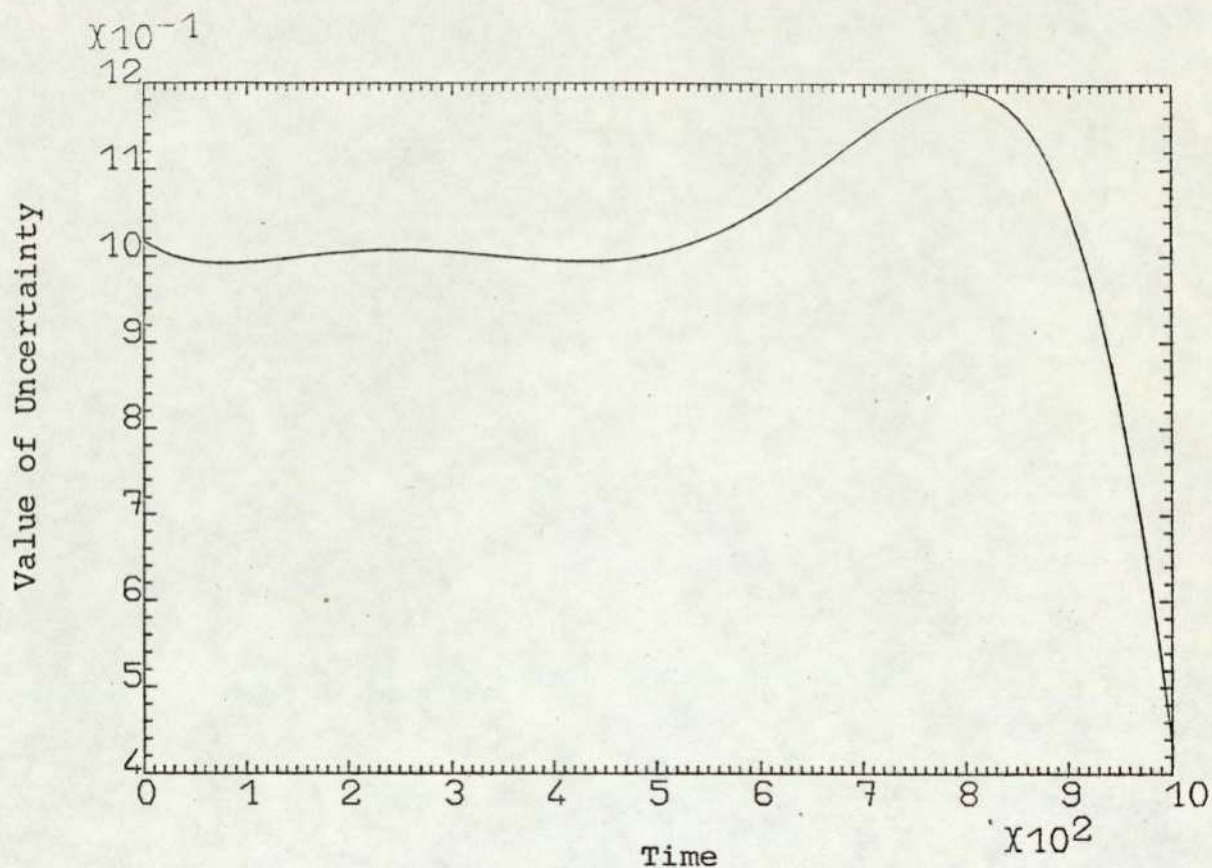
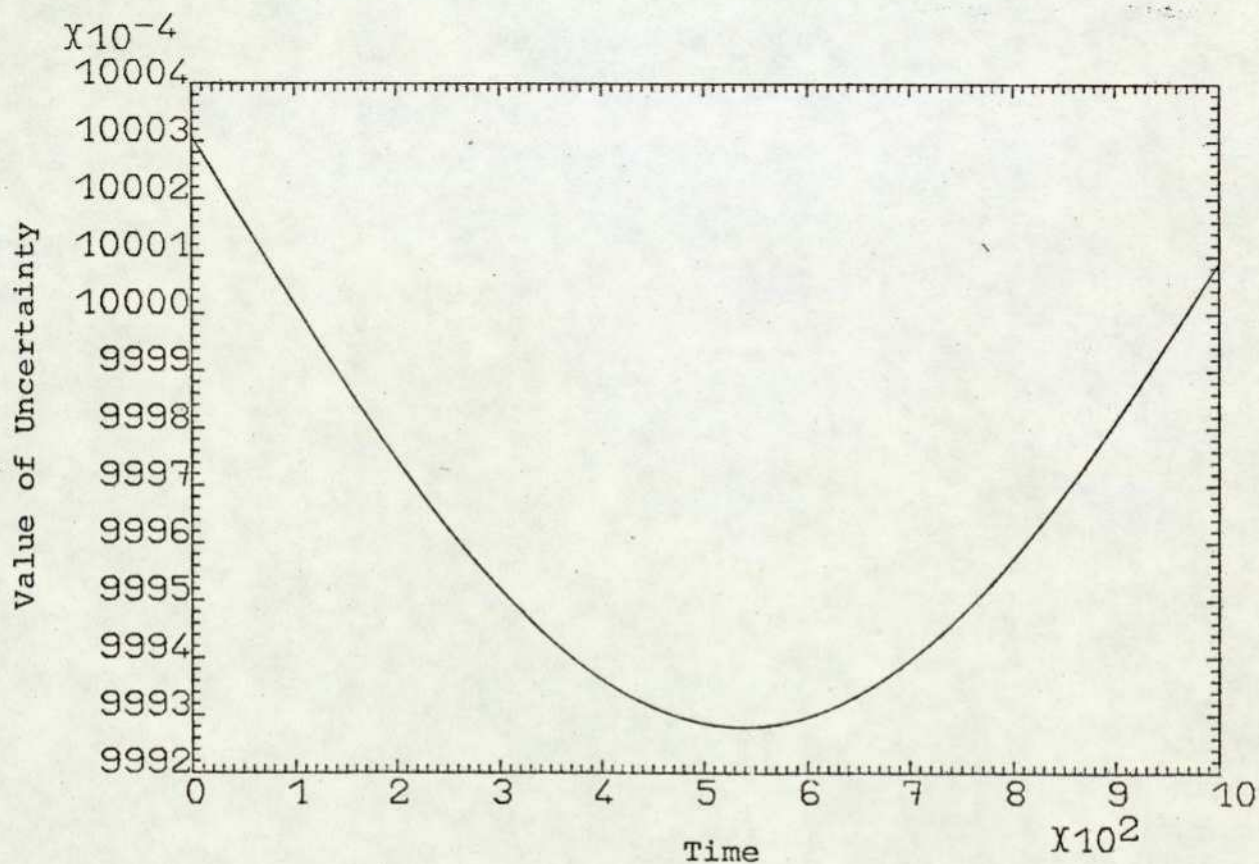


Fig. 4.3.24. The Performances of the Classical Least Squares and the Smoothed Least Squares for the Weightings of $W(1) = 10$, $W(2) = 0.5$ and $R = 20.0$.

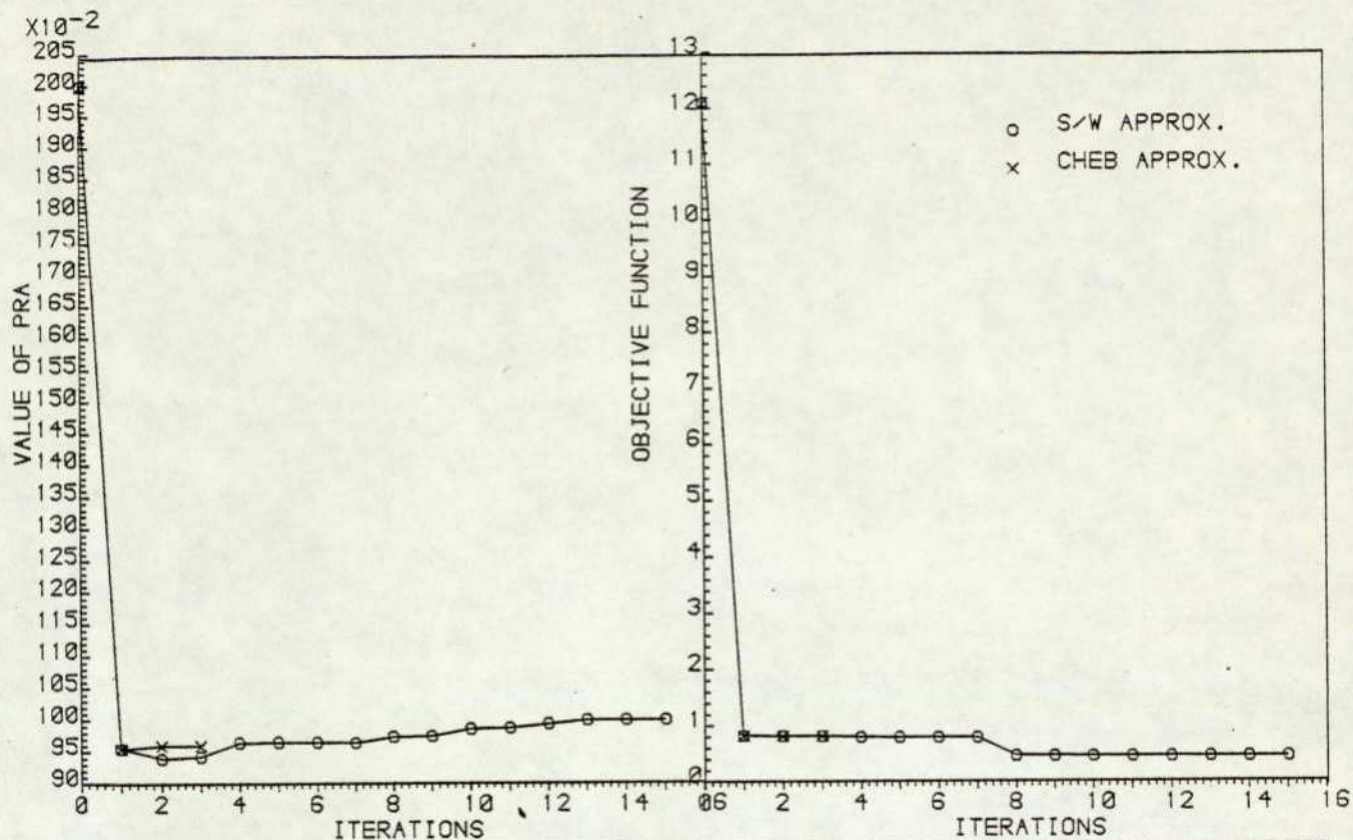


(c) Chebychev form Uncertainty



(d) Sinewave form Uncertainty

Fig.4.3.25 The Two Forms of Time Dependent Uncertainties the Smoothing Parameters Correspond to Fig.4.3.24 .



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE.

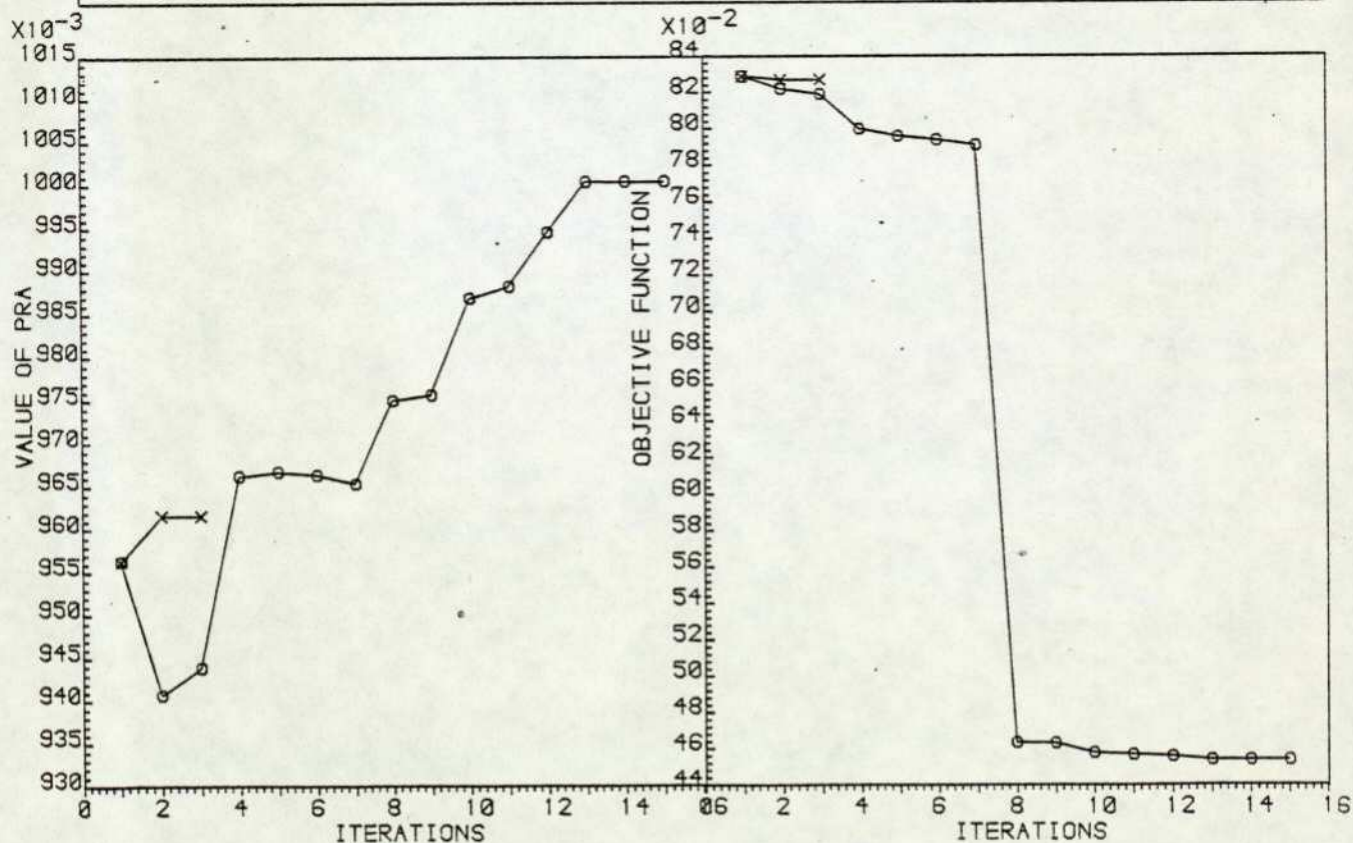


Fig.4.3.26 The Performances of the C.L.S. and S.L.S. Techniques for weightings of $W(1) = 10$, $W(2) = 0.5$, $R = 20.0$.

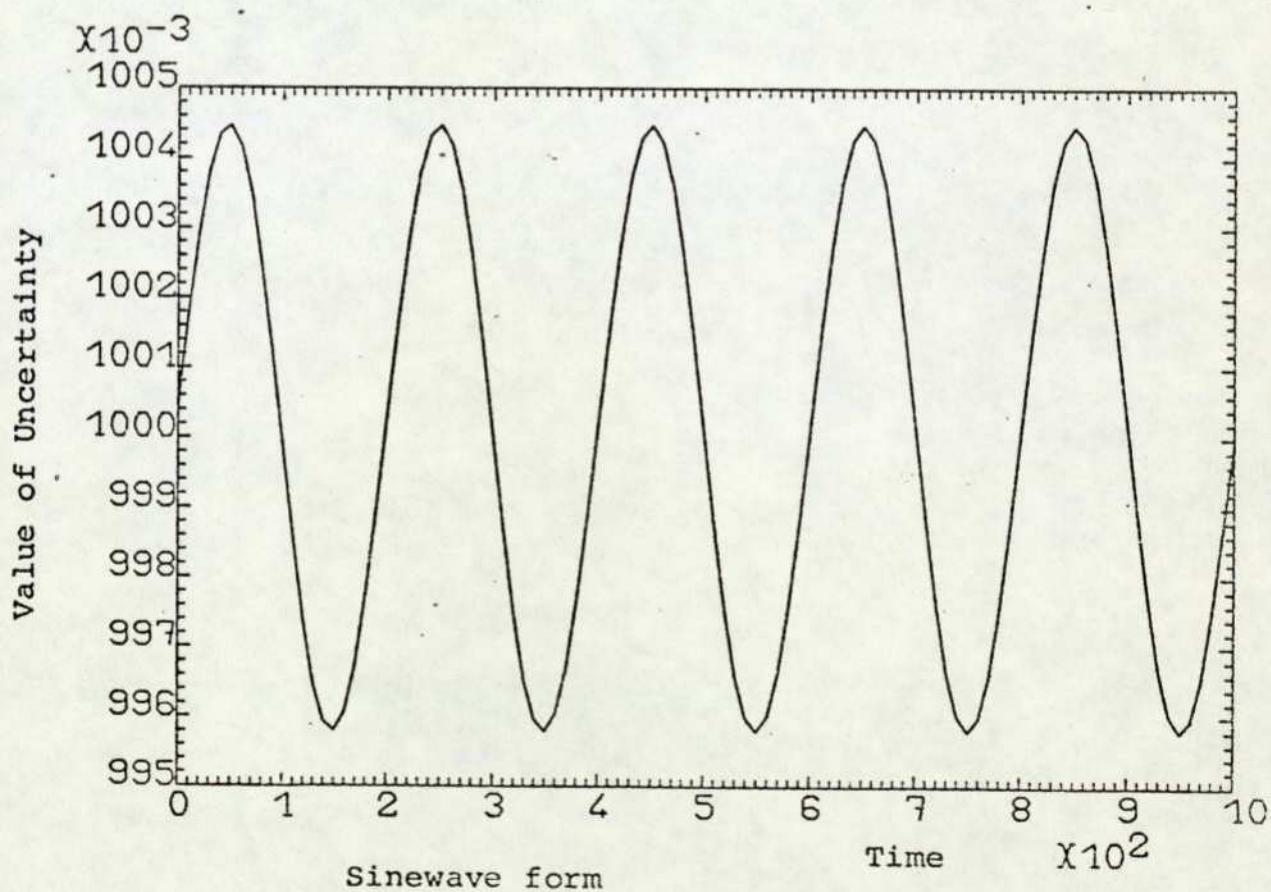
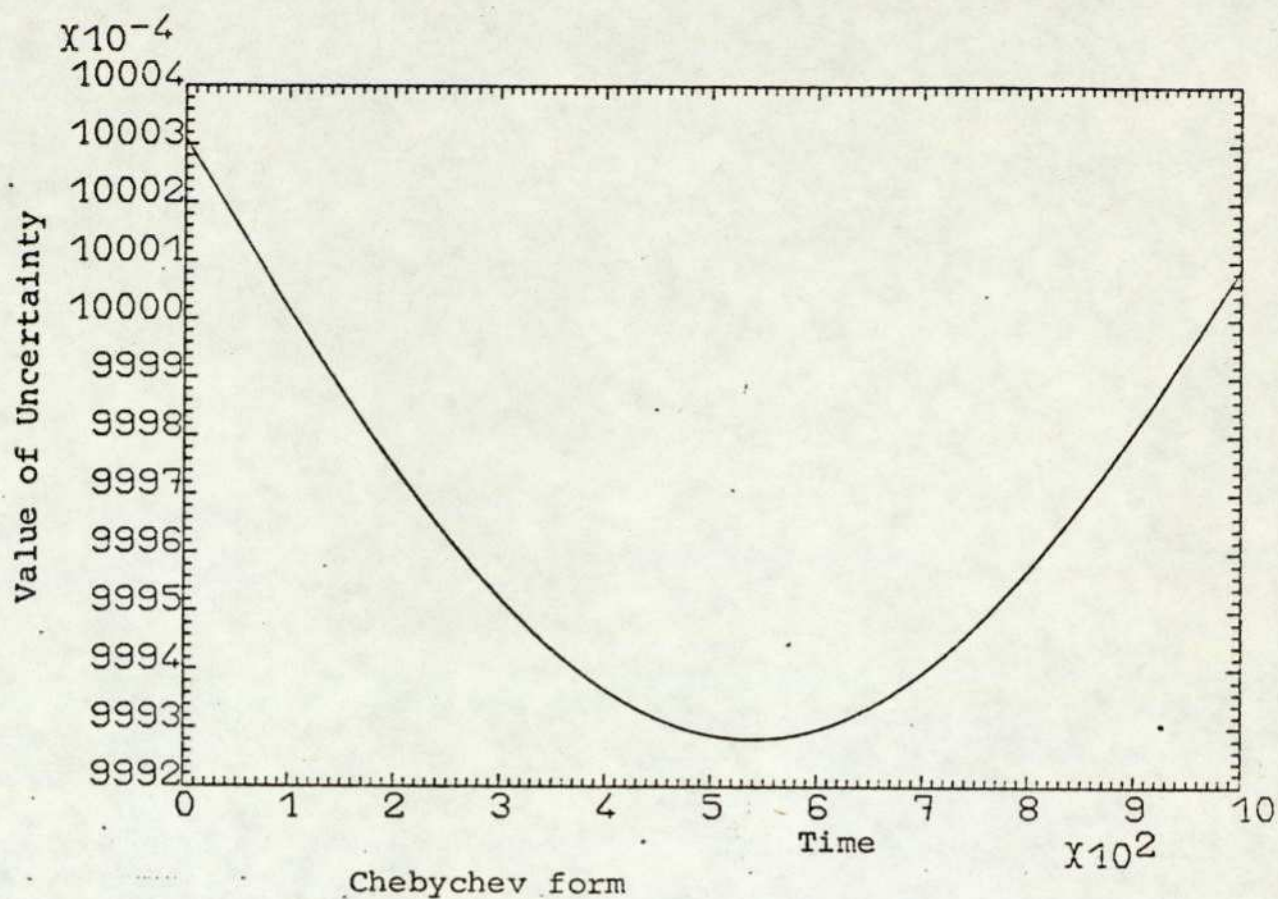
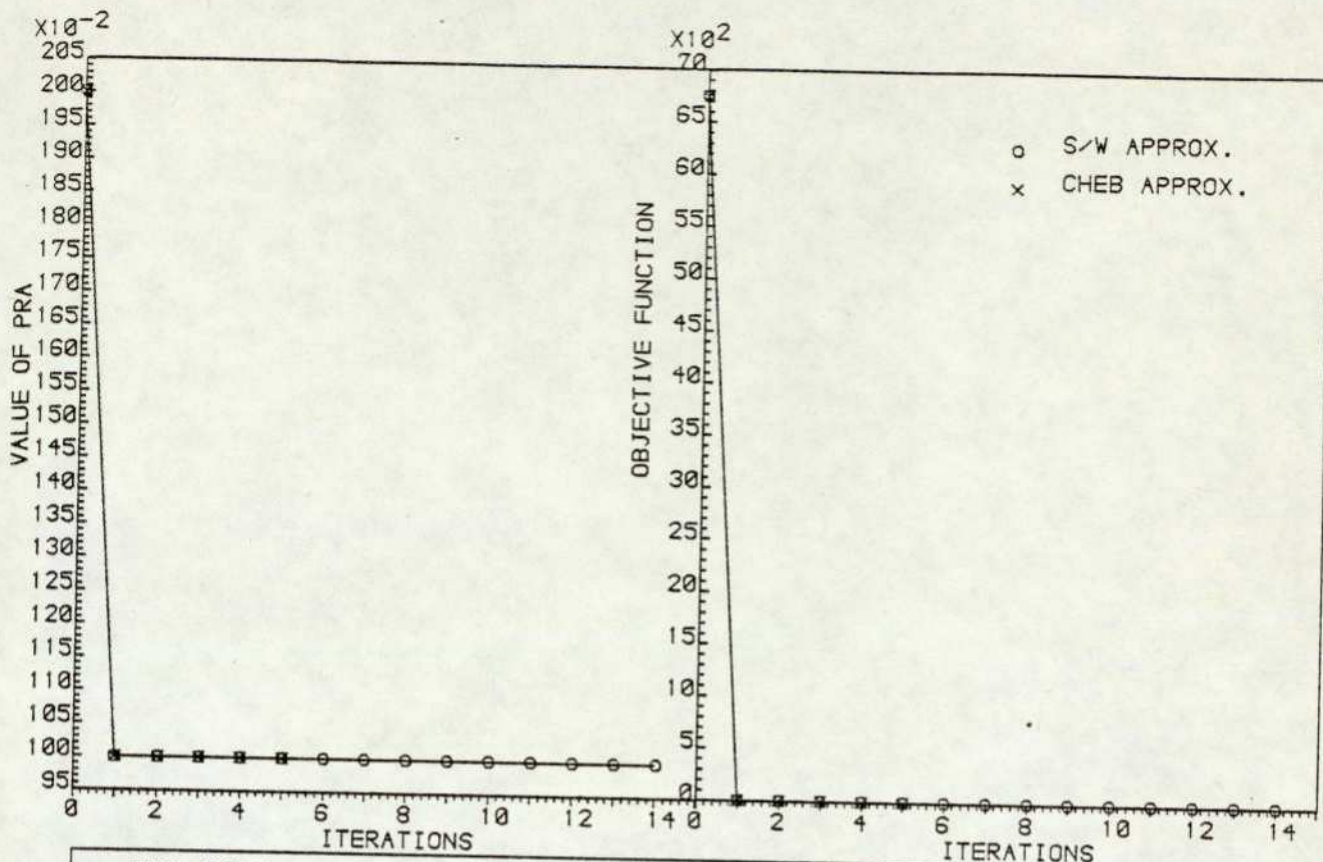


Fig.4.3.27. The Resulting Uncertainties obtained using the smoothing Parameters corresponding to Fig.4.3.26.



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE

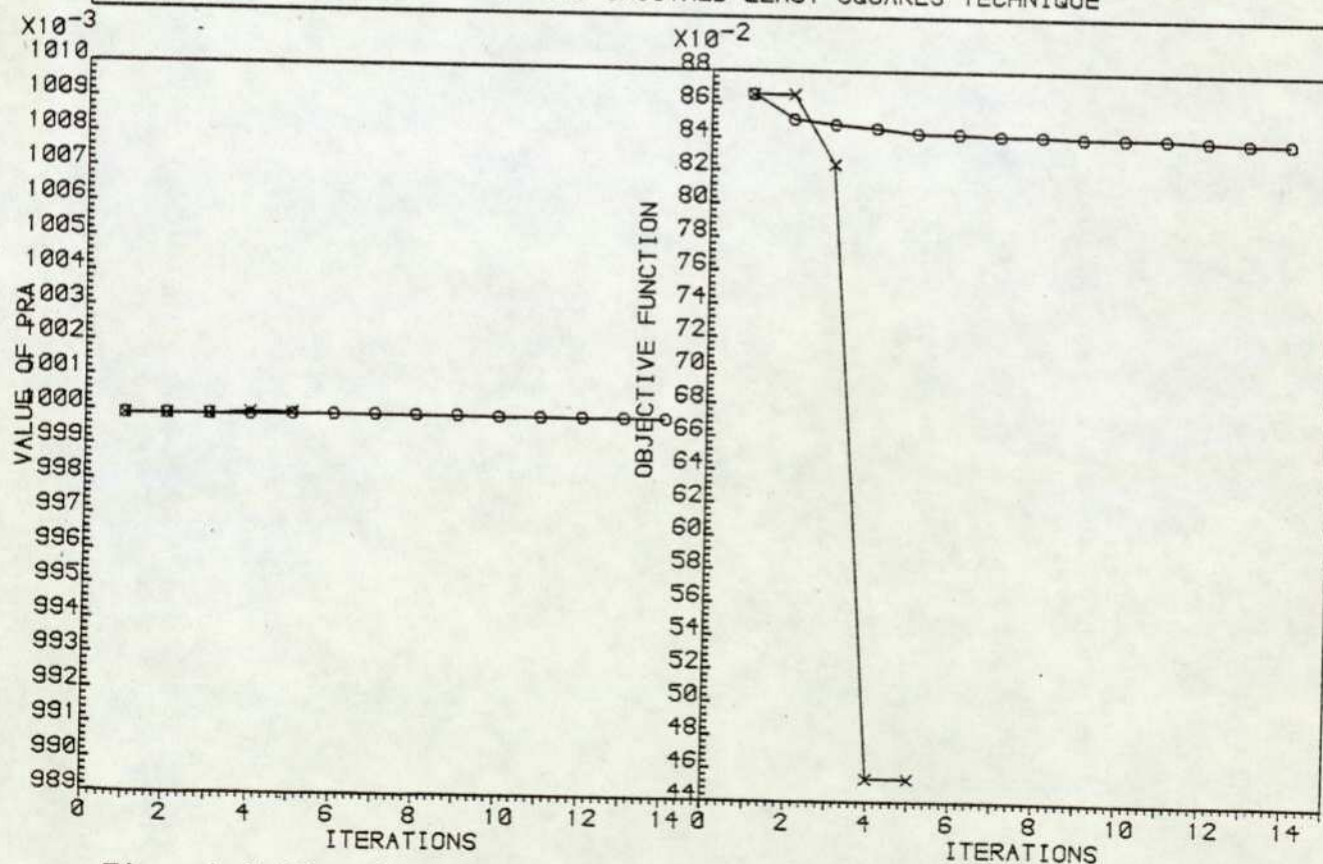
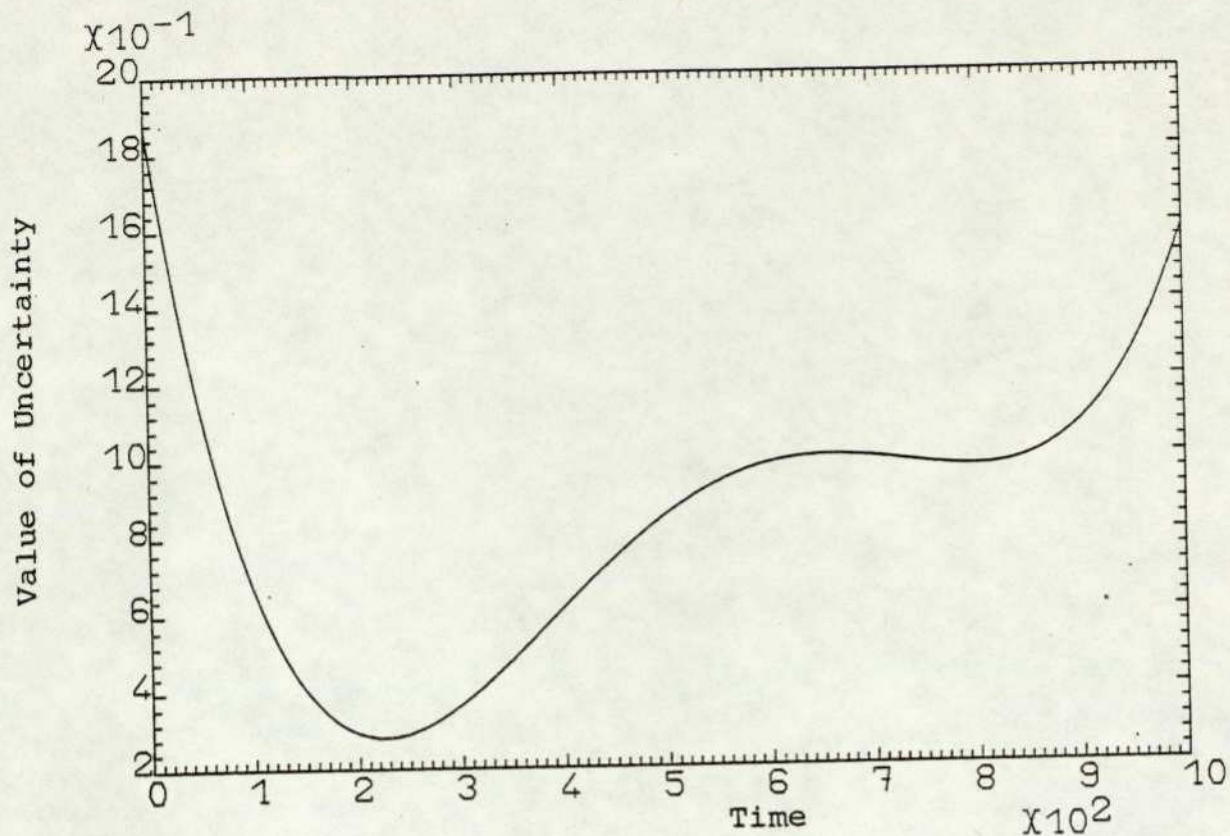
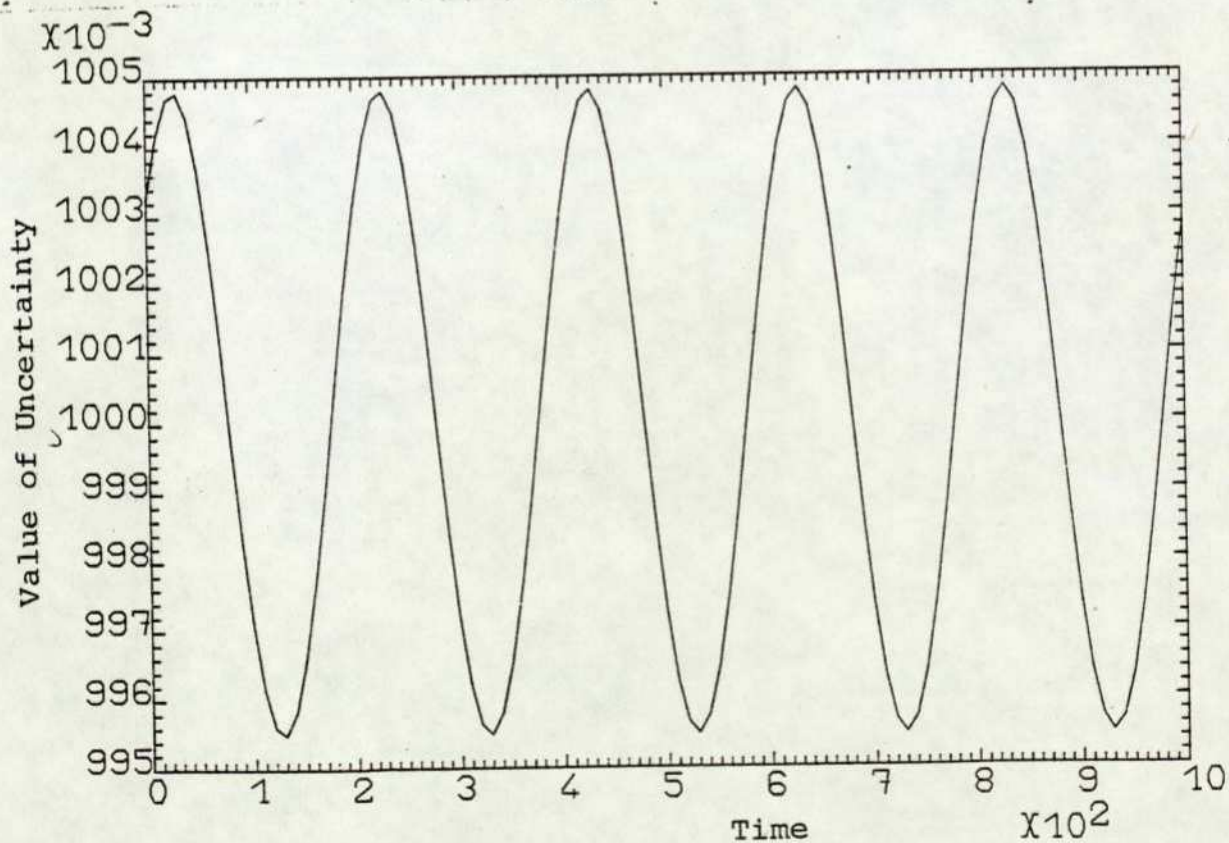


Fig. 4.3.28 The Performances of C.L.S. and S.L.S. techniques for $W(1) = 100.0$, $W(2) = 0.5$ and $R = 10.0$.

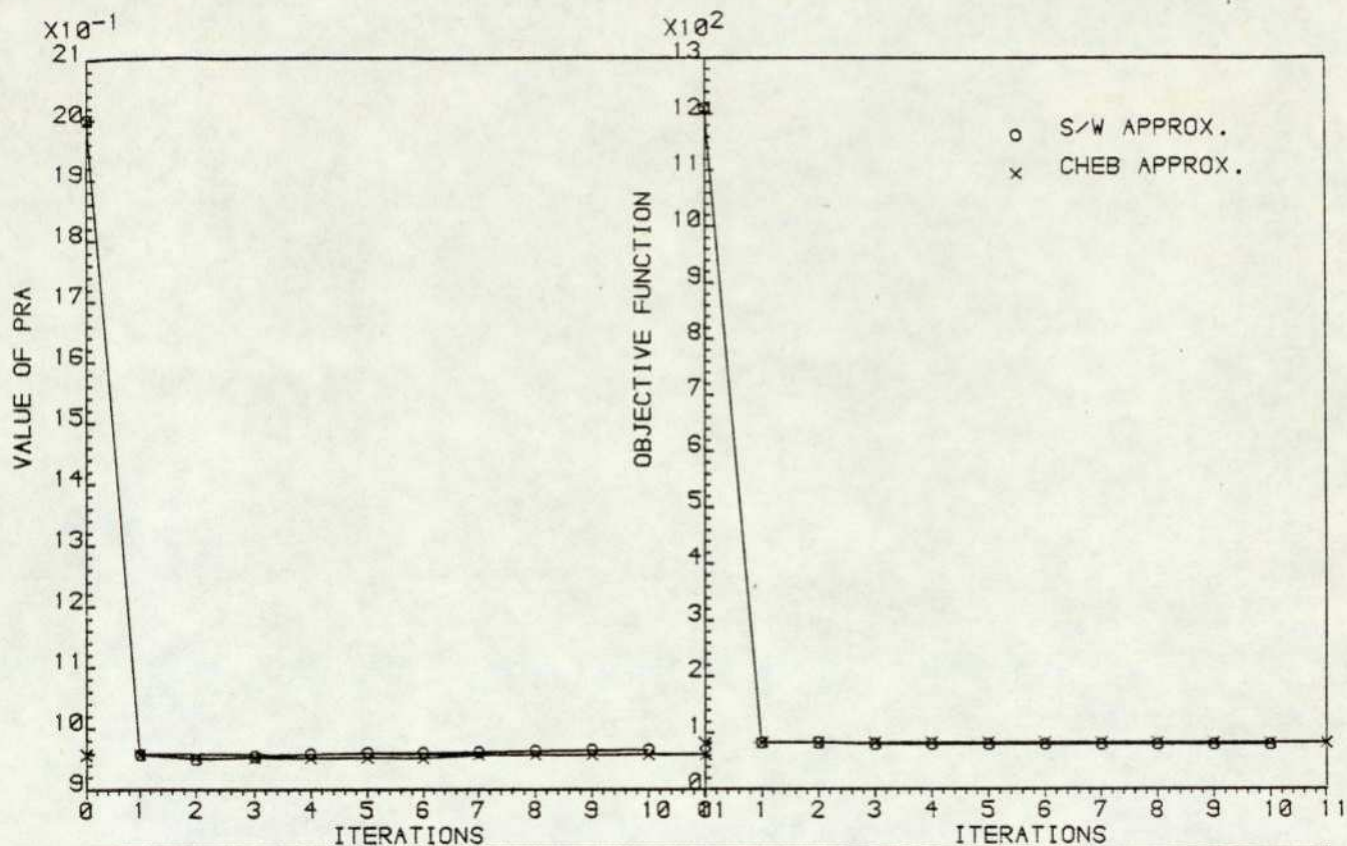


Chebychev Form



Sinewave Form

Fig.4.3.29. The Resulting Uncertainty using the Converged Estimates of the Smoothing Parameters corresponding to Fig.4.3.28.



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE

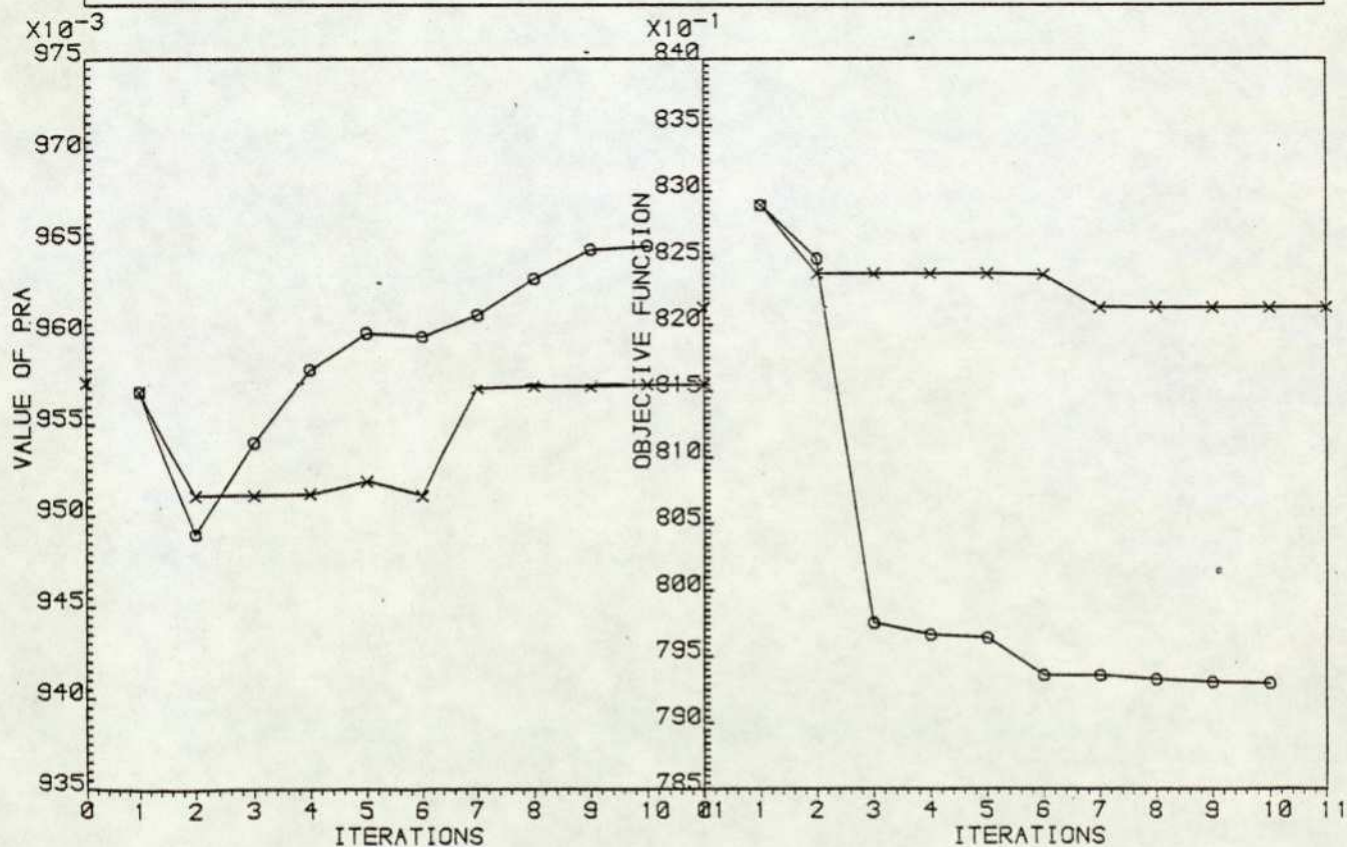
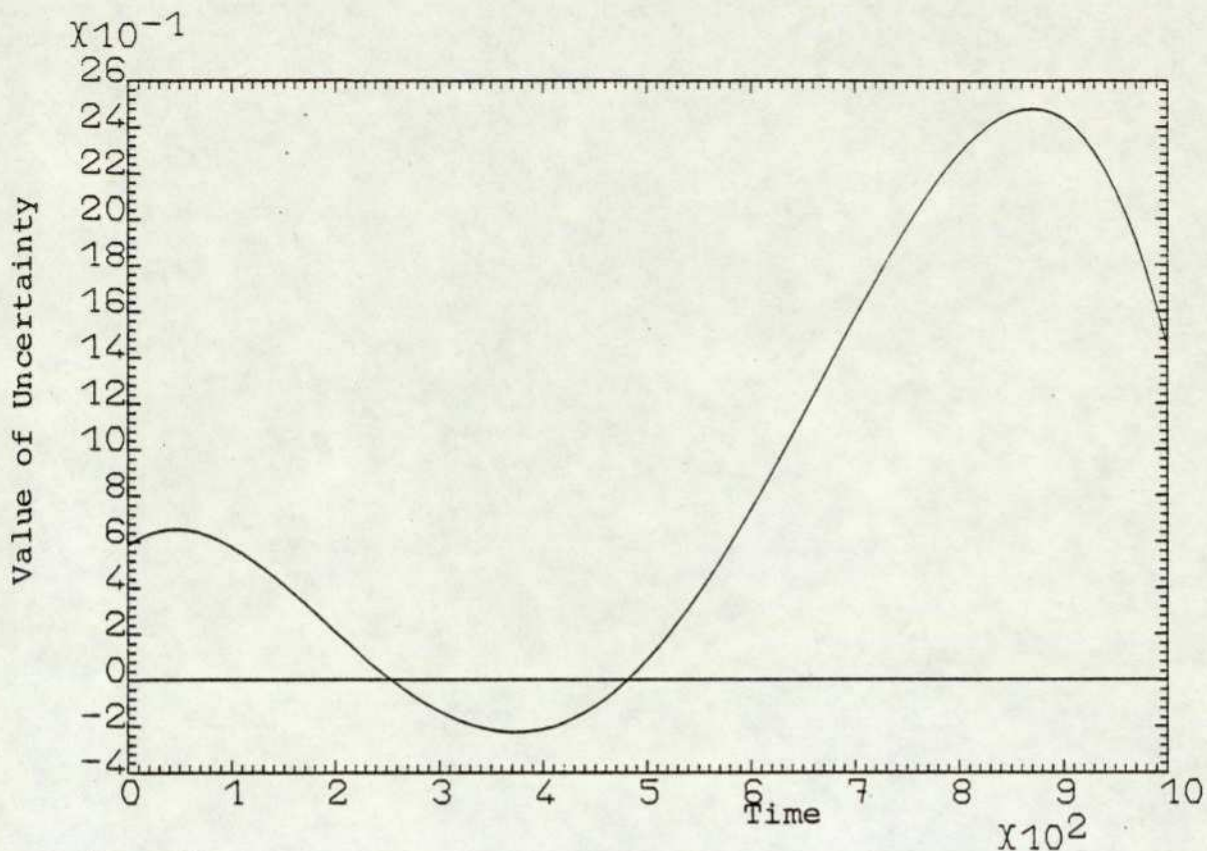
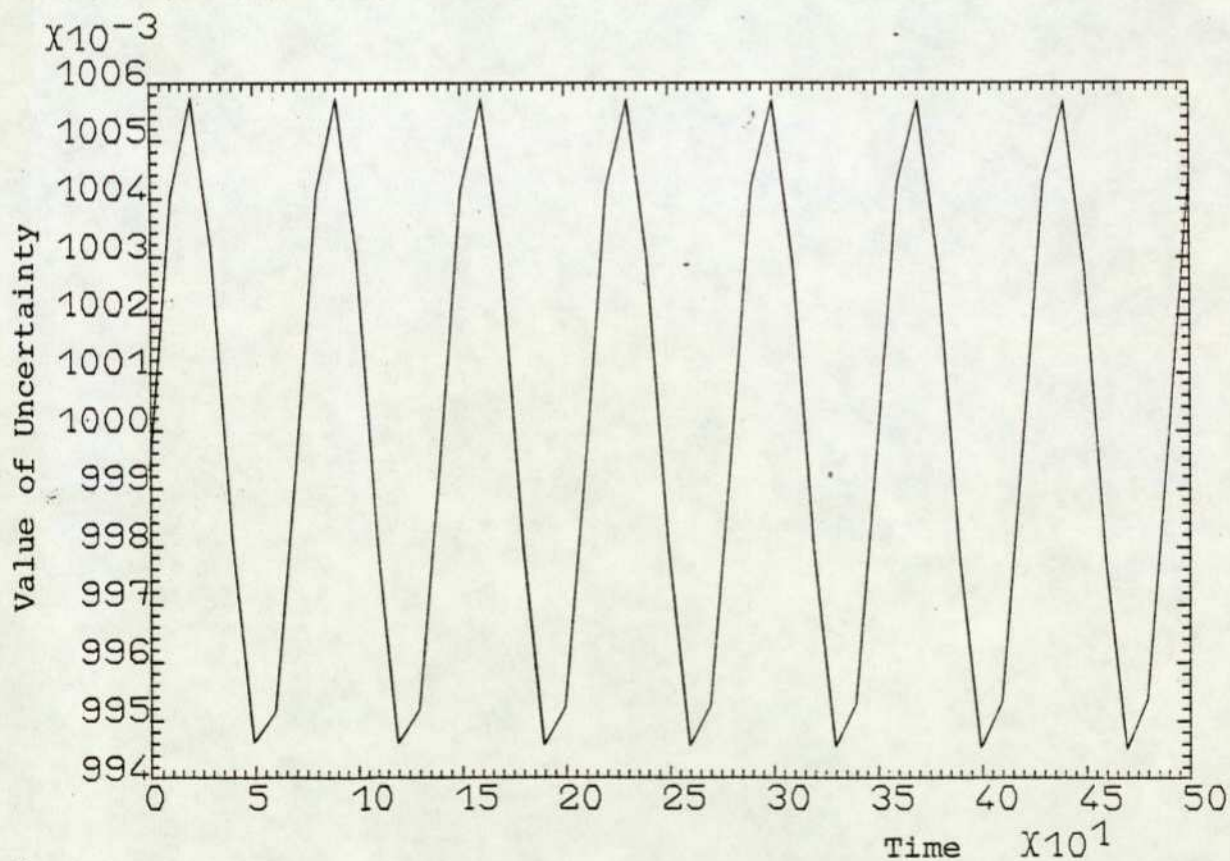


Fig. 4.3.30. The Performance of C.L.S. and S.L.S. Techniques for $W(1) = 10$, $W(2) = 5.0$ and $\rho = 10.0$.

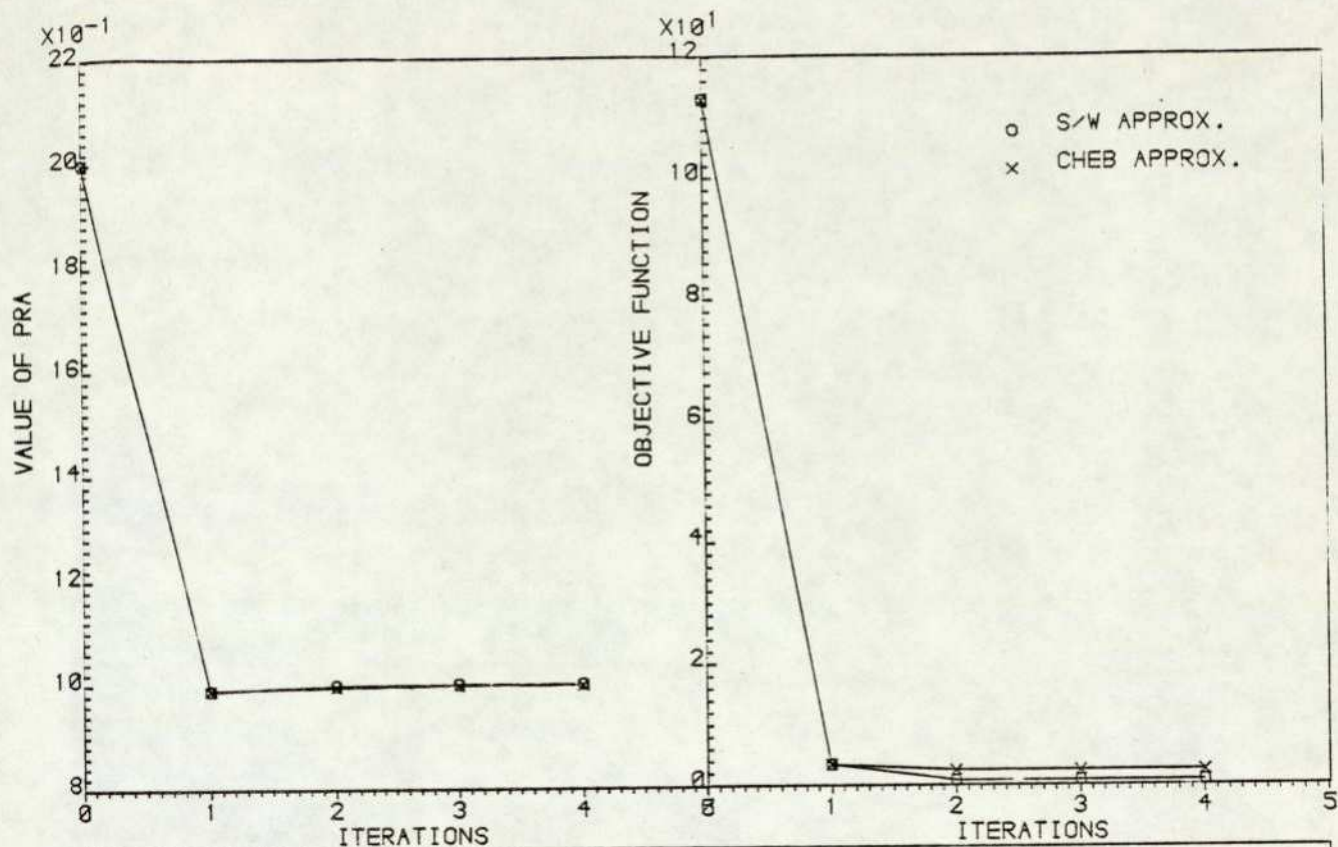


(b) Chebychev Form Uncertainty



(a) Sinewave Form Uncertainty

Fig. 4.3.31. The Resulting Uncertainties using the Converged Estimates of the Smoothing Parameters corresponding to Fig.4.3.30.



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE

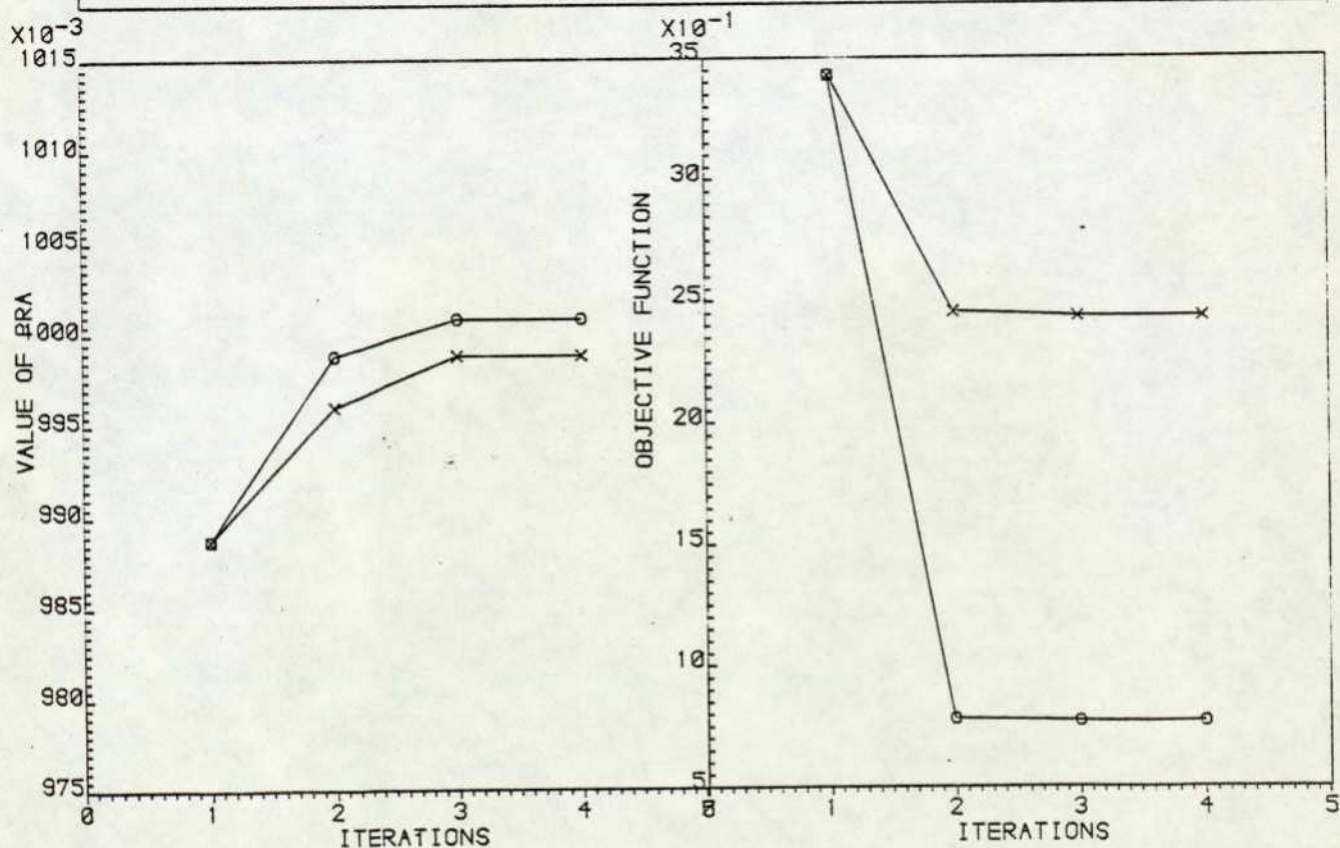
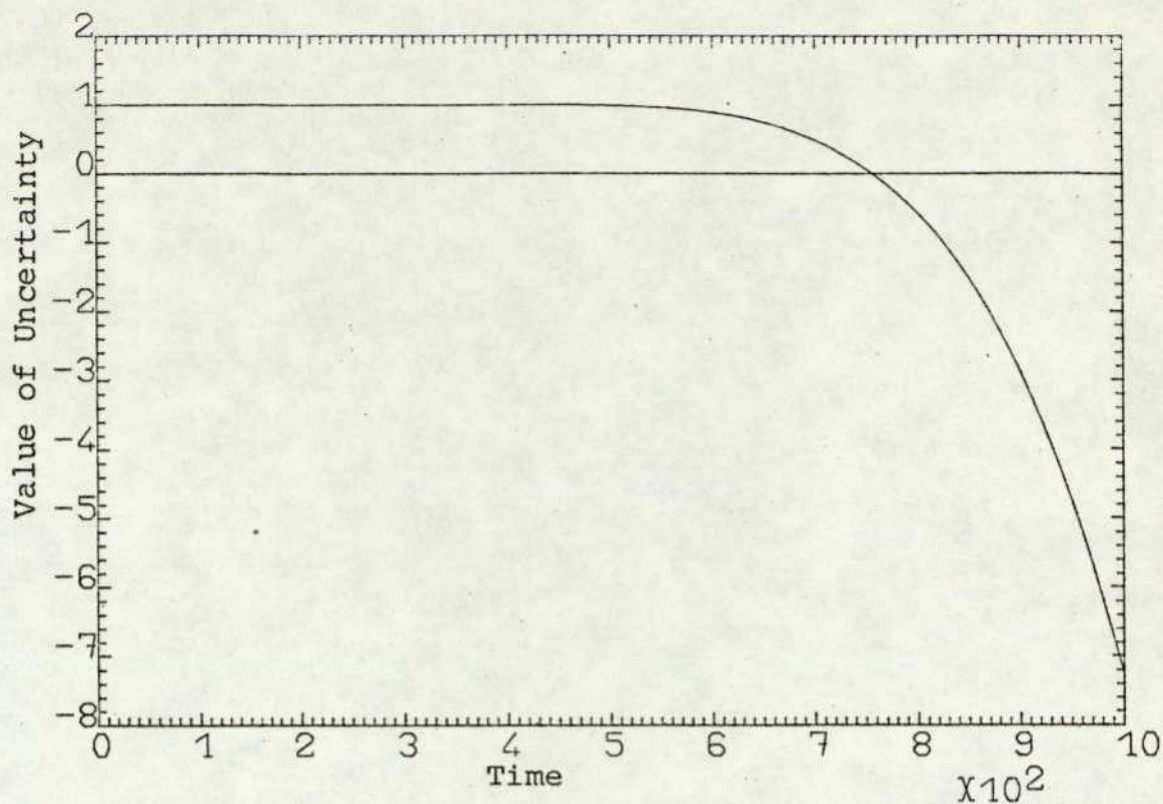
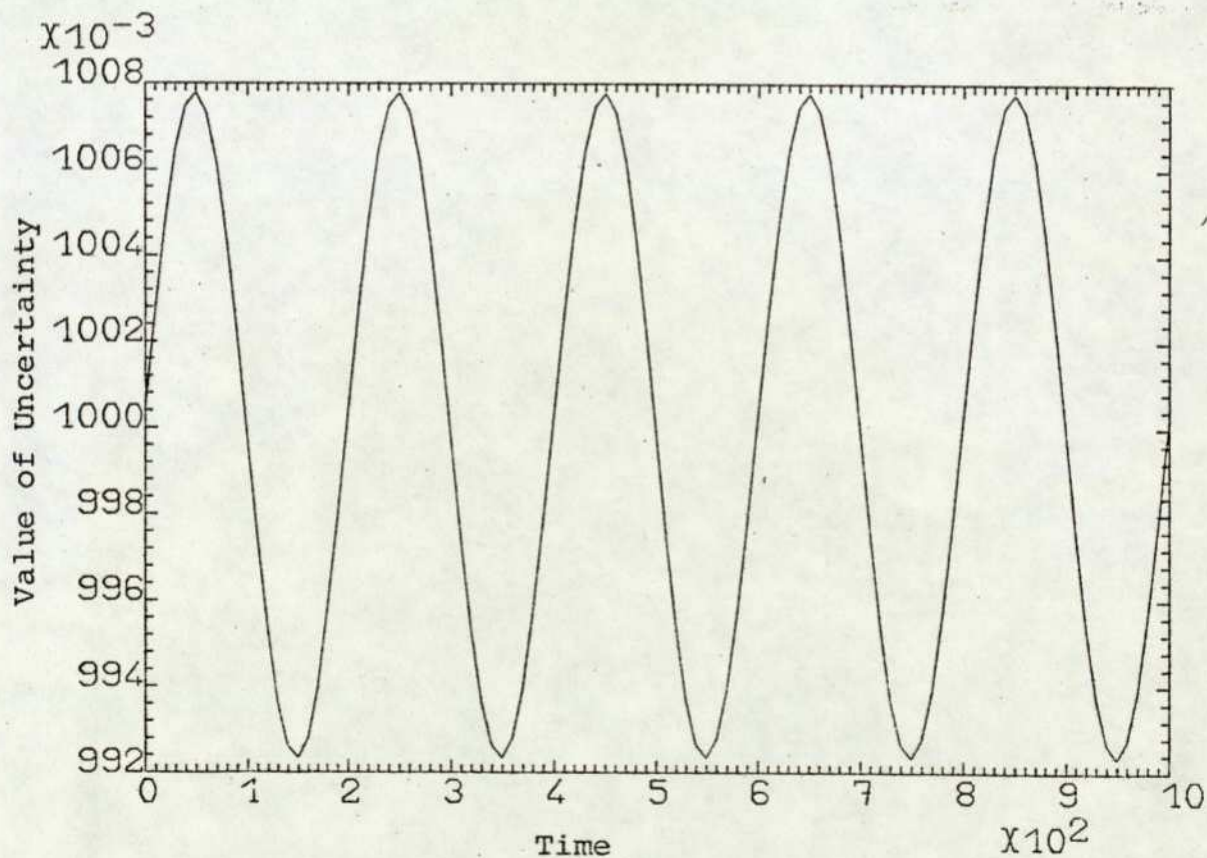


Fig.4.3.32 The Performances of C.L.S. and S.L.S. Techniques for Weightings of $W(1) = 10.0$, $W(2) = 1.0$ and $R = 20.0$.



(a) Chebychev Form Uncertainty



(b) Sinewave Form Uncertainty

Fig.4.4.33. The Resulting Uncertainty using the Converged Estimates of the Smoothing Parameters corresponding to Fig. 4.3.32.

4.3.2. SYSTEM WITH LOSSES TO THE ENVIRONMENT

The introduction of a heat losses term in the heat balance equation causes more complication and assuming the modelling process knows nothing about this, there will exist structural deficiencies in the model which will result in a non-faithful representation. In this case, compensation for the structural errors has been effected by the introduction of time-varying uncertainty to the equation of $\dot{T}_O$ in addition to that attached to the hot water temperature. The overall uncertainty comprises of two parts; a sinewave variation attached to T_H and a Chebychev polynomial attached to $\dot{T}_O$. The results obtained by the identification process, which comprises of the parameter estimation problem to estimate values of the constant parameter (k_O) and the smoothing problem to estimate the parameters of the time-varying uncertainty for varying values of weighting matrices are summarised in Table 4.3.34.

CASE	W(1)	W(2)	R	True value of k_O	PRA(k_O) C.L.S.	PRA(k_O) S.L.S.	No. of overall iterations
1	10	0.1	20.0	1.0	1.003	1.001	6
2	10	0.5	20.0	1.0	1.027	1.0205	7
3	10	0.75	20.0	1.0	0.986	0.9877	7
4	10	1.0	20.0	1.2	1.159	1.062	7
5	20	0.5	20.0	1.0	1.021	1.011	3
6	100	0.5	20.0	1.0	1.048	0.9992	6
7	10	0.5	100.0	1.0	1.0923	1.0765	11

Table 4.3.34 Summary of the results obtained for the system with heat losses.

The first three cases show that as $W(2)$ is increased, the classical least squares estimate of k_0 becomes less accurate and the need for smoothing becomes more acute. Whilst in Case 1 the error in the classical least squares estimate is only 0.3%, in Case 2 the error rises to 2.7%, in Case 3 it becomes 14% and in Case 4 it is 15.9%.

The smoothed least squares technique reduces these errors to 0.1%, 2.0%, 1.22% and 6.2% respectively. Cases 2, 5 and 6 show the effects of increasing the weighting on the errors in the height responses. As $W(1)$ is increased the value of k_0 obtained by the classical least squares technique becomes more accurate at first but for higher values of $W(1)$ the estimate becomes less accurate. The smoothed least squares technique manages to improve on the classical least squares estimate due to the nature of the problem whereby the model is certainly not a faithful representation of the system due to the inherent system uncertainties.

Increasing the weighting on the errors between the uncertainty and its nominal value has resulted in less accurate estimates. In all these cases, the true value of k_0 (PRA) could not be predicted and only improved estimates have resulted from the use of the smoothed least squares technique.

Now the height and mixed water temperature responses of the simulated system and the identified model corresponding to case 1 in the table 4.3.34 are shown in Figs. 4.3.35 and 4.3.36 respectively. Since accurate estimate of k_0 has been achieved the system and model height responses are indistinguishable. The mixed water temperature response yielded by the model does not fit exactly into the system response and does not predict its periodical variations. On the other hand

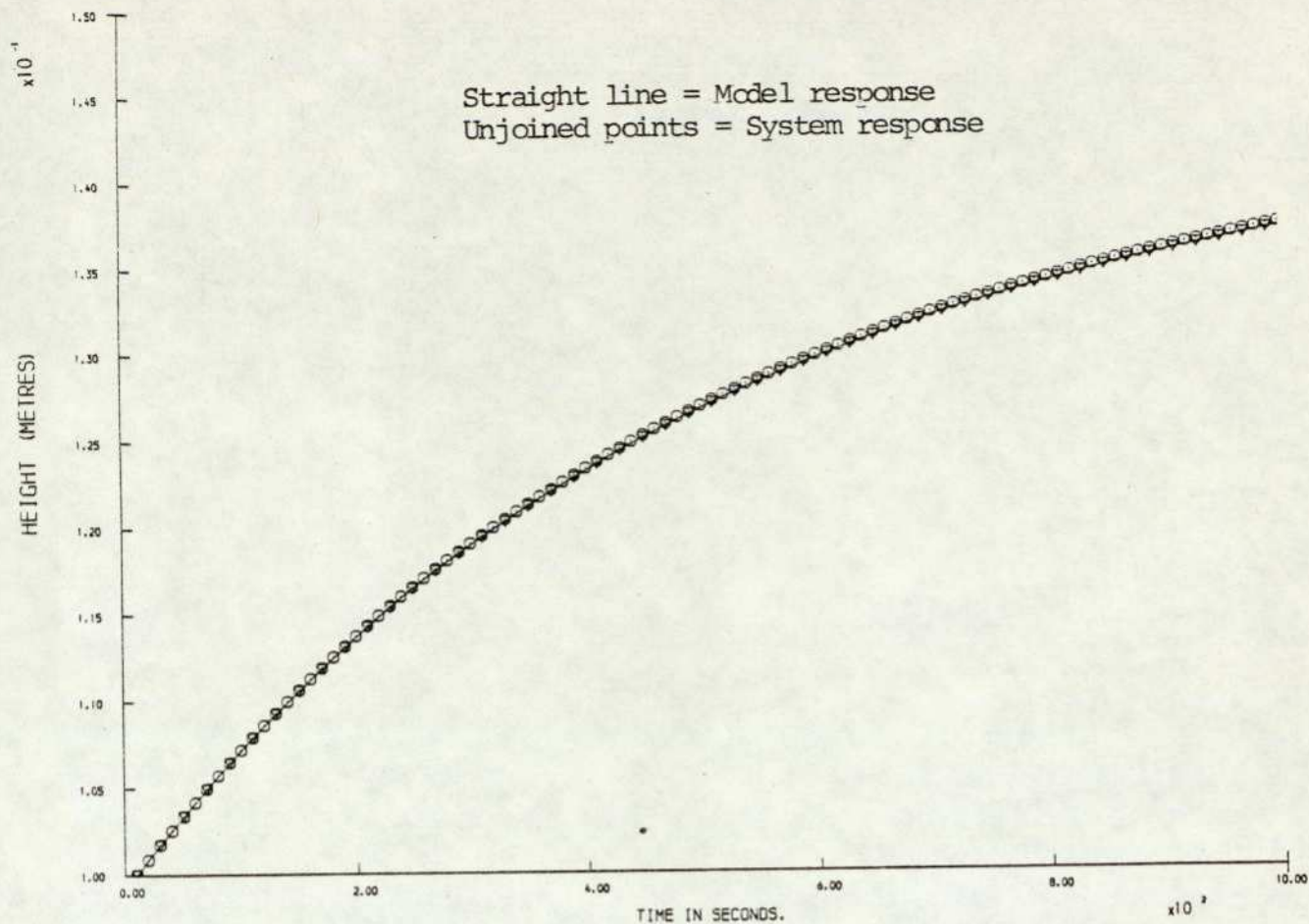


Fig.4.3.35. System and Model Freon Height Responses corresponding to Case 1 of Table 4.3.34.

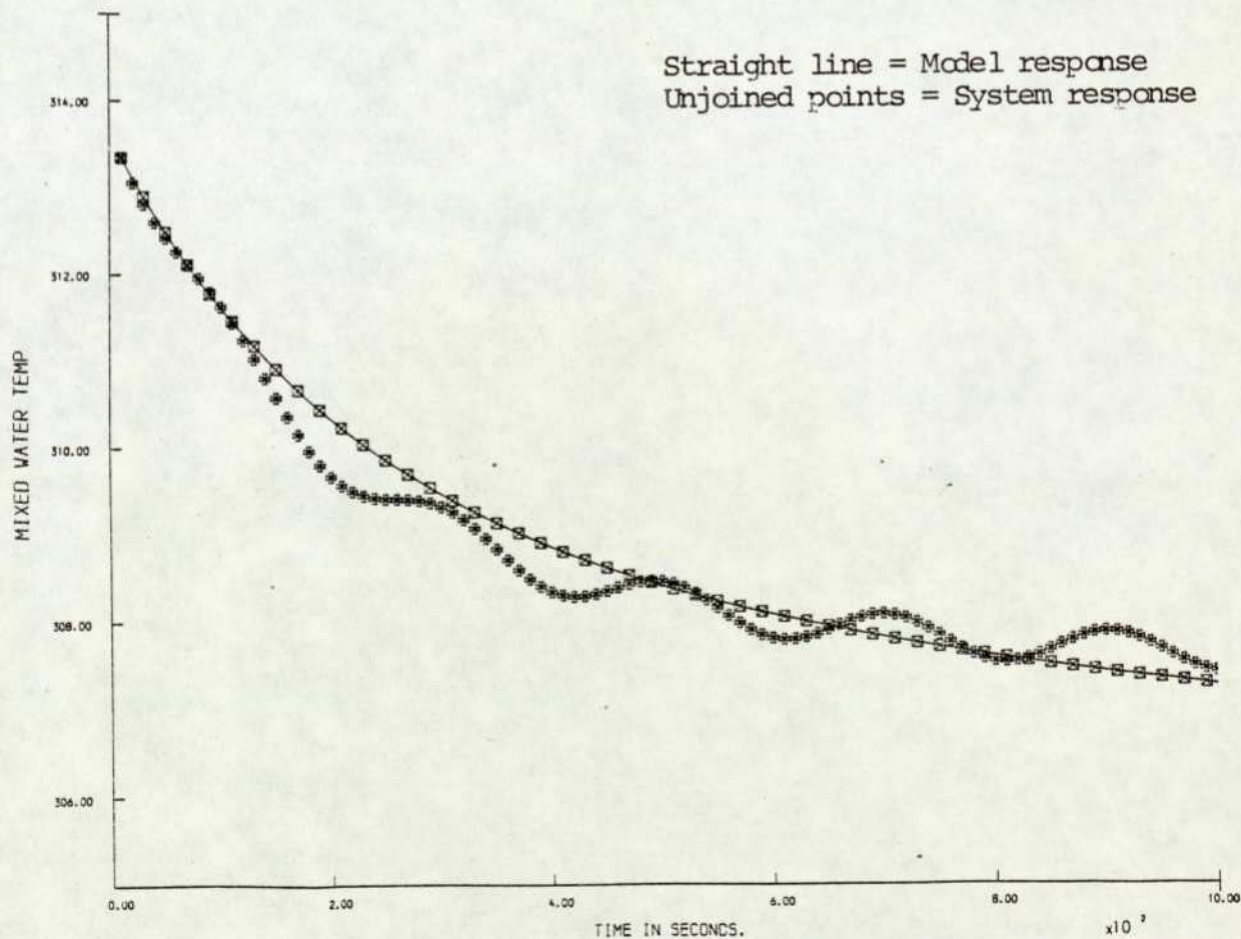


Fig.4.3.36 System and Model Vapour Pressure Responses corresponding to Case 1 of Table 4.3.34.

responses corresponding to Case 4 shown in figs 4.3.37 and 4.3.38 reflect the opposite effect. The system and model height responses do not have good agreement (due to inaccurate estimate of k_0) whilst the corresponding mixed water temperature responses reflect a reasonable fit except for the periodical fluctuations which have not been reproduced by the model. These two sets of responses represent the smallest and the largest values of $W(2)$, and thus, give an insight into the effects of using improper weighting values. Similar responses have been obtained for small and large values of $W(1)$ but these are not being presented here to avoid repetition.

Comparison between the two techniques

The performances of the classical least squares and the smoothed least squares techniques are shown for cases 1, 2, 6 and 7 by figs. 4.3.39 and 4.3.40 respectively.

Fig. 4.3.39 shows the performances of both the classical least squares technique and smoothed least squares technique ^{for} low weighting on the errors in the model and system responses of ^{the} mixed water temperature. Although the smoothed least squares technique has contributed to the reduction of objective function especially after the first and second overall iterations, the converged value of the parameter estimate differs only little from that obtained by the classical least squares technique.

In fig. 4.3.40 the contribution of the smoothed least squares to the reduction of objective function is very clear and exceeds that of the classical least squares technique. However, the improvement due to the smoothed least squares in the parameter estimate

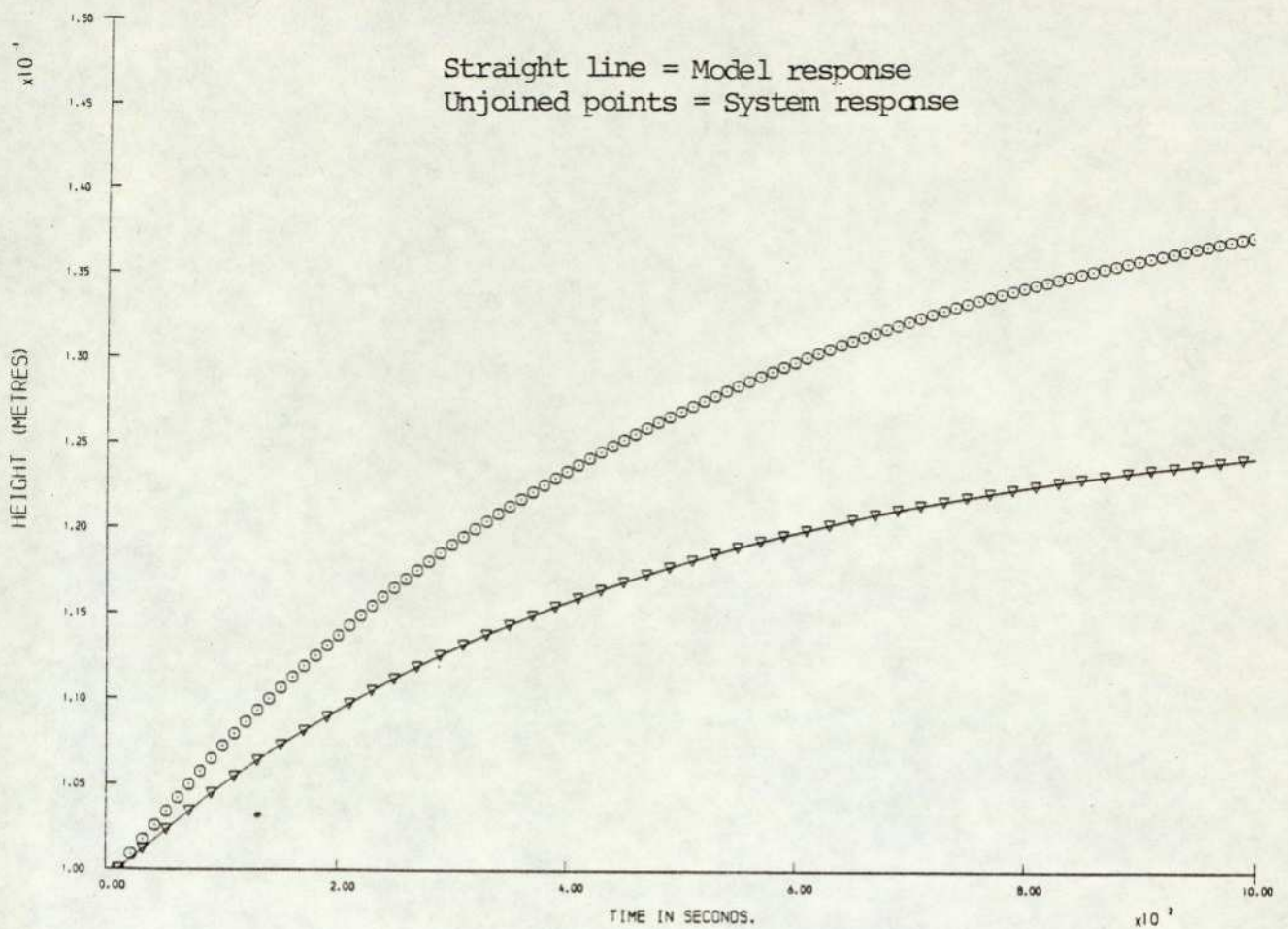


Fig.4.3.37. System and Model Height Responses Corresponding to Case 4 of Table 4.3.34.

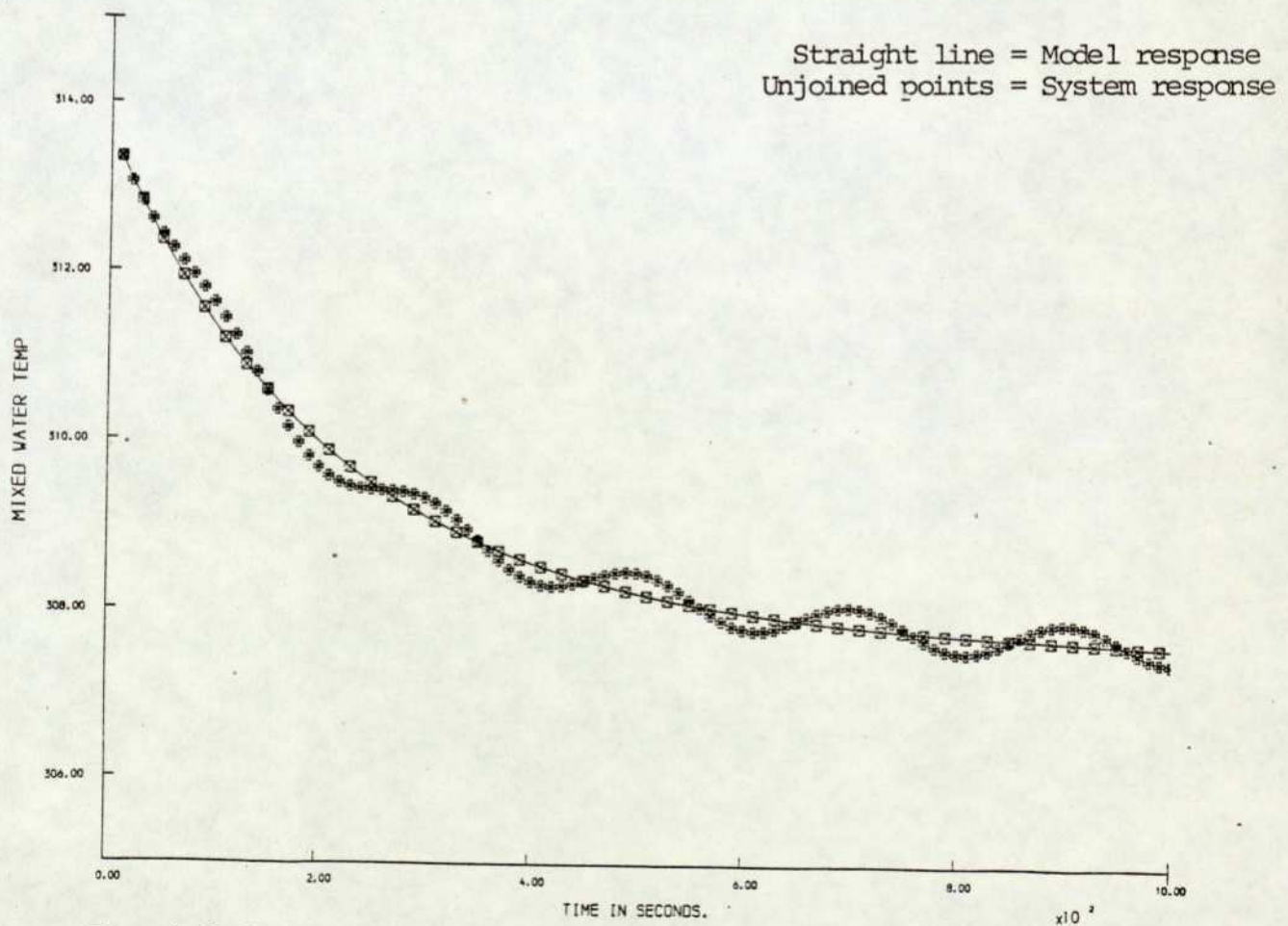


Fig.4.3.38 System and Model Vapour Pressure Responses Corresponding to Case 4 of Table 4.3.34.

k_0 is not remarkable. The time-varying uncertainties corresponding to figs. 4.3.39 and 4.3.40 are shown in fig.4.3.41.

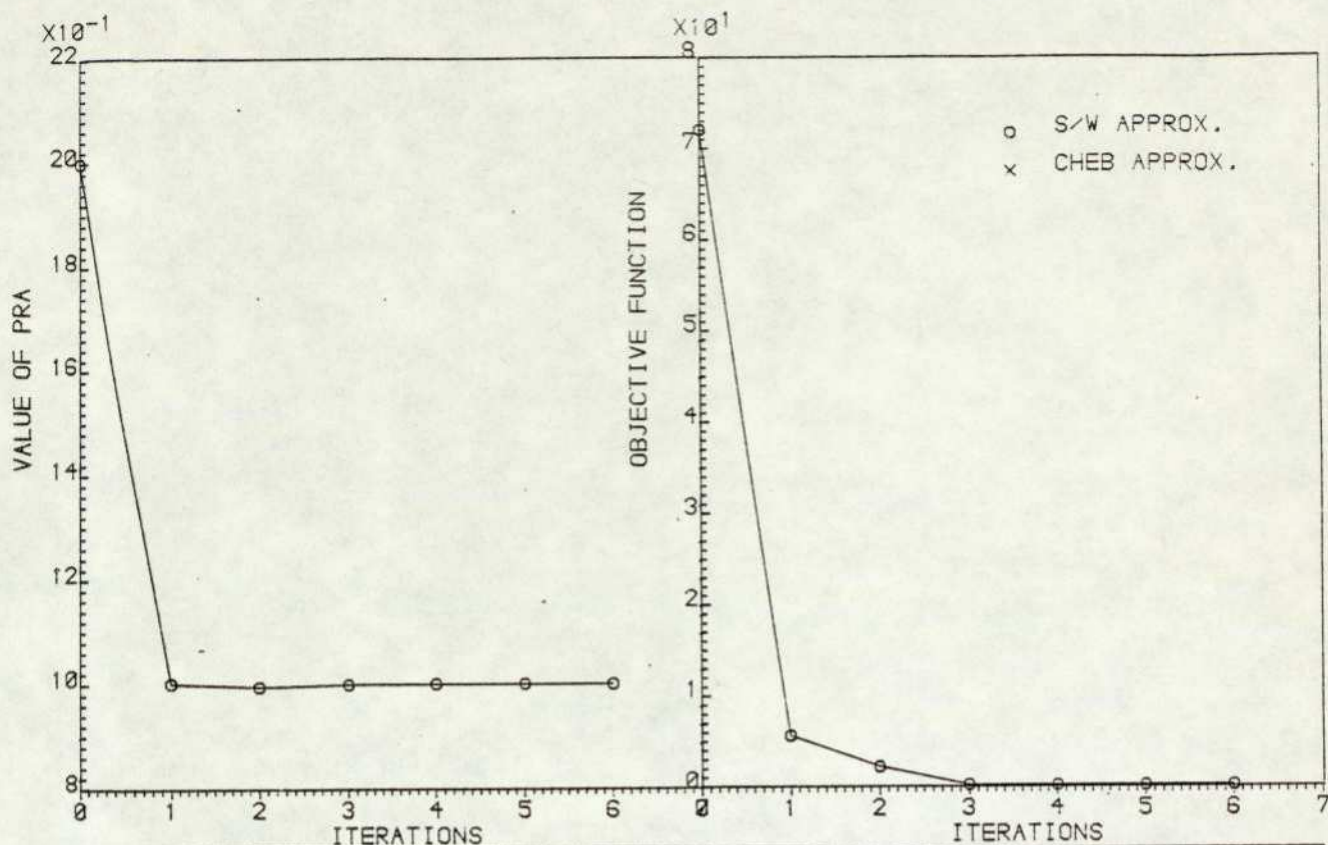
Fig. 4.3.42 which shows the effect of using large value of weighting matrix on the errors in the system and height responses shows some improvement on the value of the parameter estimate k_0 due to the smoothed least squares technique together with some improvement on the value of objective function. The use of smoothing has resulted in a very good estimate of k_0 . This may be due to the idea that with large emphasis on the errors in height response which is related to the estimation parameter k_0 , the technique tends to yield an accurate estimate so that this part of the objective function which has become dominant is reduced remarkably.

The effect of a large value of R is shown in fig. 4.3.43, where although the smoothed least squares technique yields some improvement, this happens at a slow rate. After 10 overall iterations, the improvement amounts to only about 1.6%, thus requiring unaffordable computing time for total convergence.

The time-varying uncertainties corresponding to these two conditions are given by fig. 4.3.44.

In all these cases, the true value of the parameter k_0 is normalised to 1.0. However, unlike the time varying uncertainty which has been introduced into the system discussed in section 4.2.1 in which a perfectly insulated system has been considered, the time-dependent uncertainty here consists of two parts. The first is similar to that used in section 4.3.1.

where sinewave variations have been attached to the hot water temperature. The second is the introduction of the heat losses term into the system. The resulting time-dependent uncertainties whose coefficients have been estimated by the smoothing problem consist of a sinewave part and a Chebychev polynomial part. The introduction of these uncertainties into the model has resulted in improved parameter estimates and has served as a compensation term to overcome model structural deficiencies.



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE

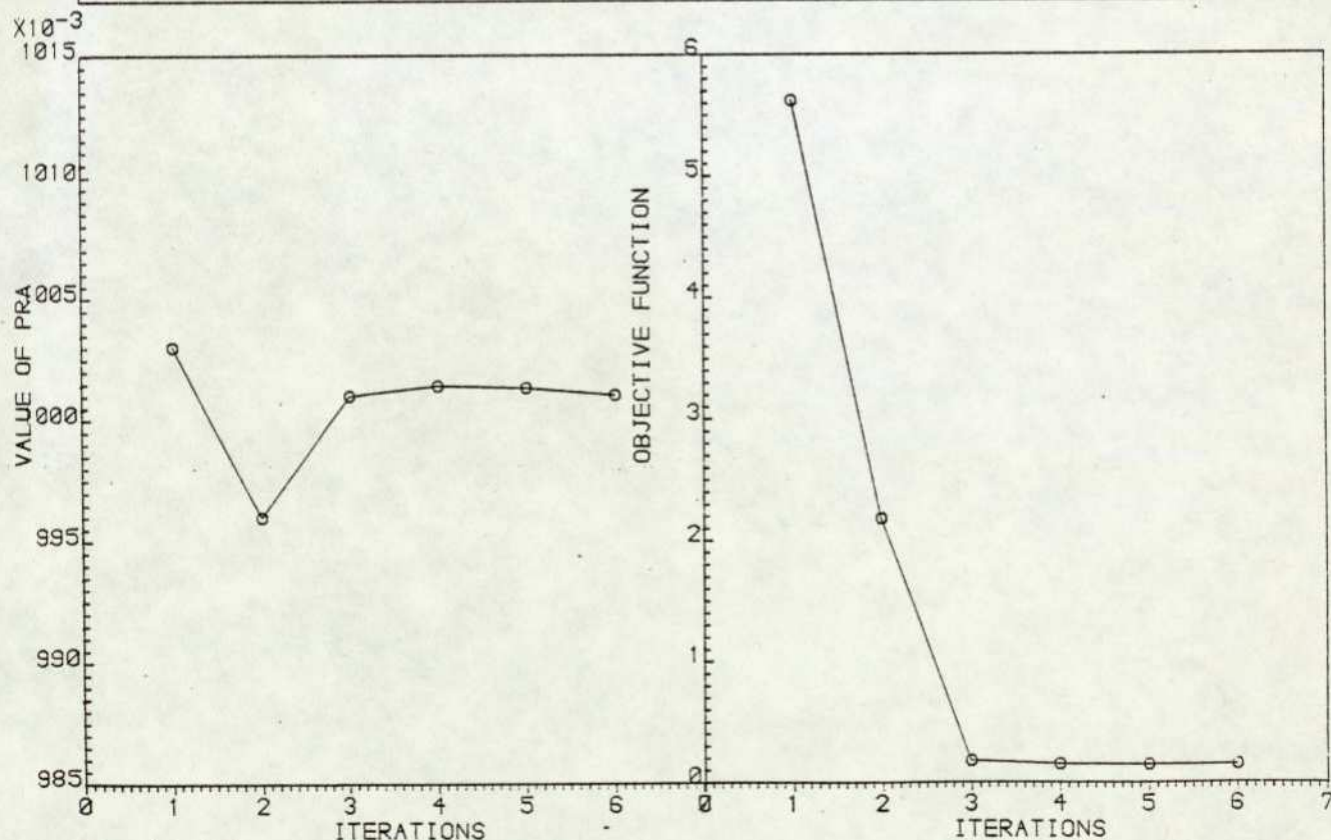
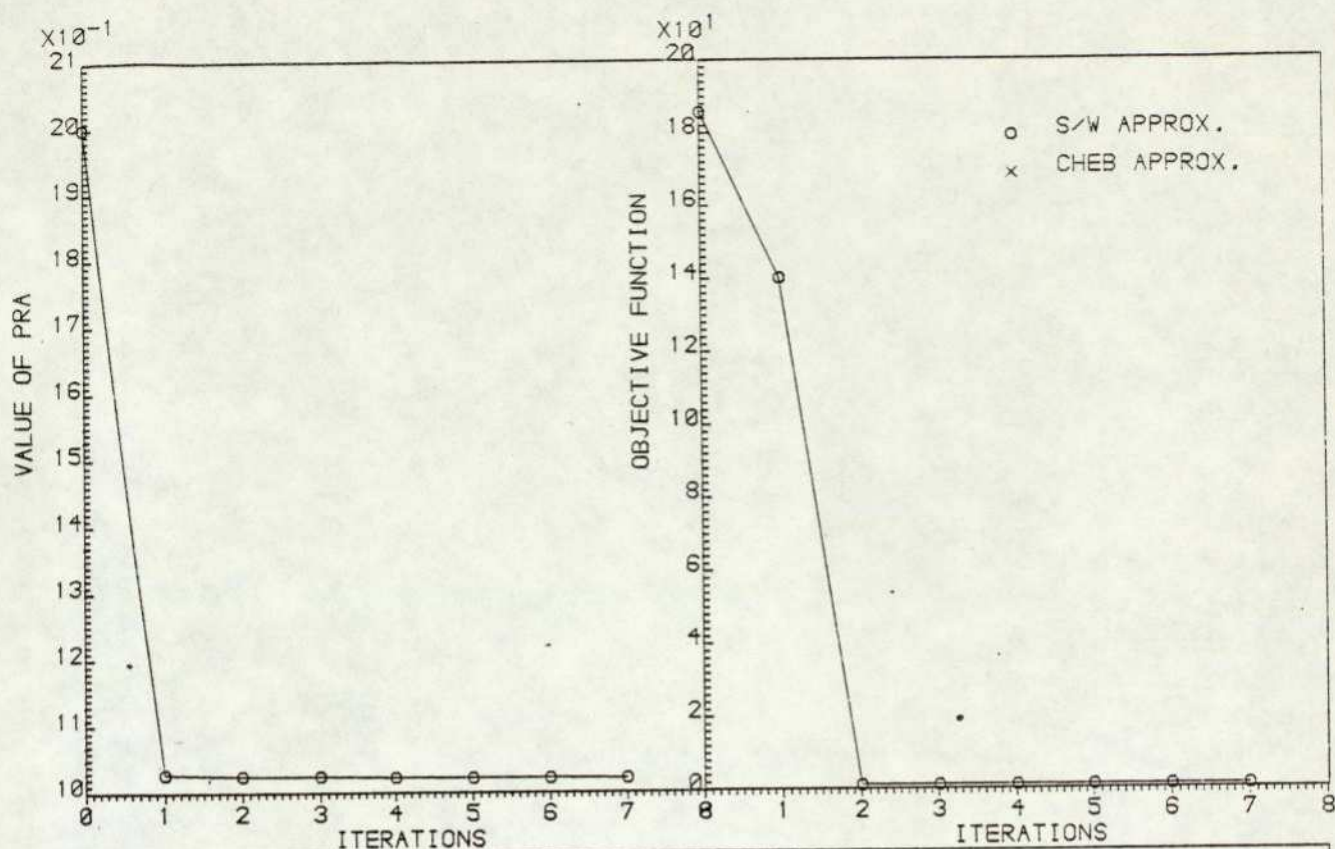


Fig.4.3.39 The Performances of C.L.S. and S.L.S. Techniques for $W(1) = 10.0$
 $W(2) = 0.1$ and $R = 20.0$.



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE

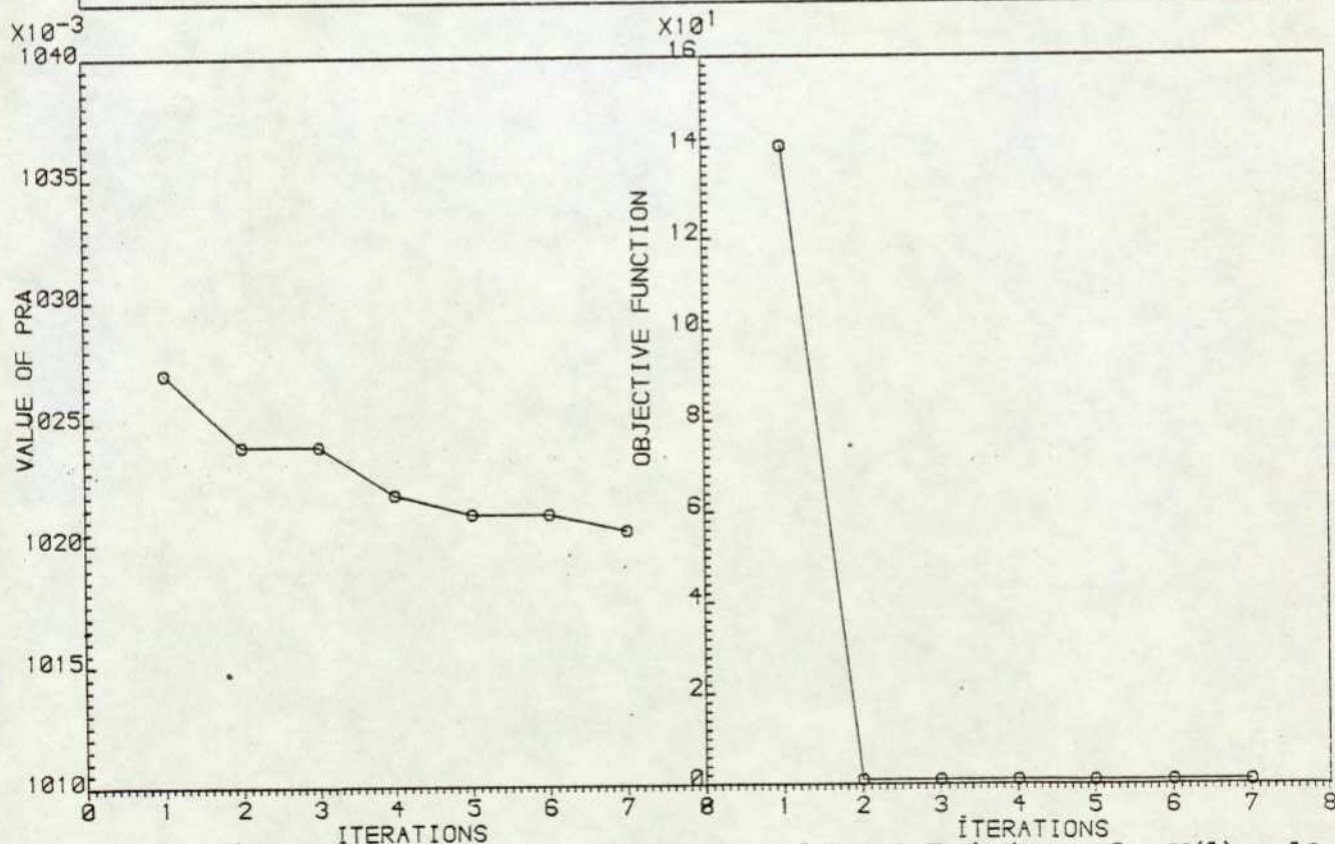


Fig 4.3.40. The Performances of C.L.S. and S.L.S. Techniques for $W(1) = 10.0$
 $W(2) = 0.5$ and $R = 20.0$.

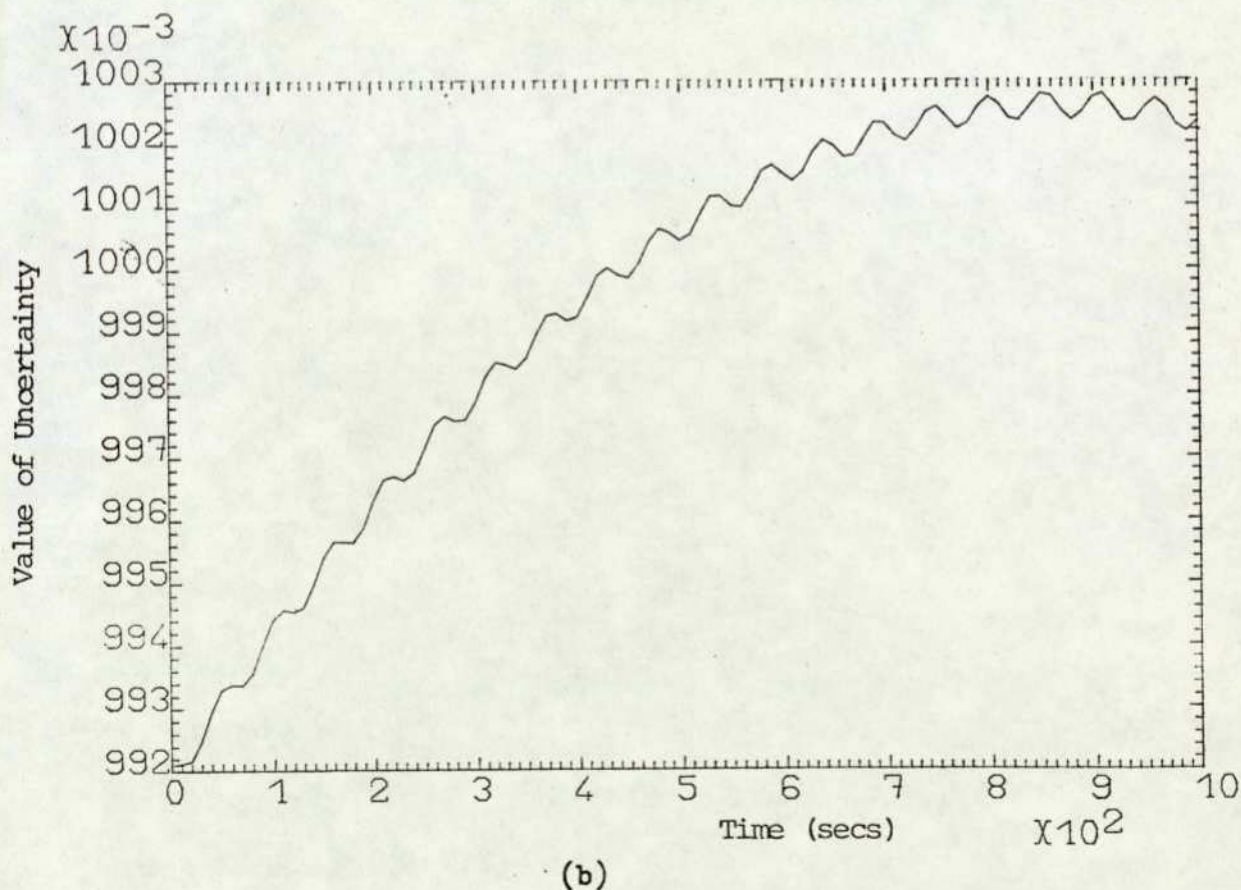
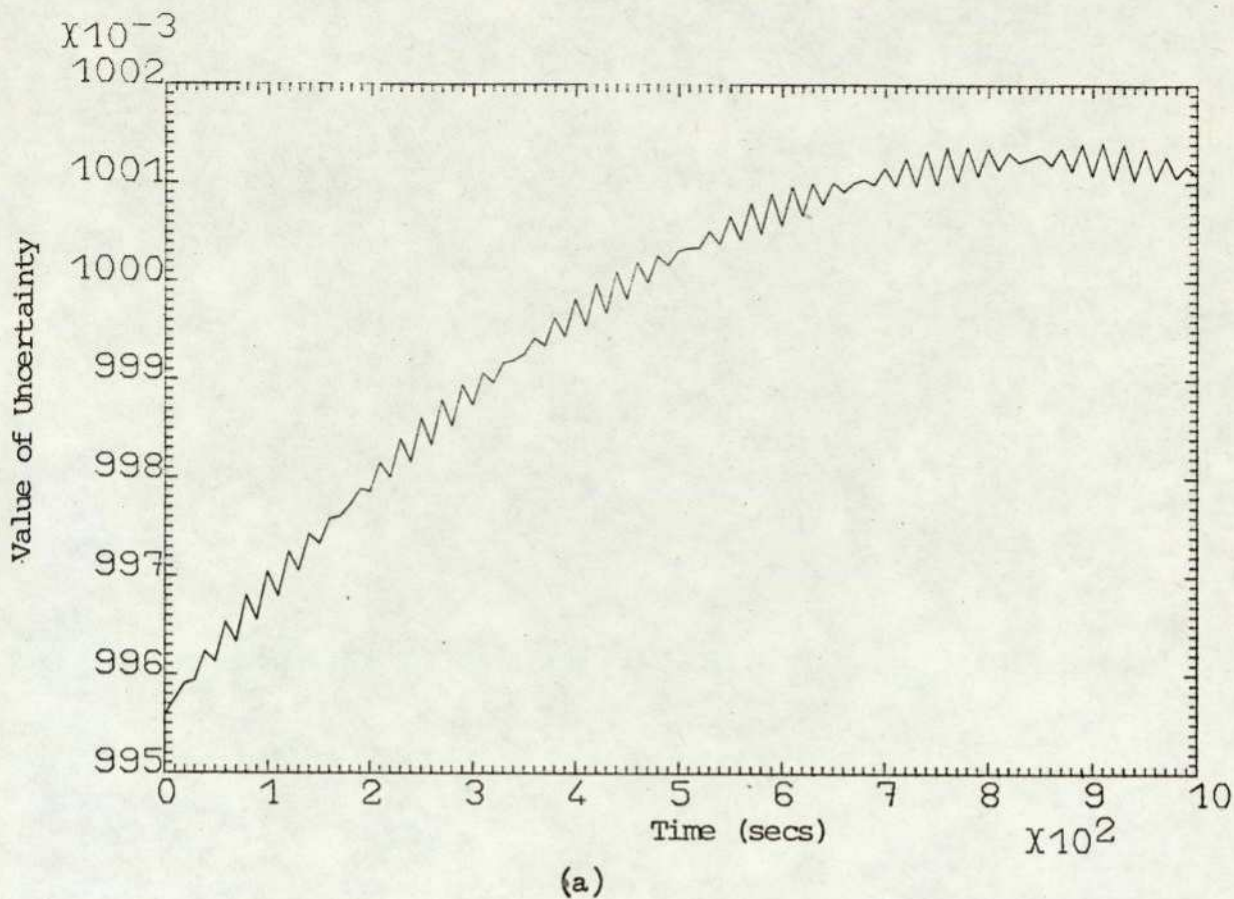
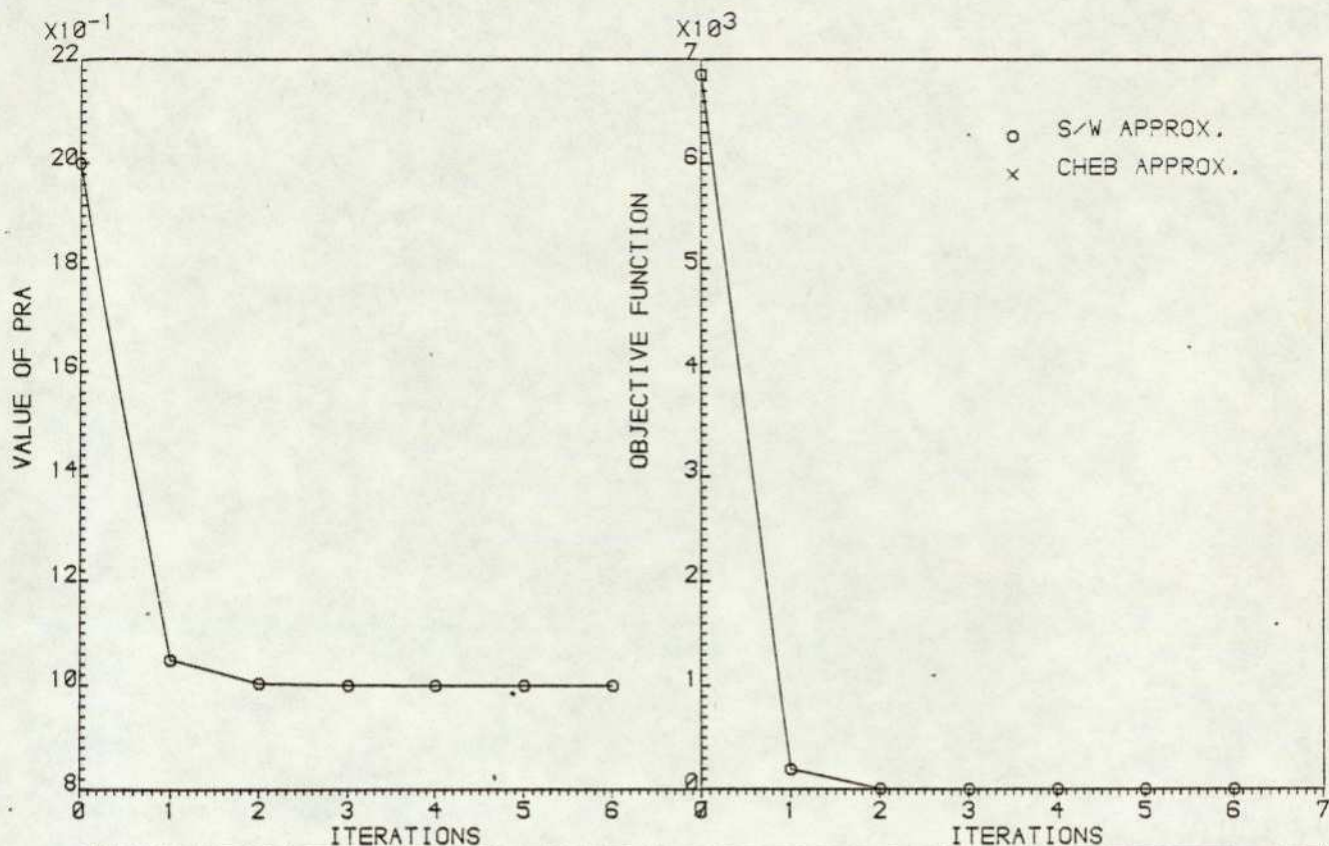


Fig.4.3.41. The Resulting Uncertainties using the Converged Systems of Smoothing Parameters where (a) corresponds to Fig.4.3.39 and (b) corresponds to 4.3.40.



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE

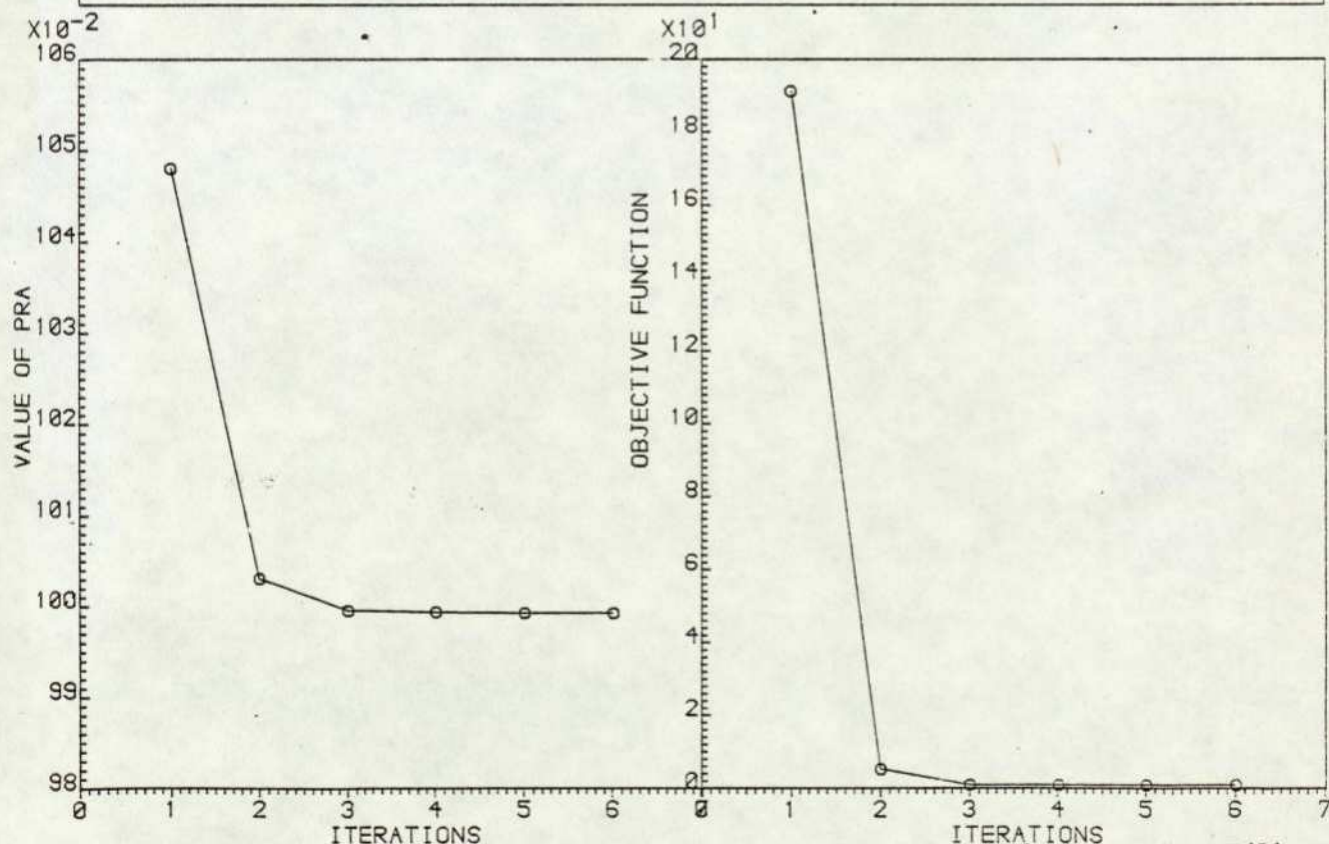
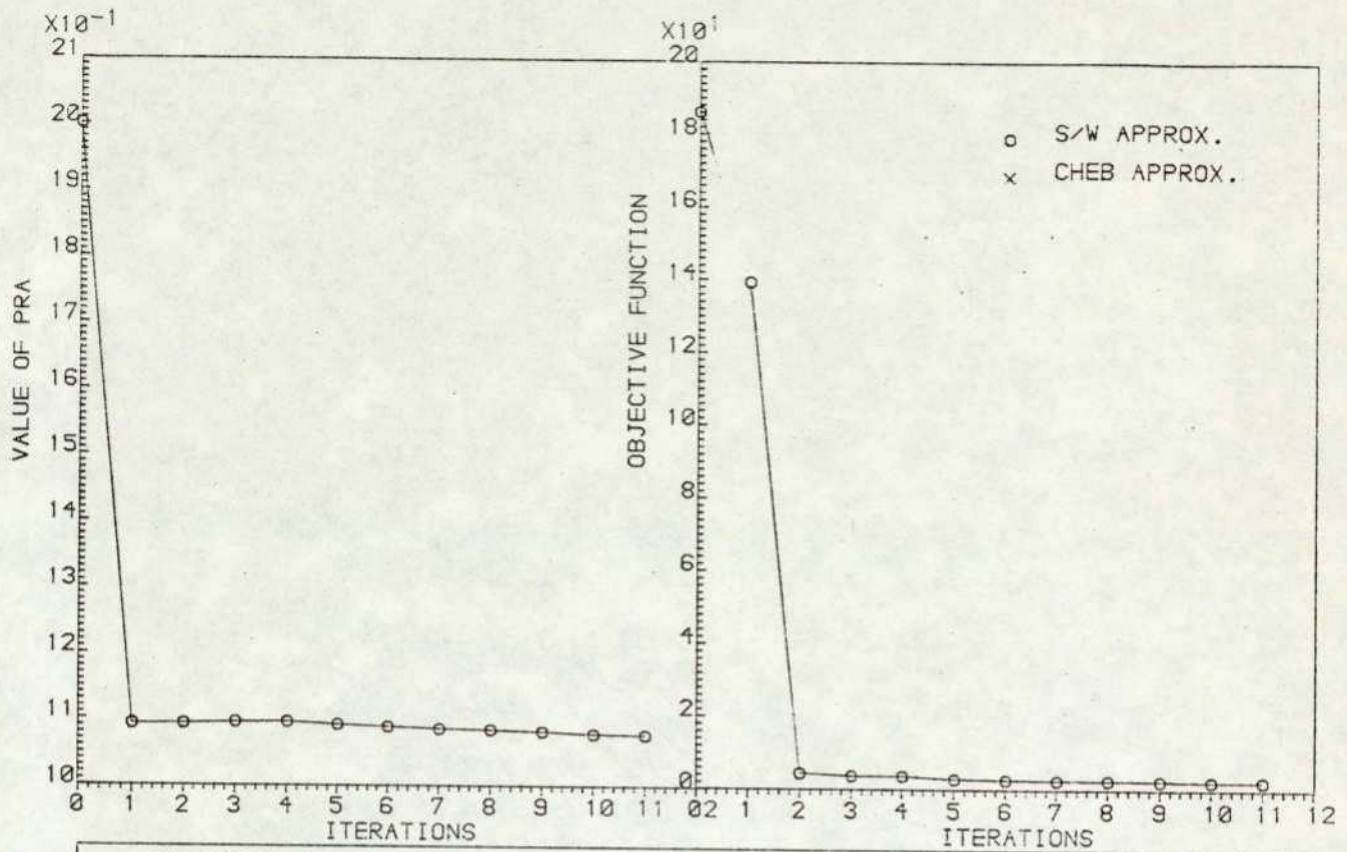


Fig.4.3.42. The Performance of the C.L.S. and S.L.S. Techniques for $W(1) = 100$, $W(2) = 0.5$ and $R = 20.0$.



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE

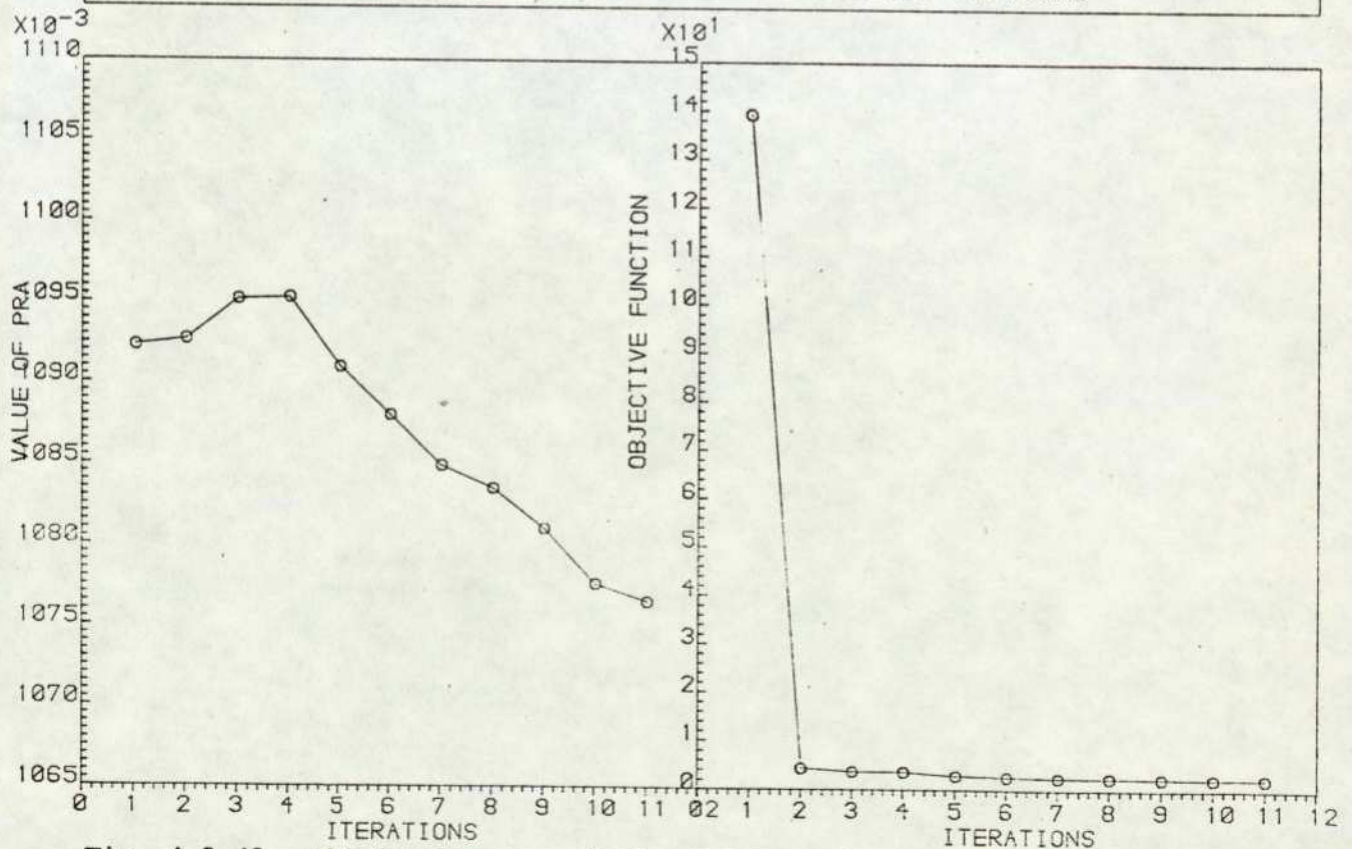


Fig. 4.3.43. The Performance of the C.L.S. and S.L.S. Techniques for $W(1) = 100$, $W(2) = 0.5$ and $R = 100.0$

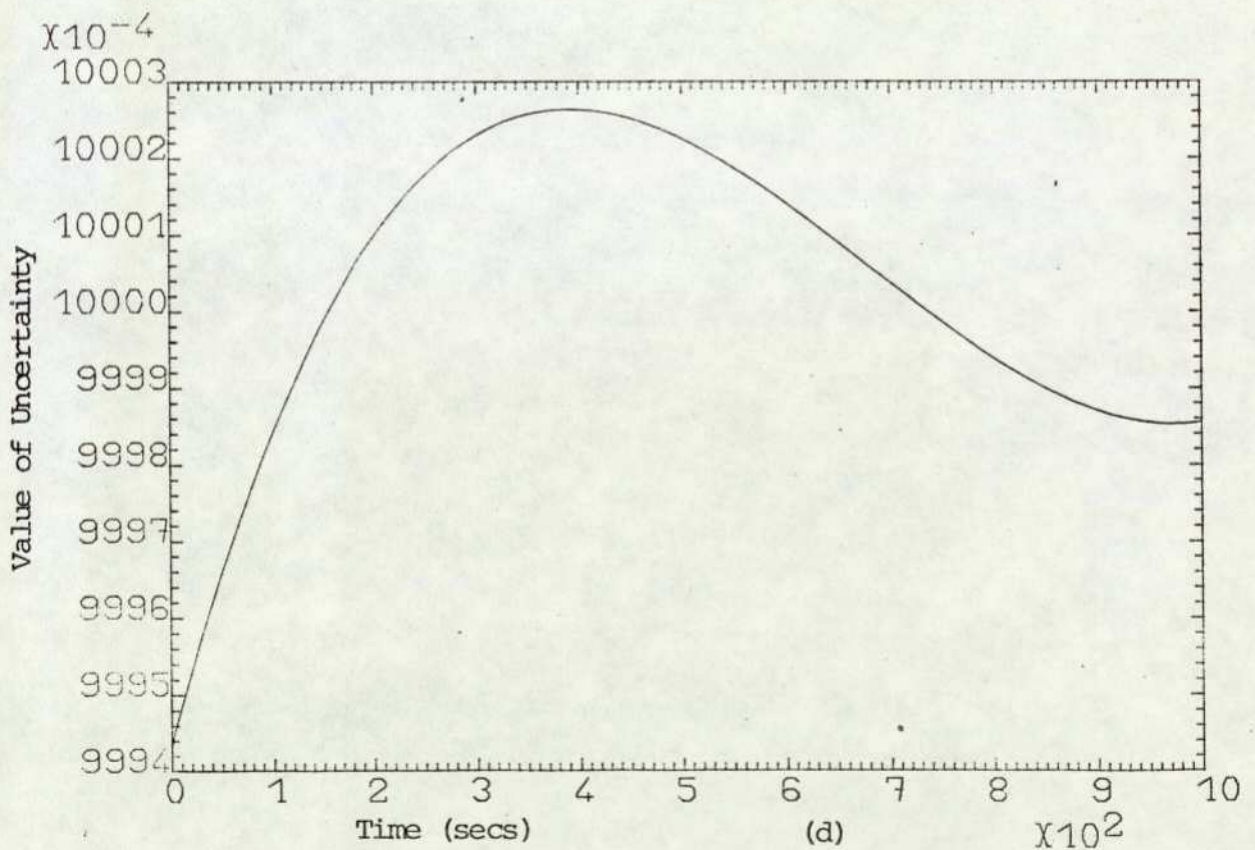
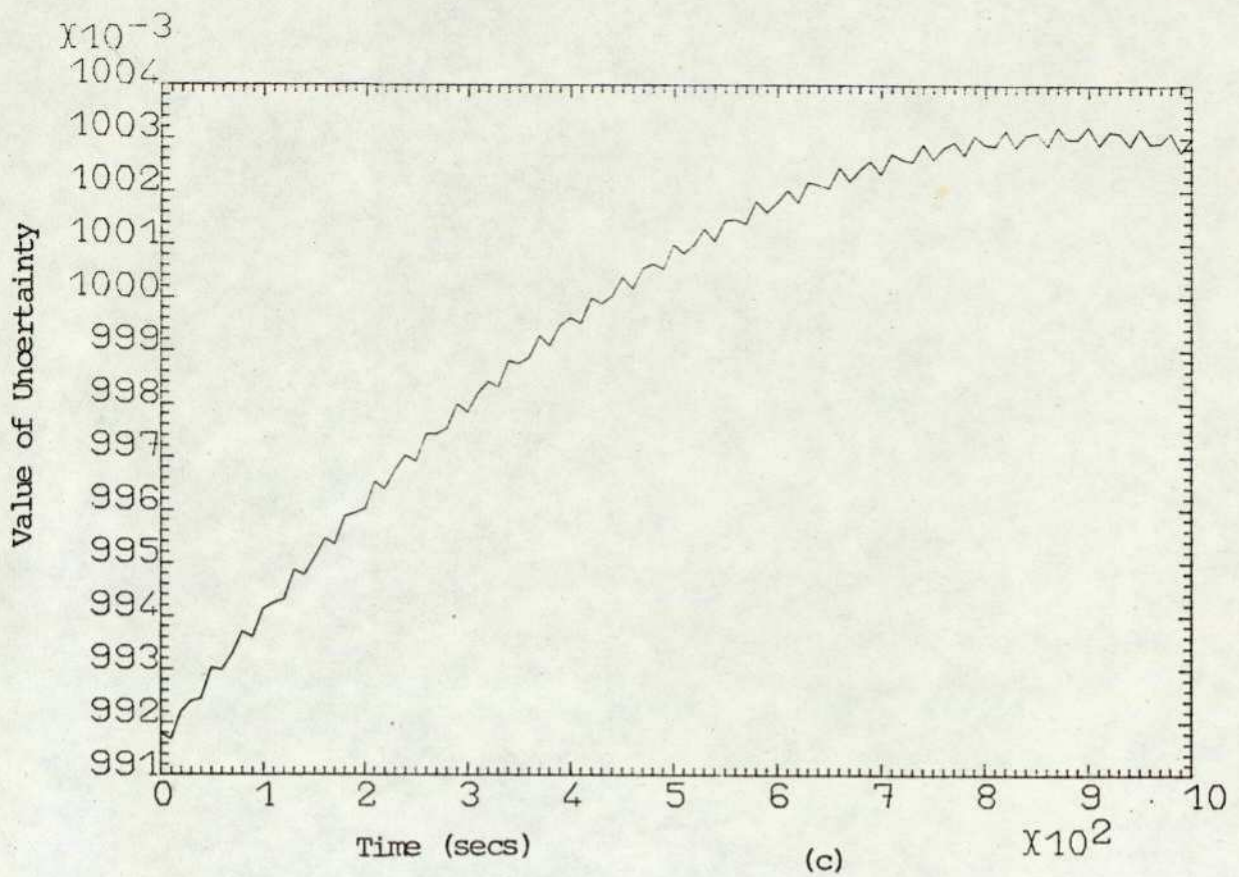


Fig.4.3.44. The Resulting Uncertainties using Estimates of Smoothing Parameters where (c) corresponds to Fig.4.3.42 and (d) corresponds to Fig.4.3.43.

Chapter 5

VAPORISER SYSTEM

5.1 Introduction

Vaporisation is the process through which a non-aqueous liquid undergoes a phase change by the addition of heat. A distinction must be made between vaporisation, evaporation and flow-boiling processes. The common connotation of evaporation is the removal of water from a solution by boiling, usually in a vessel, and withdrawing the vapour, leaving a more concentrated solution. It is one of the main methods used in the chemical industry for the concentration of aqueous solutions. In flow-boiling processes, a flowing liquid undergoes a phase change due to the absorption of heat. These processes, which can be seen in a wide variety of industrial environment, such as in steam generating plants, take place whenever the boiler is either of the recirculating or once-through type.

Unlike the evaporator, whose function is the separation of the components of a solution, the prime function of a vaporiser is to effect a phase change in a non-aqueous liquid. It is of a vertical structure with the working fluid entering at its base under forced flow conditions. The liquid is heated, usually with steam that provides enough heat to fully convert the total liquid flow to vapour by the time the fluid reaches the upper region of the device.

In this research, which is concerned with the application of identification techniques to real and simulated processes, a pilot vaporiser is considered as the real system from which real observations, required by the identification processes, are obtained.

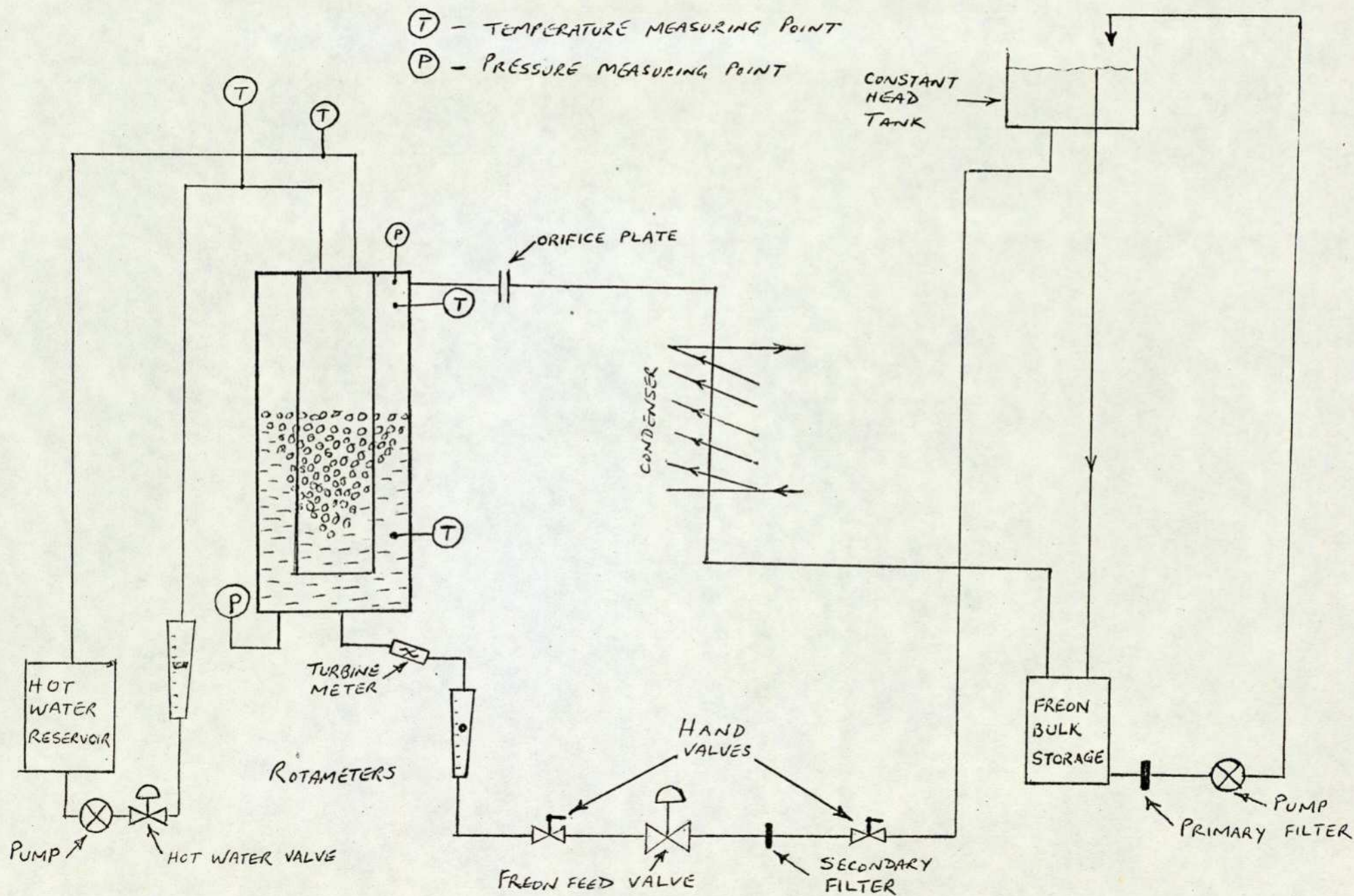
The vaporiser rig was constructed at the department more than ten years ago with the intention of extending the limited knowledge of the class of flow boiling processes of which vaporisers are part thereof. Throughout its life span, the pilot plant has passed through several stages of development. Since Collins (1971) initiated its construction, other workers (Collins 1971, Stephenson 1973, Yiakoumettis 1974, and El-Taji 1975) were concerned with the development of the system including the implementation of a single loop direct digital control scheme. But due to many physical difficulties, as cited by El-Taji (1975), none of these works resulted in fully successful operation of the system when under control. It was Ellis (1979) who, after elaboration on the earlier vaporiser models which always assumed perfect mixing conditions, managed to produce a successfully functioning vaporiser system with reliable hardware and able to operate under direct computer control. With this system, single or multivariable control may be used together with the facility of opening or closing loops.

The computer control had been achieved by the use of Ferranti Argus 500 computer, which, due to technological advancements in the computer field, is being replaced by process control I-MIC Kratos Instem micro computer.

5.2 Plant Description

The overall structure of the vaporiser assembly is shown in Fig. 5.2.1. The control element of the system is the vaporiser tube, shown in Fig. 5.2.2. and comprises of a glass tube sealed off at both ends by brass flanges which are secured together by steel rods. The heating part consists of two concentric tubes, where hot water passes down the inner tube and returns through the outer one whose

Fig. 5.2.1 The overall structure of the vaporiser rig.



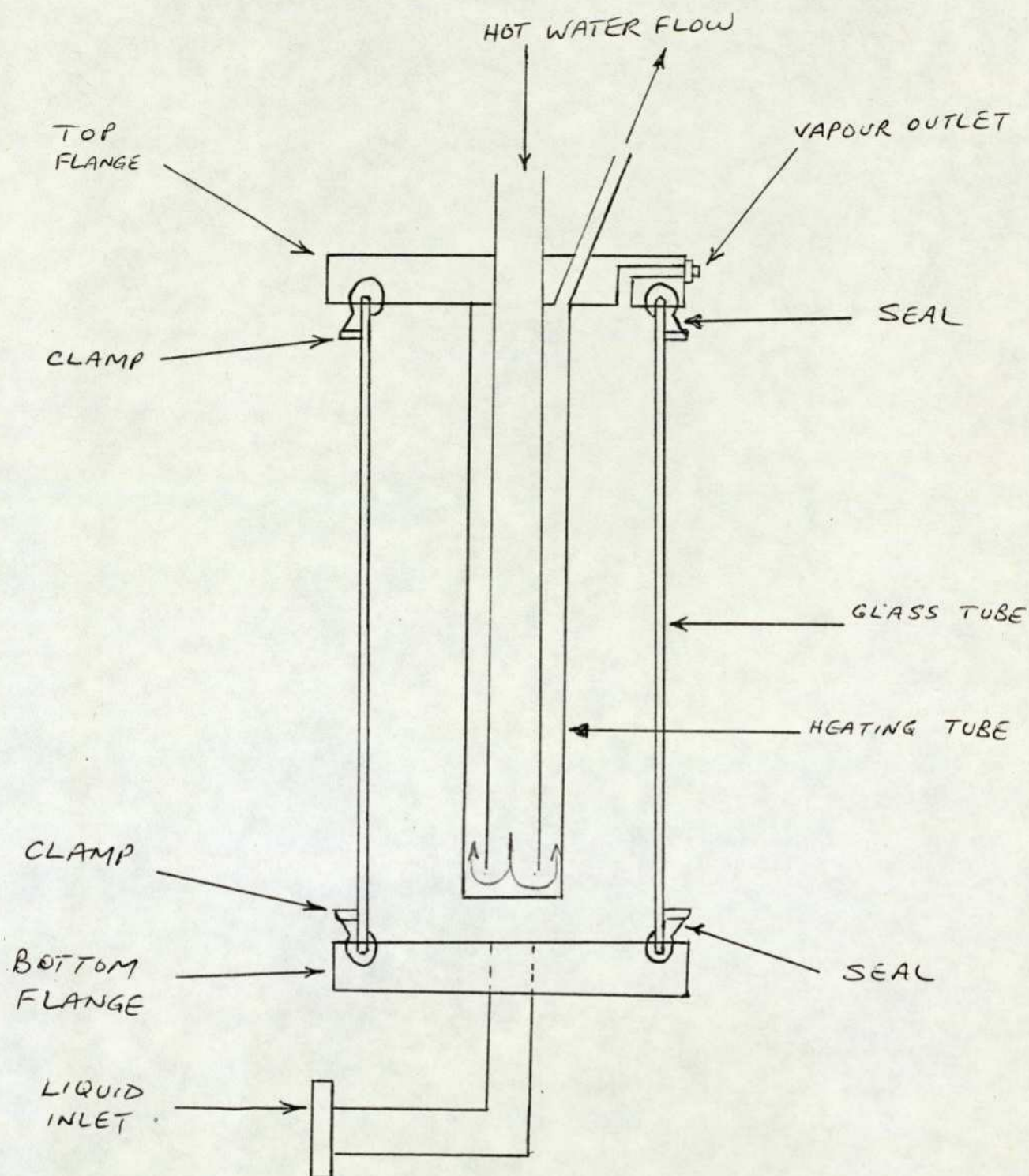


Fig. 5.2.2. The vaporiser tube and the two concentric heating tubes.

lower end is blanked off. The hot water is drawn, by a centrifugal pump, from a temperature-controlled reservoir tank which has a capacity of 7.5 gallons (34 litres approximately) and is well lagged, and passes through the hot water control valve and a rotameter to the heating tube returning back for recirculation.

The hot water control valve is of the needle type and is actuated by a stepper motor which is geared to the cam spindle. The hot water flow rotameter gives a qualitative indication of the hot water flow but not accurate measurement.

A constant head tank supplies liquid freon to the vaporiser tube. A centrifugal pump is used to pump freon liquid from a bulk storage tank to the constant head tank; the overflow being returned to the storage tank. A ceramic primary filter is fixed in the line from the storage tank to the constant head tank to prevent dirt or scale present in the storage tank from entering the system. A secondary ceramic filter is encountered by the freon liquid on the line from the constant head tank to the vaporiser tube to remove any remaining particles which may have become present in the system. Both of the filters are extremely important components to prevent blockage of the freon feed control valve. Other instruments on this path include two hand valves, a control valve, a rotameter and a turbine meter. The freon feed control valve, like the hot water valve, is of the needle type where the needle is displaced by an eccentrically mounted circular cam via a thrust arm, and is actuated by a stepper motor. The two hand valves, located one on the upstream side of the freon feed valve and one on the downstream of the secondary filter, are incorporated for easy removal of the filter or the valve during

system operation. Qualitative assessment of freon flow is achieved by the freon rotameter as with the hot water rotameter, whilst actual flow of freon is monitored by the turbine meter.

As the liquid freon enters the vaporiser tube, it receives heat from the heating tube and starts to convert into vapour. The freon liquid boils at 47.6°C at atmospheric pressure, and thus, the hot water which is at about 78°C is ideally suitable as the heat source.

The freon vapour passes through the top of the vaporiser tube to a cold water flow condenser, the condensate being returned to the storage tank. A measure of the vapour flow is obtained by passing it through an orifice plate which has a mercury "U" tube connected to it. Thermocouples are incorporated with the intention of measuring the temperature of the liquid present at the lower portion of the vaporiser tube, the freon vapour at the upper section of the tube and the inlet and outlet hot water flows. All the thermocouples are made of copper constantan material and are electrically insulated, The ambient temperature is measured by a thermistor.

Freon vapour pressure is obtained by the use of a bridge transducer at the top of the vaporiser tube whilst the base pressure is obtained by the use of potentiometric transducer positioned at the base of the tube. Freon height in the vaporiser tube is obtained by inference from the two pressure measurements.

The two valve positions are obtained by the use of two circular potentiometers situated, one on each control valve.

In a multivariable mode the measured values of height and vapour pressure are taken as the control variables - these being operated on by an Argus 500 control computer (which is being replaced by a I-MIC Kratos computer system). The computer provides control signals to two stepper motor actuators for the freon feed valve and the hot water feed valve. Either measurement of the controlled variables can be routed to either of the actuators with either or both loops performing in an open or closed loop mode.

5.3 Instrumentation and computer control

Pressure Transducers:

The height of freon liquid in the vaporiser is inferred from measurements of vapour pressure and base pressure. Vapour pressure is measured by way of a strain gauge bridge pressure transducer whose positive displacement range of 0-30 ins.wg. out of its overall range of ± 30 ins.wg. is employed. A nominal output of 10mv for an applied pressure of 30 ins.wg. is obtained with the input set at 3.93 volts, permitting the transducer output signal to be read by the computer as a low level analogue input of 0-10mv.

Base pressure is measured by a wire wound potentiometric type pressure transducer of 0.2 psig. With an applied 10v, an output signal of 0-10v enters the computer as a high level signal giving measurement of base pressure. Both transducers exhibit a high degree of linearity.

5.4 Final Control Elements

The two stepper motor actuated needle valves form the final control elements. By virtue of their nature as positional devices, a stepper motor is stepped by output pulses from the computer without the necessity of converting these pulses into analogue form, and with or without the setting of the direction line. This means that if a direction bit is set (equals unity) the valve will open and if it is not set (equals zero) the motor will close. These pulses generate a switching operation energising the motor stator coils leading to the desired step rotation. A compensation network is used between the driving circuit and the stator windings to make amends for the inherent inductance in the stator windings and to shape the drive pulses for an appropriate rate of rise.

The motor spindle rotates 3.75° for each computer pulse and 330° of cam rotation is achieved for a full cycle. The arrangement of the cam is so arranged that a valve position of 2.5v corresponds to fully closed valve whilst a reading of 7.5v corresponds to fully open position. This arrangement is implemented by the software so that whenever a value outside the range 2.5-7.5v is encountered during start up, rotation can be made so that the working range is entered.

5.4.1. Thermistor:

A bead thermistor and its associated circuit are used for ambient temperature measurement. To avoid the effect of brief temperature fluctuations, the thermistor is embedded in an aluminium block which is positioned at the thermocouple cold junctions so that the temperature of the cold junction can

be determined accurately. An operational amplifier is introduced to enable the differential voltage of the bridge network, to which the thermistor is connected to obtain its value with respect to zero. When the thermistor has been calibrated, linear range was obtained only within 14-34°C. However, this range is adequate, since the system is unlikely to be operated outside this range of values of temperature.

5.4.2 Turbine Meter

This device contains a vaned rotor whose speed of rotation depends on the velocity of the liquid flow. The vanes break a light beam to a photodiode at a frequency proportional to the flow velocity. When in use, the turbine meter must always be inclined at an angle so as to ensure that it is filled for all flows, otherwise, for low flow rates, the turbine meter will not be filled with liquid which may pass the rotor without rotating it. The turbine meter exhibits a good degree of linearity.

5.4.3 Temperature Control of Hot Water Supply

The temperature control of the heating tank operates independently from the process computer control loops. The purpose of this control is to keep the hot water supply at constant ^{temperature}/within certain limits. Thus, as heat is lost by hot water either to the surroundings or to the system, the control circuit comes into effect and compensates for these losses.

The heater control circuit is shown in Fig.5.2.2b. Power supply to the immersion heater which is used to heat the water is controlled by a pulse fired triac. The temperature of the hot water is sensed by a thermistor which forms one of the four arms of a resistive bridge. Another arm is formed by a resistor which is used to set the temperature at which the hot water is to be maintained. The remaining two arms form an equal rate arm across the 4v D.C. bridge supply. The bridge output voltage forms the input to an operational amplifier whose gain is such that a temperature change of about 2° causes an output voltage change of 0 to +5v applied to the control input of the pulse firing zero crossing switch shown in Fig. 5.4.1. The resistor R determines the rate at which the voltage produced by the ramp generator rises. In the vaporiser operation R has been adjusted to give a cycle time of 0.5secs. When the output voltage reaches +5v the ramp resets to 0v and restarts. The comparator gives a logic 0 when $V_c < V_{\text{ramp}}$ and a logic 1 when $V_c > V_{\text{ramp}}$. A positive pulse is produced by the zero crossing detector at the beginning of each half cycle of its a.c. supply. The triac is triggered by the output of the AND gate. Since the mains supply which operates both the heater and the zero crossing detector has a frequency of 50 Hz, a maximum of 25 cycles are admitted to the heater in each 0.5 secs. ramp generator period. If the water temperature is more than 1°C below the required temperature, the system is adjusted to provide full power but when it is 1°C above that required, the power is linearly reduced to zero.

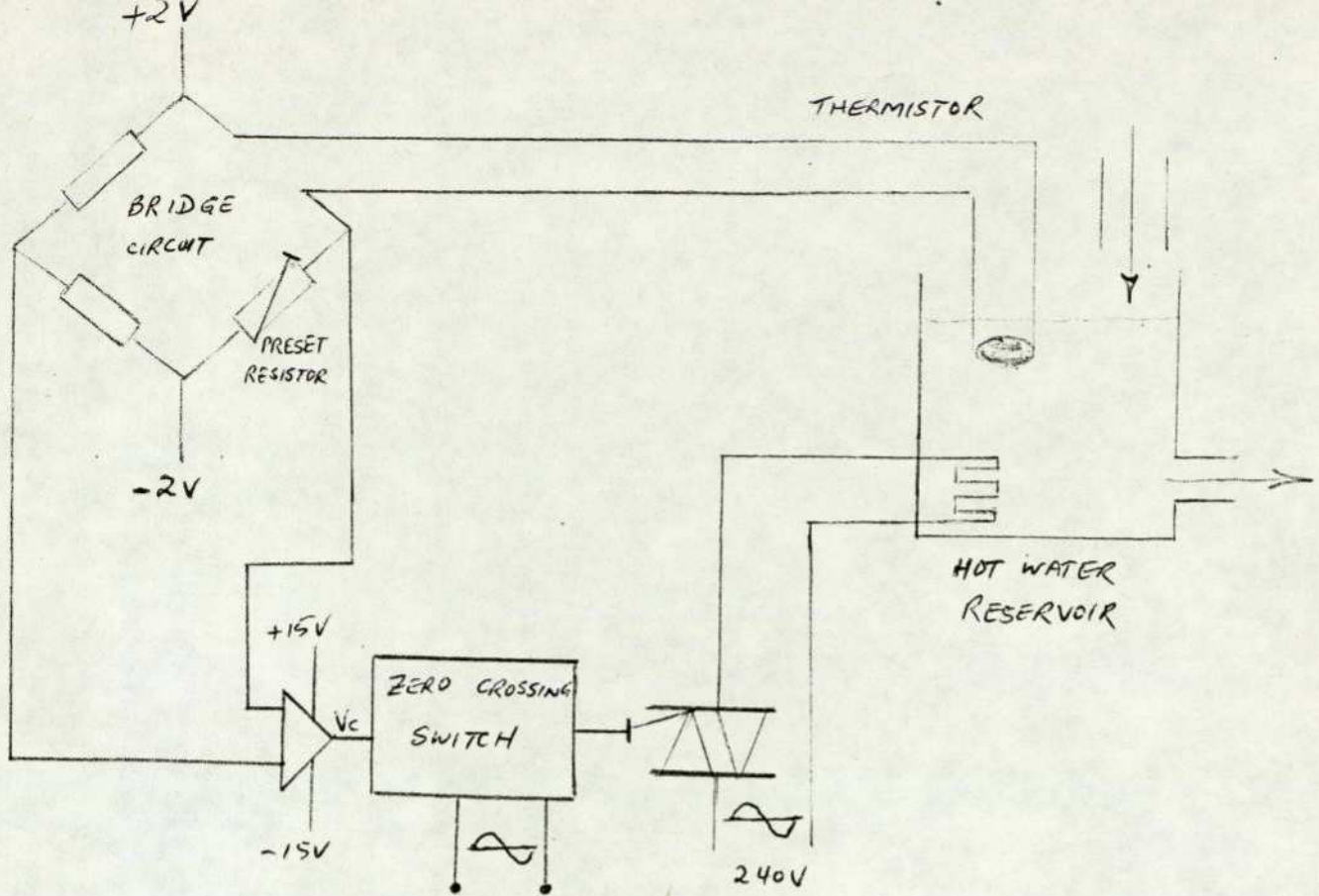
During rig operation, heat is lost by the hot water to the process causing the inlet hot water temperature (the temperature of the hot water returning to the tank) to be less than the outlet. In addition heat is being lost to the surroundings causing the outlet hot water temperature to settle between the 1°C limits. In fact, the present resistor in the bridge circuit has been adjusted to yield hot water outlet temperature of about $78^{\circ}\text{--}80^{\circ}\text{C}$.

These temperature fluctuations have a direct effect on the vapour pressure inside the vaporiser tube. It is likely that the apparent periodical fluctuations on the vapour pressure response are caused by these temperature fluctuations. So far these fluctuations have been ignored in the modelling processes on the assumption that their effects are negligible.

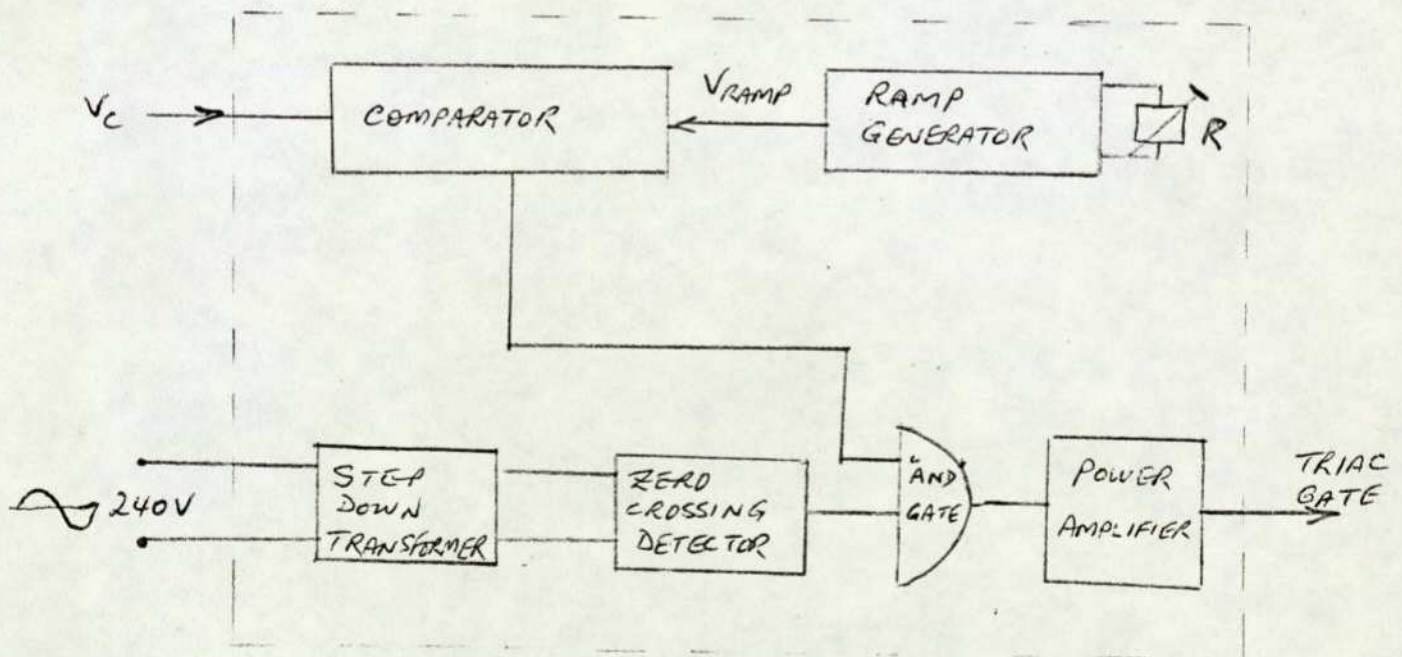
In this research, an attempt is being made to account for these variations by attaching to the hot water temperature a time-dependent entity on the assumption that ignoring them causes model structural errors. This implementation will be discussed in Chapter 6.

5.5 Computer Control

The software package of the vaporiser system for use on the Argus 500 computer (which is being replaced by I-MIC Kratos computer) had been started by earlier workers but was completed by Ellis (1979). The programming was done in Astral - one of the languages of Argus.



(a) General Arrangement of Hot Water Temperature Control



(b) Zero Crossing Switch (Type RS-305-800)

Fig.5.2.2b Hot Water Temperature Control

The control program accepts analogue inputs from the vaporiser instrumentation via an ADC interface and after manipulation, supplies the relevant control signals to the actuators. The program includes facilities for data logging, plotting and printing as well as a conversational mode which allows an operator to set flags and adjust parameters during the running of the system.

The program suit consists of two separate sub-programs; the foreground program and ^{the} background program. The foreground program contains the main activities of the computer and consists of six separate routines; the organiser routine, the initialisation routine, the control routine, the stepper motor routine, the plotter routine and the logging routine. The background program contains the conversational facilities. Ellis (1979) gives details of these two programs with a full description of the function of each routine. Facilities obtained with this program suite include single or multivariable control and open or closed loop operation.

5.6 Open Loop Response

The usual method to operate the system in an open loop mode has been to adopt the following procedure:

- 1) the vaporiser is first operated under closed loop mode. For this purpose the required setpoints are fed into the computer together with the gains and the integral action times of the two control loops (these are required by the control algorithm employed by the computer).

The computer is left in this mode until the system settles down (a continuous monitoring is obtained by an on-line teletype which outputs selected results at intervals of 10 seconds apart).

- 2) Once the system settles down to a steady state condition, the last few position values of the two stepper motors are averaged out.
- 3) These average values of the two stepper motor positions are fed into the computer as new set point values. At the same time the closed loop control is abandoned and the system is operated under an open loop mode, until a steady state condition is reached.
- 4) A step change in one of the two valve positions is applied and the system is left to operate under this open loop mode for a certain period of time. The responses obtained for the freon liquid height and vapour pressure are the open loop responses of the system.

Since, for identification purposes, only open loop responses are required, the vaporiser rig has been operated under different conditions in an open loop mode following the procedure above. The conditions under which the system has been operated included variations in the environmental conditions, such as atmospheric pressure variations, ambient temperature and freon feed temperature. Under the same environmental conditions, responses were also obtained for different changes in the two control valve positions, as well as the initial steady states.

In the next chapter, some of these responses will be presented to provide real observational data needed for identification purposes. The model of the vaporiser system, which is discussed in Section (5.7.1.) is operated under the same conditions in order to compare the model performance with that of the real system. However, for the sole purpose of shedding some light on the behaviour of the vaporiser, Figs. (5.2.3) and (5.2.4) which show the vapour pressure and the height responses, are presented. Starting from steady state conditions with a height of 0.1m and vapour pressure of 10' wg, a 20% step change was applied to the freon feed control valve. As more freon entered the vaporiser tube, the heat available from the hot water was diverted to heat the incoming flow, causing an initial drop in the vaporisation process, and consequently, an initial drop in the vapour pressure before it rises to its new value, causing a non-minimum phase response to occur. This is clearly shown in the vapour pressure response. Of importance in these responses is their oscillatory nature despite their overall trend of rising with time. The causes behind these oscillations are for speculation. They may be due to the bubbling nature of the boiling processes, or to unknown disturbances within the system. Certainly, the hot water temperature which exhibits some sort of variations may have some effect on this. For these reasons, the identification process is of prime importance especially on such systems which exhibit unpredictable variations. In the next Chapter, which is concerned with the identification of the vaporiser system, this problem will be dealt with and solutions will be attempted. However, it must be emphasised here that the identification process cannot uncover the right causes of these disturbances but, rather, the engineering judgement regarding these causes will contribute greatly towards overcoming their undesirable effects.

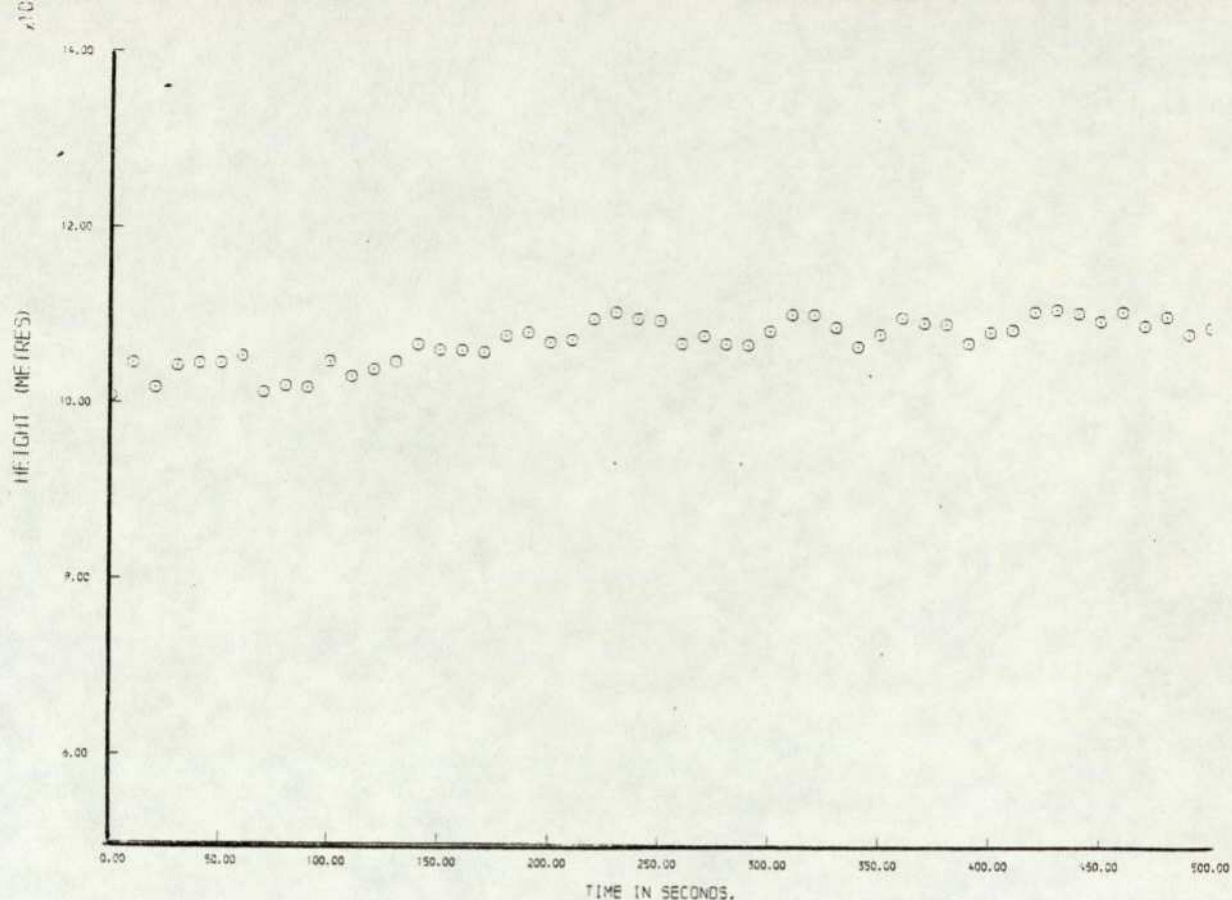


Fig. 5.2.3. Open Loop Height Response of the Vaporiser Rig to a 20% Step Change in Freon Valve Position VP1.

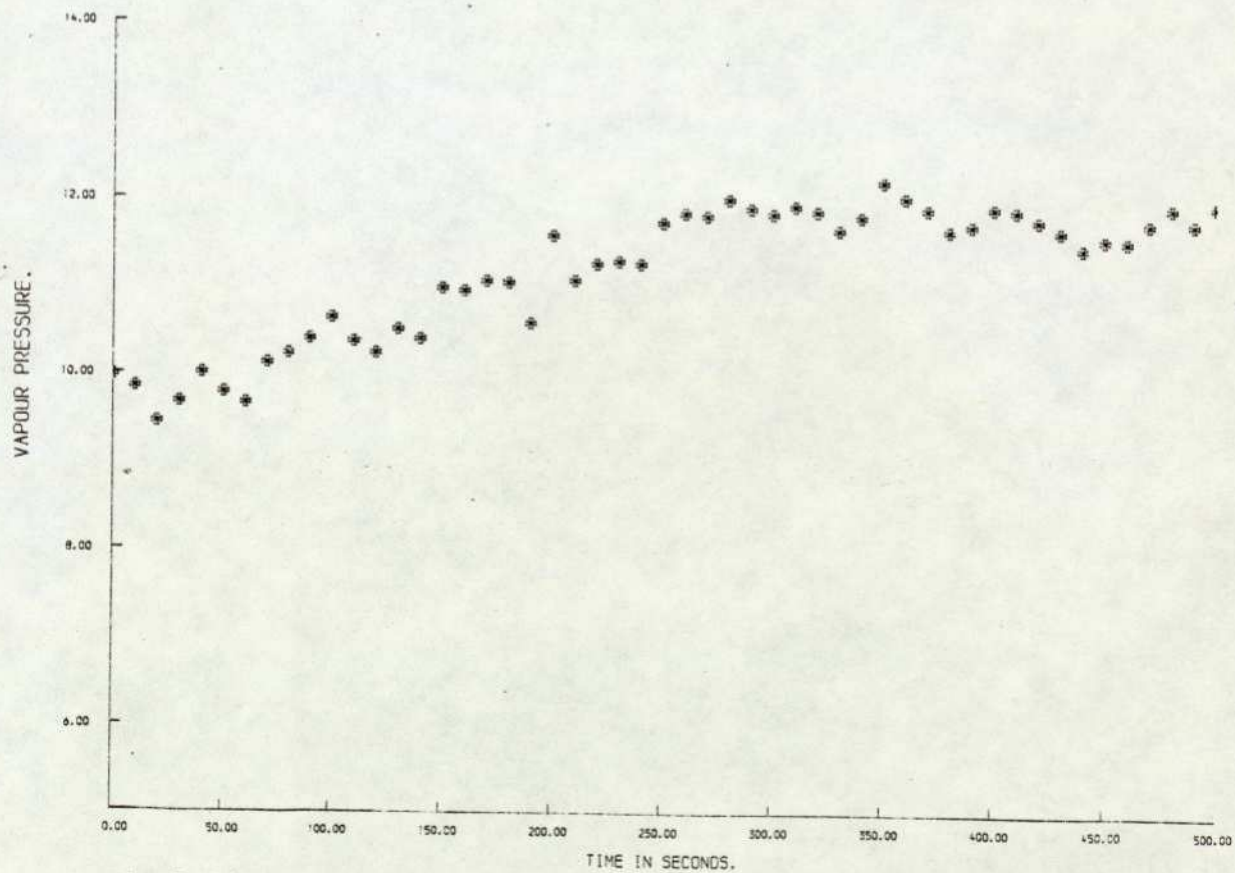


Fig. 5.2.4 Open Loop Vapour Pressure Responses of the System to a 20% Step Change in VP2.

5.7 Vaporiser System Models:

When modelling a dynamic system, the assumptions made about its behaviour play a crucial role in determining the nearness of the model to reality.

The vaporiser system is of the flow boiling class, but the working fluid flow rates encountered are very low. This state of affairs allows for the assumption that two distinct regions of perfectly mixed pure liquid and also perfectly mixed pure vapour exist in the vaporiser. Earlier workers on the vaporiser system developed mathematical models making use of this assumption. But in flow boiling processes of high flow rates, consideration is given to the existence of a two-phase region with liquid and vapour together in a simultaneous flow. A simple technique based on this assumption is provided by homogeneous flow, whereby no relative velocity is taken to exist between the phases. Ellis (1979) presented these two groups of vaporiser system models with only limited attempts made at model simplification (the two groups being those models based on the assumption of the existence of a two phase region). Using the perfect mixing assumption, three types of models were developed, the first was based on the assumption that freon boiling temperature possessed fast dynamics, the second based on the assumption of slow boiling dynamics and the third considered the heating tube in its actual construction of concentric tubes. The homogeneous models were then examined for fast and slow dynamics. The system model considered by Ellis for either

group is essentially a two input/two output model, with the control signals to the valves as the inputs and the measured variables of freon liquid height and vapour pressure as the outputs.

In this research only perfect mixing, fast boiling dynamic model is considered. This is because the identification process is a lengthy procedure due to its iterative nature, and if highly complicated models are considered, convergence may not be guaranteed within the limited computing facilities available. On the other hand, this relatively simple model of the vaporiser reflects the general behaviour of the system, and, at the same time, suffices for the purpose of investigating the performance of the identification techniques of interest. If needed, the results obtained using this simplified model may be extended to the models mentioned above which were developed by Ellis.

Also Ellis (1979) found that the simple model was adequate for control system design purposes.

5.7.1. Perfect Mixing Model - fast dynamics assumptions:

For this model, the operation of the plant is shown by the schematic diagram in fig. 5.2.2. In this diagram two distinct regions of pure liquid and pure vapour are taken to exist, with the heat provided by the central tube. The assumptions underlying this model are:

- (1) Perfect mixing takes place between the boiling liquid and the freon feed as soon as the incoming flow enters the tube, i.e. an average freon temperature is assumed. This is the basic assumption of this model type and is justified on the grounds of low fluid flow rate which give the incoming liquid time to mix properly with the boiling liquid present in the vaporiser tube due to the turbulent nature of the boiling process.
- (2) The freon liquid height in the vaporiser tube is well defined i.e. sharp distinction exists between liquid and vapour.
- (3) Due to the low flow rates considered, momentum effects are negligible.
- (4) The heat losses to the vaporiser structure and vapour are either of negligible amount or are included in the heat losses term.
- (5) Vapour and liquid contents are in equilibrium. Hence, majority of heat losses occur in the liquid section, and,
- (6) liquid density, specific heat and latent heat of vaporisation of freon liquid are constant. Due to the small temperature variations at any given operating point this assumption is justified.

- (7) The heating tube is of single tube construction with the hot water entering from the base and leaving from the top of the tube. The actual tube is formed from two concentric tubes, with the hot water entering through the central tube and leaving through the outer. This can be justified on the basis that the heating tube runs down to almost the bottom of the vaporiser tube, thus enabling the hot water to flow upwards.

In addition to these assumptions, the heat flux into the freon liquid is assumed to be determined by freon level in the vaporiser. The heat flux is considered to be used in the following ways: part of it is used to raise the temperature of the incoming liquid to the boiling point, part is used to provide the latent heat of vaporisation and the remainder is lost. If, for example, a step change is applied to the freon flow in order to increase the vapour pressure, then part of the heat is used to supply latent heat to the increased liquid flow resulting in a reduction of vaporisation and hence a transient drop in vapour pressure. This pressure drop allows the liquid level to rise even faster and continues until the vaporisation rate again builds up (due to the increased heat transfer area) increasing the pressure until, together with the hydrostatic head, it balances the inlet pressure. The heat balance of the liquid in the model derives from this proposition and thus involves the pre-supposition that the boiling dynamics are very fast.

Valve Characteristics

Both valves have a non-linear relationship between valve position and flow of the form

$$R_{A1} = f_1 (VP_1) \quad \dots \quad 5.5.1.$$

$$Q_W = f_2 (VP_2) \quad \dots \quad 5.5.2.$$

where VP_1 and VP_2 are the valve positions of the freon feed and hot water feed valves respectively.

R_{A1} is the relative aperture for the freon valve and Q_W is the hot water flow.

Freon Inlet Flow

The equation of flow through the inlet pipe and freon valve is obtained by combining the equation of flow (Coulson, 1964) through the inlet pipe (ignoring the dynamic term since the time constant is small) and the equation of flow through a valve (Franks, 1972) thus

$$Q_L = \sqrt{\frac{P_I - P_B}{K_1 + K_2/R_{A1}^2}} \quad 5.5.2.$$

where Q_L = freon flow (m^3/S)
 P_I = the freon valve inlet (N/m^2)
 K_1 = the inlet pipe constant (SI units)
 $K_2 = 1/C_d^2$, the valve constant (SI units)

Vaporiser Base Pressure:

The pressure at the vaporiser base is taken to be the sum of the vapour pressure P_v and the pressure due to the head of freon liquid in the vaporiser, i.e.

$$P_B = P_v + \rho_L g z \quad 5.5.3.$$

where

ρ_L = density of liquid freon (kg/m^3)

g = gravitational constant (m/s^2)

z = height of freon liquid in the vaporiser (m)

Vapour Outlet Flow

It is assumed that the vapour outlet friction factor is substantially constant where the following equation is used to calculate the vapour flow:

$$Q_v = \frac{K_G}{\ell_g} \sqrt{\frac{P_v^2 - P_s^2}{T_B}} \quad 5.5.4.$$

where

Q_v = the vapour flow (m^3/s)

ℓ_g = density of the vapour (kg/m^3)

P_s = vaporiser downstream pressure (N/m^2)

T_B = the saturation temperature of liquid freon
at pressure, P_v ($^{\circ}K$)

Vapour Mass Balance:

$$\dot{M}_G = \ell_L Q_B - \ell_g Q_v \quad 5.5.5.$$

where

$$\ell_g = M_G / (V_{olv} - A_v z) \quad 5.5.6.$$

where M_G = the mass of vapour present in the
vaporiser (kg)

Q_B = the boil-off rate (m^3/s)

V_{olv} = the total internal volume of the
vaporiser (m^3)

A_v = area of vaporiser (m^2)

Equilibrium Relationships:

Due to the equilibrium assumptions of the model, the vapour temperature is the same as the boiling liquid temperature and will be the saturated vapour temperature. The temperature and pressure of the saturated vapour is related to the vapour ℓ_g by the following relationships:

$$T_B = f_3 (\ell_g) \quad 5.5.7.$$

$$P_v = f_4 (\ell_g) \quad 5.5.8.$$

Using the available data, the following linear relationship is obtained when vapour pressure P_v is plotted against vapour density (Ellis 1979)

$$P_v = (-0.79 + 0.0148 \ell_g) \cdot 10^5 \quad 5.5.9.$$

Also from the plot of P_v against $\log (\ell_g T_B)$, the following relationship is obtained over the operating range of interest:

$$P_v = 53.7 (\ell_g T_B)^{0.971} \quad 5.5.10.$$

Liquid Mass Balance

Applying the principle of the accumulation of liquid mass in the vaporiser tube gives the following differential equation:

$$\dot{z} = \frac{(Q_L - Q_B)}{A_v} \quad 5.5.11.$$

Boil-Off Equation

The assumption that the heat input is instantly used for sensible and latent heat of vaporisation together with an amount of heat lost yields the following boil-off equation (Franks, 1972):

$$Q_B = \frac{\pi D_v z H_{tc} (T_w - T_B) - \rho_L Q_L C_V (T_B - T_i) - L_A}{\ell_L \lambda} \quad 5.5.12$$

where

- D_v = diameter of the vaporiser tube (m)
 T_w = the hot water temperature ($^{\circ}\text{K}$)
 H_{tc} = heat transfer coefficient (SI units)
 C_v = specific heat of liquid freon at constant volume ($\text{J/kg}^{\circ}\text{C}$)
 T_i = freon inlet temperature ($^{\circ}\text{K}$)
 L_A = the losses to the surroundings J/S
 λ = latent heat of vaporisation of freon J/kg

Hot Water Heat Balance:

According to the assumption that heat is supplied by a single tube at the centre of the vaporiser, hot water flows uni-directionally, that is, water flows from the bottom to the top of the vaporiser.

$$\frac{d}{dt} (\pi r^2 z C_p \rho_w T_w) = \begin{aligned} &= \text{rate of heat flow in} \\ &- \text{net heat flow out across boundary} \\ &- \text{heat flow to freon} \end{aligned}$$

The heat balance equation, after manipulation (Roberts and Ellis, 1977) becomes:

$$\dot{T}_w = \frac{Q_w (T_o - T_w)}{\pi r^2 z} - \frac{2 \cdot H_{tc} (T_w - T_B)}{r C_p \ell_w} \quad 5.5.13$$

where r = radius of the heating tube (m)

C_p = specific heat of hot water ($J/kg^{\circ}C$)

T_o = hot water inlet temperature ($^{\circ}K$)

5.8 Computer Implementation

The mathematical model presented in section (5.7.1) of the vaporiser system has been simulated on the CDC 7600 computer to be used as the basis for the identification process. The model consists of a set of algebraic equations and a set of linear and non-linear differential equations representing the state variables of the model. The algebraic equations include equations to calculate variables such as vapour density (ρ_g), vapour pressure (P_v), boiling temperature (T_B), vapour flow (Q_v), freon valve relative aperture (R_{A1}), hot water flow (Q_w), base pressure (P_b), freon inlet flow (Q_L) and boil off flow (Q_B). Since the two control valves have non-linear characteristics, data obtained when calibrating them are used to interpolate the values of R_{A1} and Q_w which correspond to the two valve positions V_{P1} and V_{P2} . The differential equations represent the state variables of the system which are mainly the freon height (Z), the mass of the vapour (M_g), the hot water temperature (T_w), (inside the heating tube which is different from that of the hot water tank due to the loss of heat to the freon and other losses) the measured value of the base pressure (M_{PB}) and the measured value of the vapour pressure (M_{PV}). The measured value of height (M_{VH}) is inferred from these two measurements which represent the outputs of two pressure transducers and cannot be considered an output of a height transducer since it cannot be measured directly.

The system has been simulated using the subroutine MODEL which is contained within a program VAPOUR. In this program, values of the various constants and variables of the vaporiser system are read in. These values include dimensions of the vaporiser tube, valve constants, physical properties of water and freon, data defining the valves

characteristics, setpoints and atmospheric dependent variables. Initial conditions are then calculated using the available steady state data. Valve characteristics are dealt with by subroutine FUNC (See Appendix 4).

The open loop responses of the model are obtained by the use of an integration procedure. The process is started by applying a step-change to one of the two valve positions (which are normalised to lie in the range 0-1). This step change causes changes in the values of the variables leading to changes in the derivatives of the state variables (at steady state conditions, the derivatives have the value of zero). The integration procedure (which must be chosen to suit the particular case) uses these derivative values to calculate new values of the state variables. This process is continued until the time span is covered yielding the behaviour of the state variables over this time span which characterises the vaporiser system.

The integration process employed here is the NAG subroutine D02AJF (which has been used in Section 4.2) which integrates a system of first order ordinary differential equations over a range using a divided difference formulation of Gear's method (1957) for stiff system of equations (for details see Appendix 2). This is a step-by-step integration procedure and requires the specification of the required integration accuracy (in any case it must not be bigger than 10^{-3}). The routine chooses the step size and the order of the method to try to obtain the specified accuracy with minimum computation. As has happened in this research work, the use of larger values of integration accuracy will result in inaccurate, and may be, meaningless results.

In this research, in which interest is focussed on open loop responses for the identification process different steady states conditions are considered whereby a step change is applied to one of the two control valve positions, and the ensuing responses embarked upon and compared with the corresponding real system responses obtained under the same operating conditions. Details of this will be given in the next Chapter, but an example of such conditions is given here with the intention of conveying an overall picture of the expected form of responses. Fig. 5.8.1 shows the open loop responses of freon height and vapour pressure. They were obtained when operating the model under the same conditions as those mentioned in section (5.7) whereby the steady state values of freon height and vapour pressure were 0.1m and 10'w.g. respectively, atmospheric pressure of 1.02245 bars, $T_L = 295.74^{\circ}\text{K}$, and subjecting the freon feed valve to 20% step change in its steady state position. The freon height response, as expected, rises steadily due to the increase in the incoming flow whilst the vapour pressure response exhibits the non-minimum phase phenomena for about 30 seconds and then starts to rise sharply due to the rise in the freon height and the subsequent decrease of the space available for the vapour causing this sharp increase in the vapour pressure.

Fig 5.8.2 shows the freon height and vapour pressure responses, under the same conditions as above, for a 20% step change in the hot water valve position. The immediate effect is a sharp rise in vapour pressure due to the sensitivity of vapour pressure to changes in hot water temperature. The height diminishes slowly from its steady state value due to the higher rate of vaporisation caused by the increased inlet

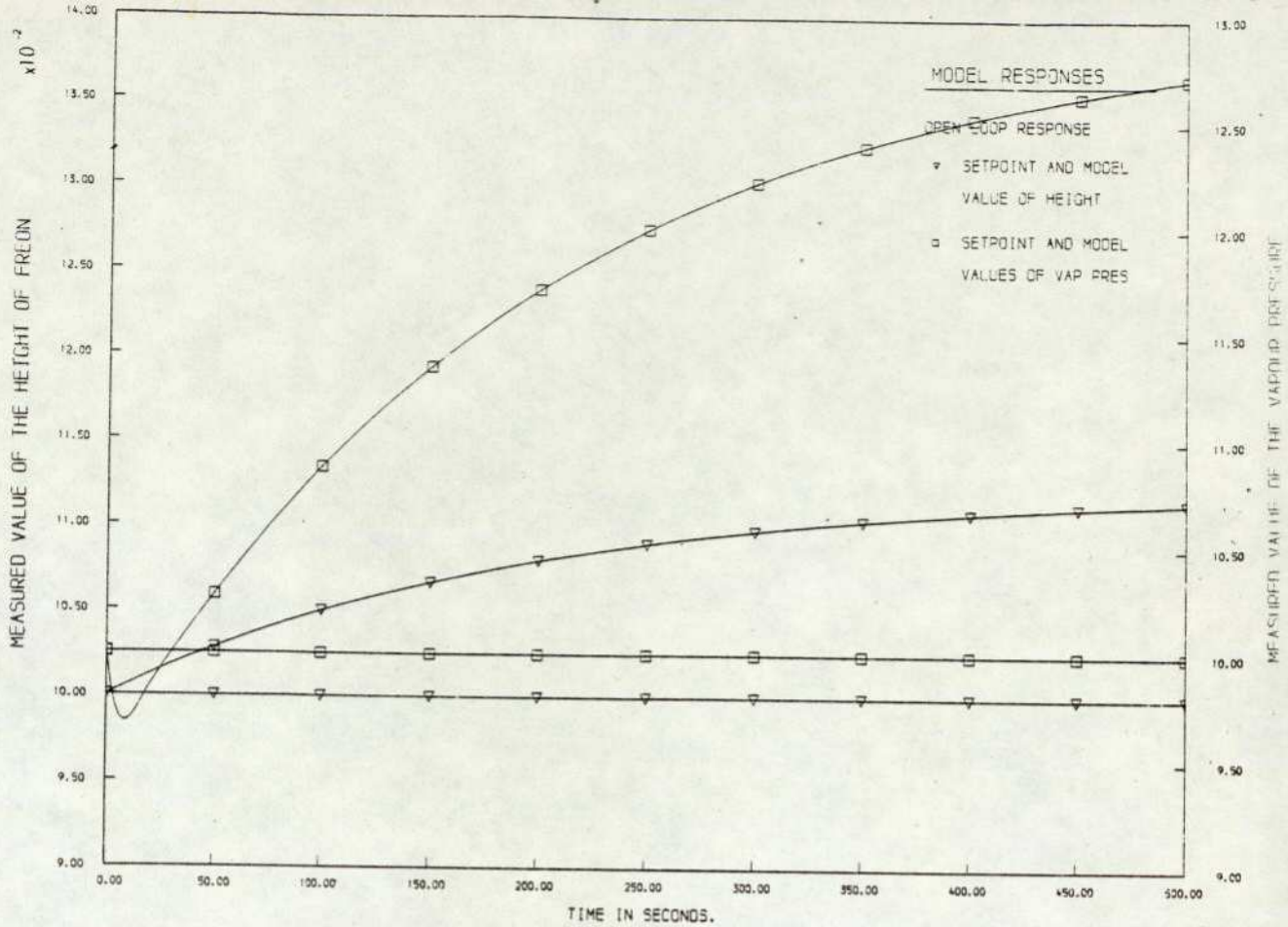


Fig.5.8.1. Open Loop Height and Vapour Pressure Responses of the Model to a 20% Step Change in VP1.

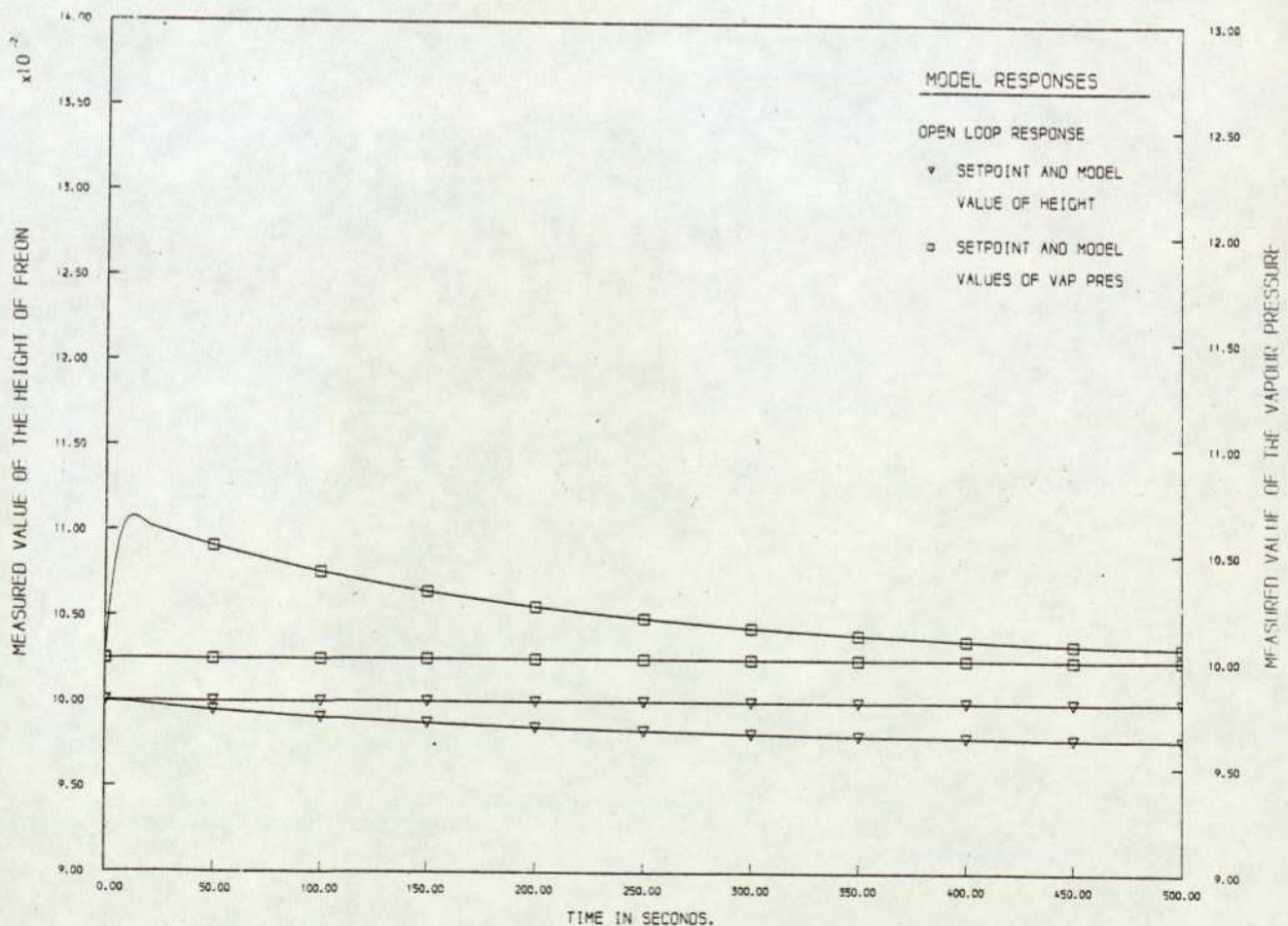


Fig.5.8.2. Open Loop Height and Vapour Pressure Responses of the Model to a 20% Step Change in Hot Water Valve Position VP2.

heat of the hot water. However as time drags on, the vapour pressure drops due to the fact that as the liquid height diminishes there is less heat transfer area, and consequently, a reduced boil-off rate and an eventual drop in vapour pressure from its transient level.

However, when comparing the model and system responses an obvious difference is the oscillations on the system responses which are not apparent on the smooth model responses. Although boiling processes are of bubbling nature, a feature to which such oscillations may be attributed a deeper and more elaborate account must be made of this phenomenon. Possible reasons for such undetected disturbances are; inaccurate model parameter values, such as the heat transfer coefficient between the heating tube and freon liquid, or model structural deficiencies. These problems will be dealt with extensively in the next Chapter.

Initially, model parameters were calculated using steady state relationships. For example, the steady state value of H_{tc} is calculated using the following equation:

$$H_{tc} = \frac{Q_L \cdot \rho_L \left[\lambda + c_V (T_B - T_i) \right]}{\pi \cdot D \cdot Z (T_W - T_B)}$$

It remains to see whether the identification process of the next Chapter will yield the same parameter estimates especially after compensation for the apparent model deficiencies.

5.9 Closed Loop Control

The multivariable control algorithm devised by Ellis (1979) for the vaporiser has been very effective in controlling the two interacting state variables,

H_T and P_V . When operating the vaporiser rig in a closed loop multivariable control mode (Fig.5.9.1) the system seemed to respond easily to set points step changes, and eventually settled down to the required setpoint. When this multivariable control algorithm was simulated on the CDC 7600 computer in conjunction with the open loop model, the responses obtained for H_t and P_V to a 20% change in the height setpoint (i.e. S_{PH} changed from its steady state value of 0.1m to 0.12m) are shown in Fig. 5.9.2. The height rises from its steady state value trying to achieve the new setpoint, but it seems that it is quite oscillatory and it probably needs a longer time to settle down close to the setpoint. However, the pressure response displays only small departures from its desired value. The model height response is in fair agreement with that of the system although settling time is achieved earlier. However, the model does indicate the behaviour of the system for setpoint changes for most practical purposes.

Fig 5.9.3 shows height and vapour pressure responses for a 20% step change in vapour pressure setpoint. The behaviour of the model compared to the plant is not so encouraging. The vapour pressure response of the model does not agree very well with that of the real system which achieves the desired value in a relatively short time. The height response of both the model and the system only deviate slightly from the setpoint. The responses show that when the height drops slightly, the pressure drops accordingly supporting the argument that an opening of the hot water valve results in a rise in vapour pressure only to see a fall in height due to boil-off with a consequent reduction in vapour pressure.

However, the multivariable algorithm does not allow the height to fall, the freon valve acts to compensate for the height fall.

The open and closed loop system and model responses are in full agreement with those obtained by Ellis (1979). In fact, the open loop system responses discussed in Section 5.7 are those obtained by Ellis.

In the next Chapter where identification of the vaporiser system will be discussed, five different operating conditions including the one discussed here will be dealt with.

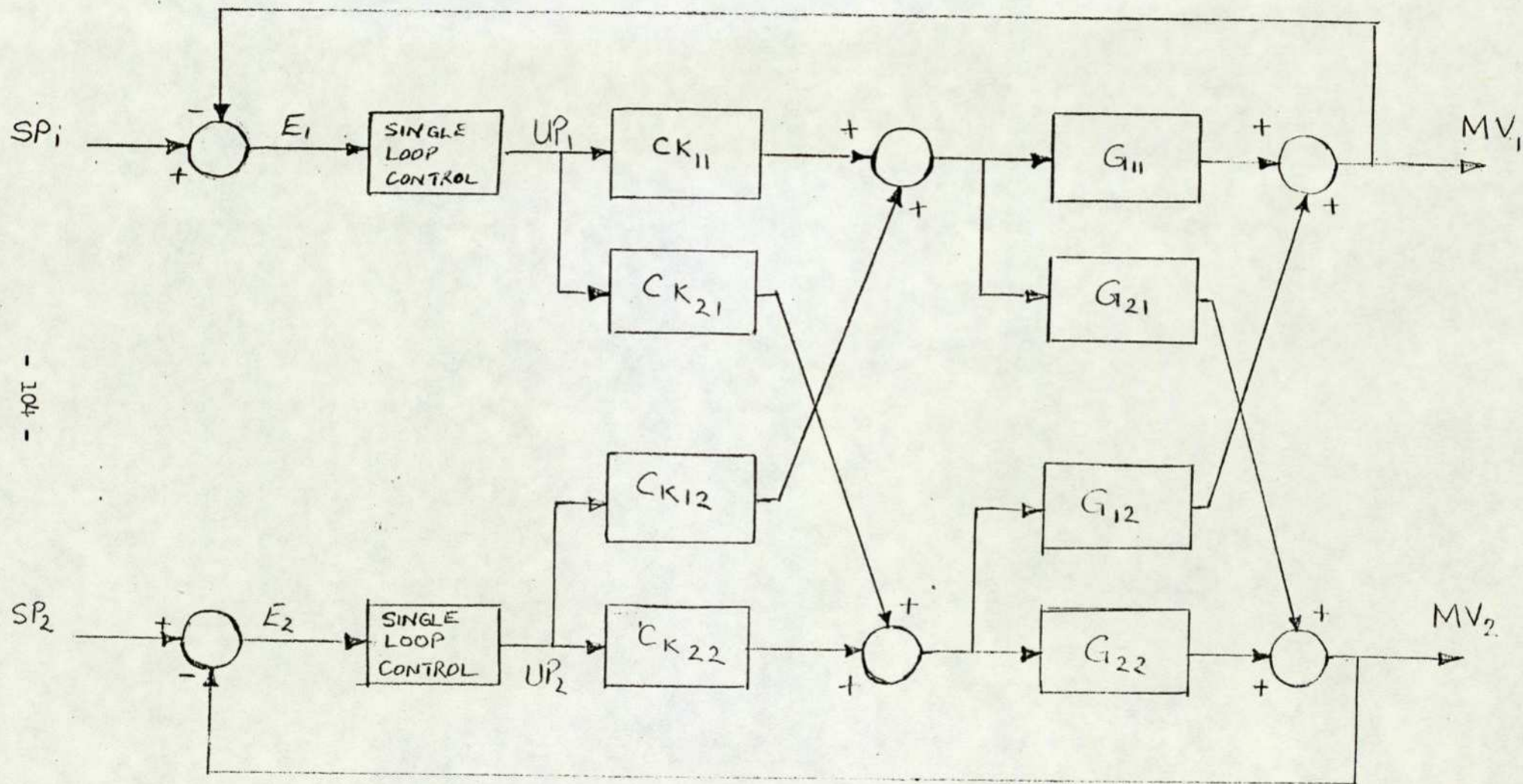


Fig. 5.9.1. Multivariable Control Scheme used on a Vaporiser System

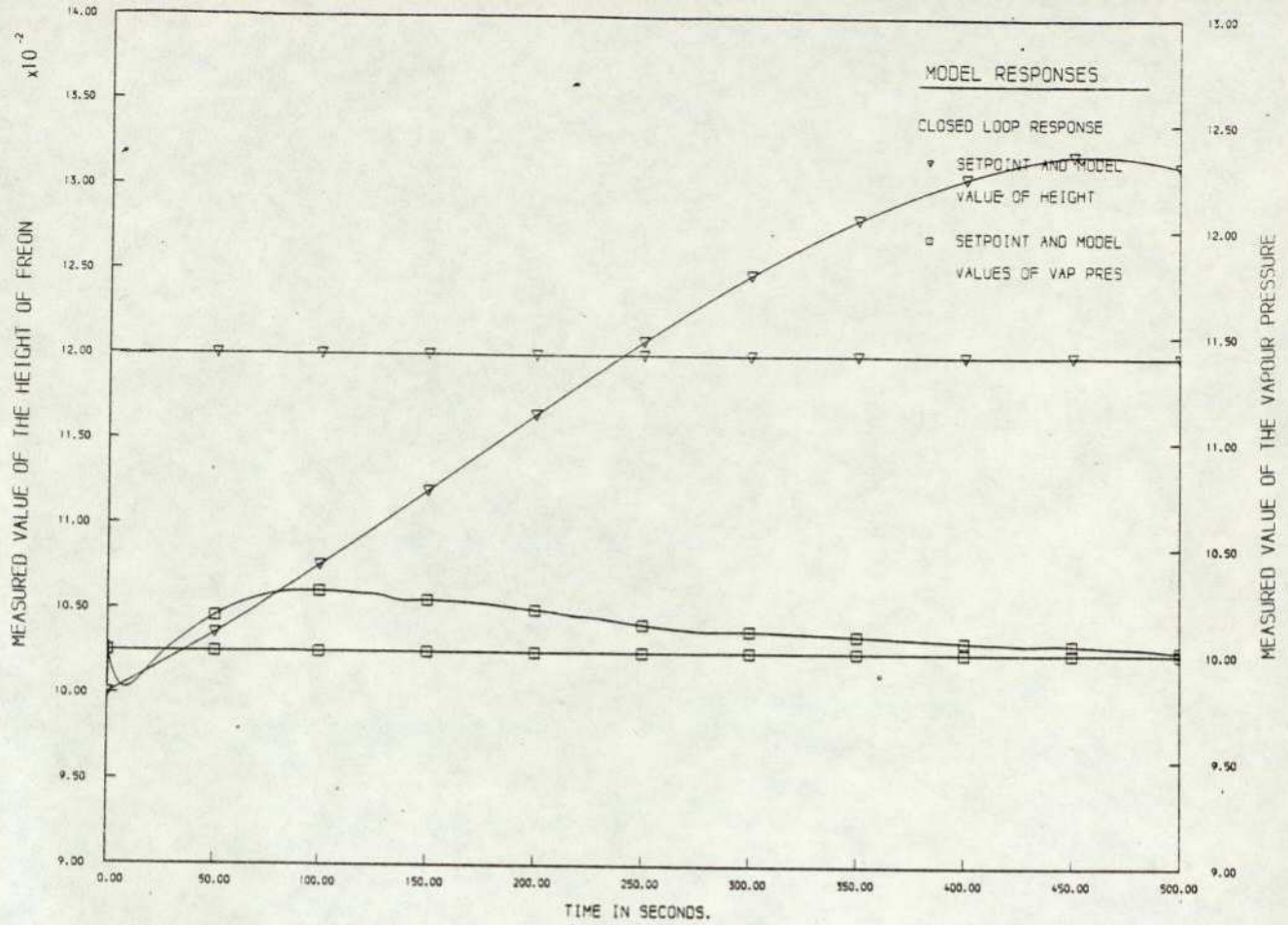


Fig. 5.9.2. Closed Loop Height and Vapour Pressure Responses due to a 20% Step Change in Height from 0.1-0.12m.

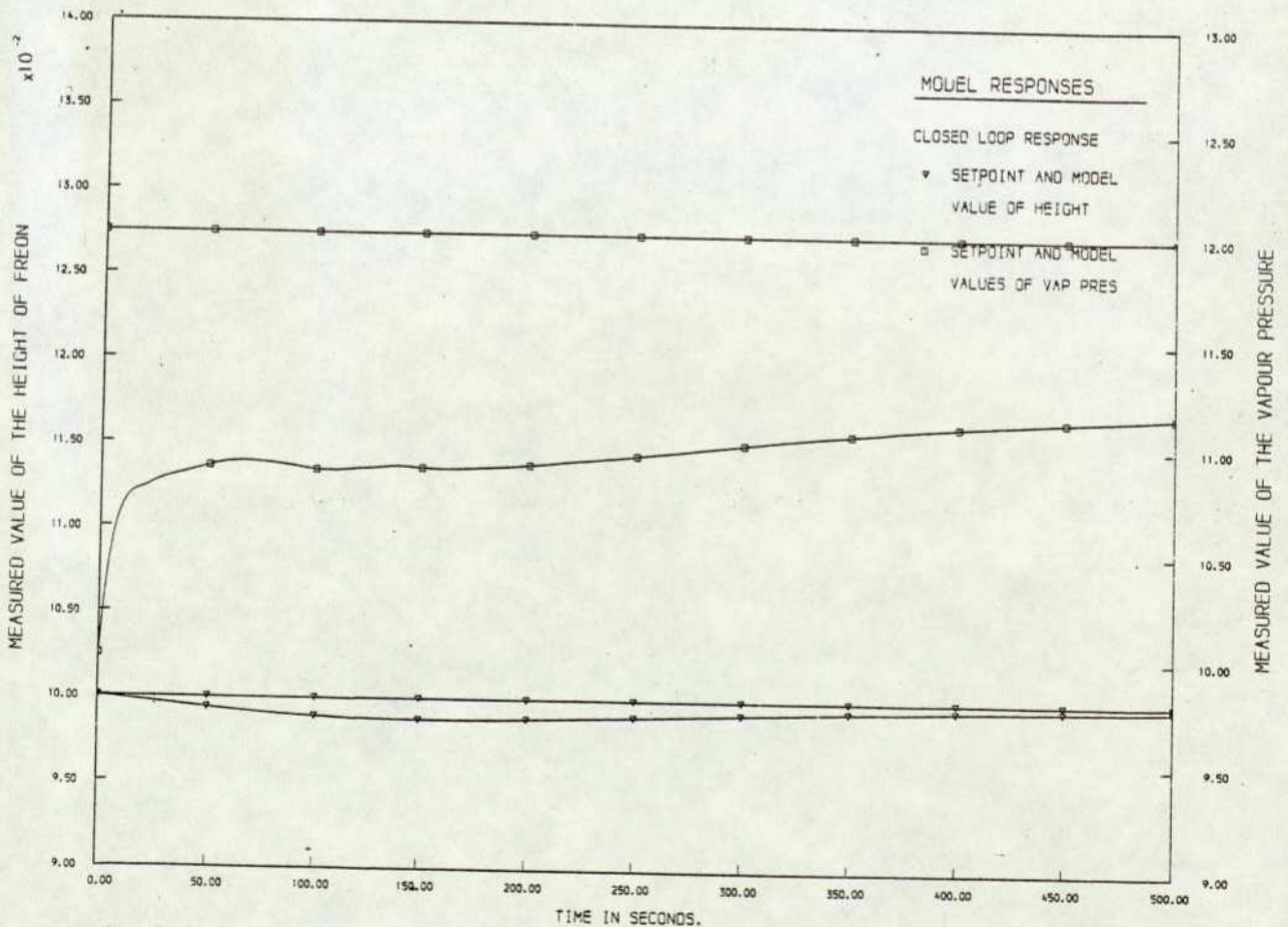


Fig.5.9.3. Closed Loop Height and Vapour Pressure Responses of the Model to a Step Change in Vapour Pressure Setpoint from 10 to 12".

Chapter 6

VAPORISER IDENTIFICATION

6.1 Introduction

The need to identify the vaporiser model arises from the desire to achieve accurate representation of the real system by the mathematical model. Of course, the mathematical model is based on knowledge of basic laws of Physics and Chemistry relevant to the system. However, this knowledge is not always complete especially with systems of relatively complex structure. After all, assumptions made about the system, often leading to simplification and approximation, play a significant role in degradation of modelling procedure. Simplicity is a notion whereby a researcher attempts to describe a high-order system (or equations) in a much lower-order form accepting the inevitable incurring errors. An example of this being Ohm's law which 'can' be of a higher order than is commonly known. Another example is where a set of data which seem to follow a straight line are joined by a straight line disregarding what may take place between each set of two points. It may be argued that such decisions are dictated by common sense, but it remains to determine the closeness of common sense to reality. Identification process is of paramount importance in such situations where discrepancies exist between model and system behaviour which may be due to inaccurate parameter estimates or structural deficiencies. In section

5.8 model open loop responses were presented and compared with corresponding system responses. Although both sets of responses were following the same trend, the oscillation on the system responses were not predicted by the model. Further cases which will be presented later in this chapter will reflect clearly the discrepancies between the system and model behaviour. In all these cases the system and the model are operated under the same conditions; that is, initial conditions, step changes in valve positions, atmospheric pressure, ambient temperature, etc. under which the system is operated, are fed into the model. Causes of these discrepancies are not known, but assumptions about them can be made which have to be validated by means of experimentation. Where parameters which cannot be measured directly exist, as is often encountered, especially when heat transfer is involved, inaccurate estimates of their values may lead to inaccurate responses of the mathematical model. Furthermore, deficiencies in model structure, which are often due to lack of knowledge leading to either invalid assumptions or approximations, have serious consequences on model behaviour which may, to some extent, differ from that of the system. In many practical situations, combination of these causes exist and complications arise when estimates of constant parameters are obtained using model formulation which is in error. Since pin-pointing to the exact causes is not always possible, a method which minimises the sensitivity of the model to structural errors must be devised. The algorithm

due to Roberts and Leal (1980) discussed in chapter 2 separates the overall identification problem into a parameter estimation problem concerned with finding estimates of constant unknown parameters, and a smoothing problem whose task is to approximate to the structural deficiencies which often result in a time-dependent variation by a time varying entity, the nature of which depends on the nature of the apparent variations on the system observations. This time-varying entity may be approximated to by a time-varying uncertainty whose parameters are estimated by the smoothing problem as discussed in Chapter 2.

In the vaporiser system, the discrepancies between the system and model responses may be attributed to incorrect estimates of certain constant parameters such as the heat transfer coefficient (H_{tc}) between the hot water flow and the freon liquid in the vaporiser tube. The seemingly periodic variations on the vapour pressure response may be attributed to variations on the hot water inlet temperature (T_o) since vapour pressure is sensitive to hot water temperature variation. To reduce model sensitivity to these hidden variations, a time-varying uncertainty is attached to the hot water temperature based on the parameterisation concept proposed by Georgantzis (1977). The overall identification process had, thus, been transformed into a joint problem of parameter estimation and smoothing problems which can be solved separately and iteratively in a similar fashion to that adopted in the identification of the mixing tank system.

However, unlike the mixing tank system, some of the steady state values of the vaporiser model are functions of the estimation parameter (H_{tc}). This means that the initial conditions of the model are part of the identification problem, that is, they will vary as the parameter estimate varies in each iteration. This requires the recalculation of the steady state conditions for each value of the estimation parameter, otherwise the supposedly more accurate estimate of H_{tc} may not be so when starting the model from different initial conditions. This idea has been incorporated into the identification process and has proved fruitful.

6.2 Open Loop Responses

The identification procedure requires open loop responses obtained for the real system, together with a model which is to be identified when both the system and model are excited with the same input. What is of significance here is the transient part of the response which characterises the system's dynamic behaviour. When model response agrees satisfactorily (i.e. according to a certain criterion) with that of the system, the model is said to be "identified".

In section 5.8 open loop responses obtained for the system and model under one set of operating conditions were presented and compared. The discrepancies between the two corresponding sets of responses were mentioned. In this section, open loop responses of the system and model obtained under various operating conditions are presented and discussed. In all, five different conditions are considered. The differences between these conditions are in the initial conditions, the step changes in valve positions, atmospheric pressure, ambient temperature and slight changes in hot water inlet and outlet temperatures, inlet freon flow, steady state valve positions, heat transfer coefficients, heat losses, valve constant, outlet friction factor and hot water valve characteristics. It has been found that whilst the freon valve characteristics remained unchanged for all the operating conditions, the hot water valve was found to possess three slightly different characteristics due to some changes in the mechanism of the valve motor and structure. In each case, valve calibration was obtained and fed into the model simulation.

For the five cases involved, the hot water valve characteristics are shown in fig. 6.2.2. where cases 2 and 3 and cases 4 and 5 have the same hot water valve characteristics. The freon valve characteristics are the same for all cases. (Fig. 6.2.1.)

Table 6.2 gives, for the five different operating conditions, the atmospheric pressure (P_A), ambient temperature (T_A), and the steady state values of liquid freon height (S_{PICH}), vapour pressure (P_V), inlet hot water temperature (T_{CHWI}), outlet hot water temperature (T_{CHWO}) and freon feed flow (Q_L). It also gives the calculated values of K_G , K_2 , H_{tc} , and L_A using steady state calculations. Open loop responses obtained under these different operating conditions are as follows:

6.2.1. CASE 1

Under the conditions summarised in Table 6.2 a 20% step change was applied to the freon feed valve position, and the transient responses of H_T and P_V were recorded by the teletype which was connected to the Argus on-line computer.

The model simulation has been subjected, under the same operating conditions, to a 20% step change in freon feed valve position (V_{P1}), and the transient responses of H_T and P_V were calculated.

CASE	P_A N/m ²	T_A °K	SPICH m	SPICP w.g.	VP_2	TCHWI °K	TCHWO °K	Q_L m ³ /s	K_G SI units	HTC W/m ² /°K	LA J/s	K_2 SI units
1	102245	295.74	0.1	10.0	0.37002	352.64	349.98	1.64E-6	1.4166 E-6	1835.7	113.68	13.85 E14
2	101653.0	293.47	0.1078	9.79	0.63	352.38	350.38	1.81E-6	2.2208 E-6	2080.0	44.812	7.14 E14
3	101653.0	293.47	0.1102	10.02	0.634	352.3	350.23	1.53E-6	1.8554 E-6	2125.0	138.77	7.14 E14
4	100400.0	293.47	0.1405	9.38	0.464	352.1	349.8	1.32E-6	1.6641 E-6	1498.8	140.58	7.14 E14
5	100400.0	293.47	0.1306	9.21	0.562	352.01	350.1	1.53E-6	1.9467 E-6	1490.4	52.121	7.14 E14

Table 6.2. Steady State Values as Measured on the Vaporiser Rig under Five Different Operating Conditions.

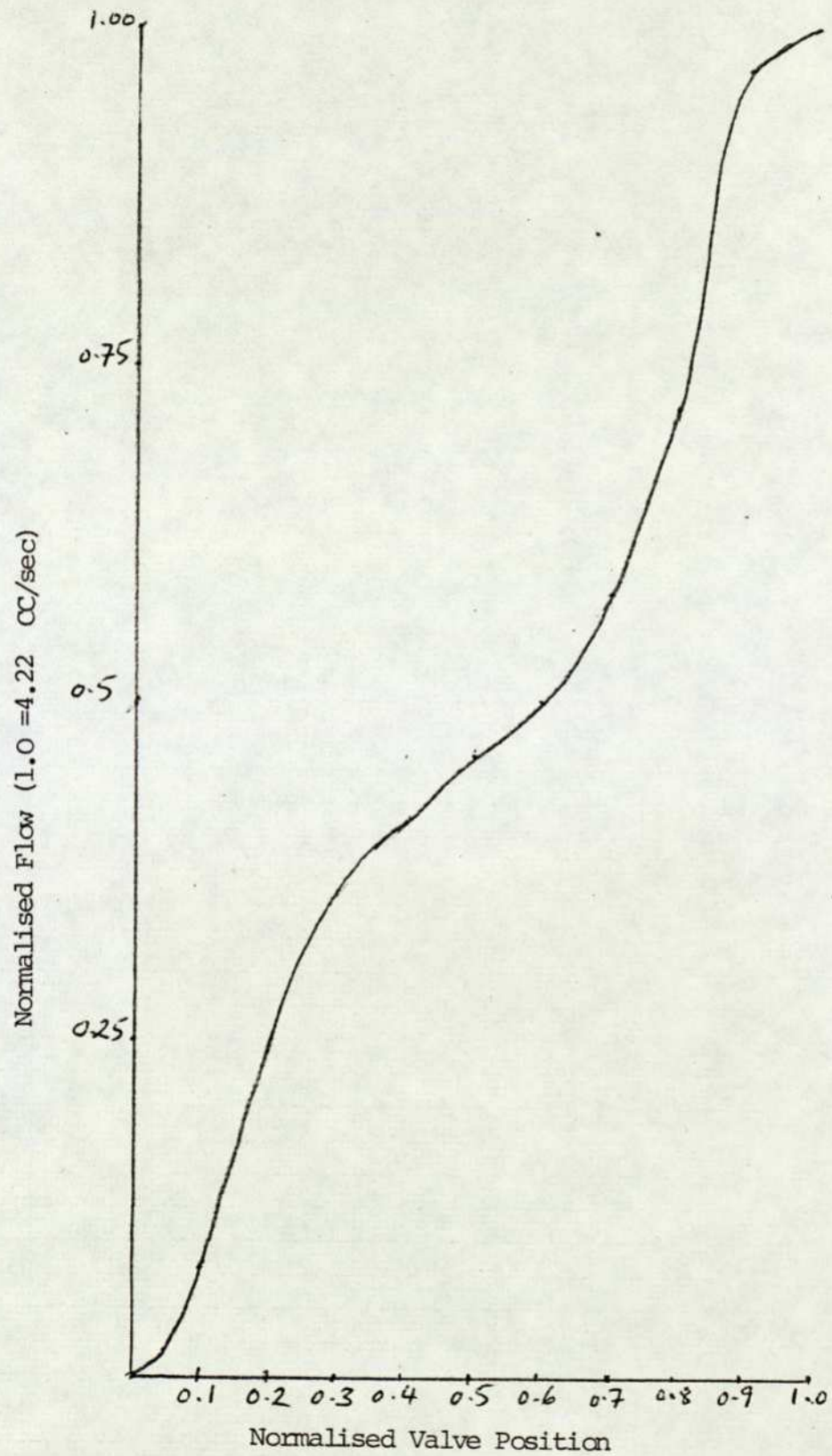


Fig.6.2.1. Freon Valve Characteristics

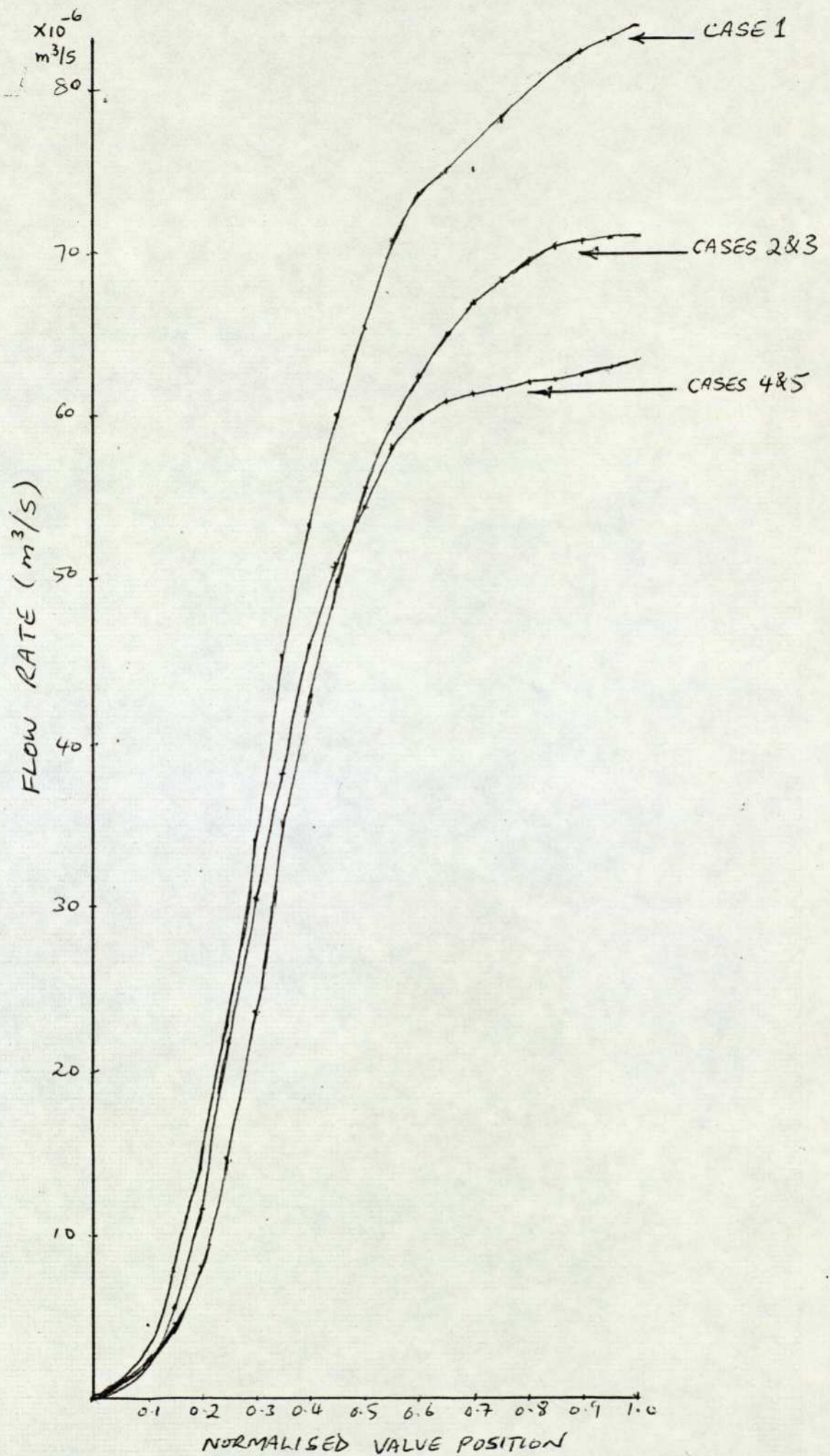


Fig 6.2.2 Hot Water Valve, characteristics under Cases 1, 2, 3, 4 and 5.

Both the system and model responses have been plotted in figs. 6.2.3. and 6.2.4. The graphs show clearly the "bubbling" nature of the responses which could not be predicted by the model which has been operated under the same conditions.

The parameter value (H_{tc}) used in the model is that obtained from steady state calculations using Eqn 6.3.1. In this case $H_{tc} = 1835.7$ SI units. In the model this value has been normalised to 1.0.

6.2.2. CASE 2

The vaporiser system was operated under the conditions summarised in Table 6.2 with the hot water valve characteristics as shown in fig. 6.2.2. The system, whilst in a steady state condition, was subjected to a 20% step change in the position of the freon feed valve, and the ensuing height and vapour pressure responses were recorded by the computer-operated teletype for a running time of 500 seconds.

The model was subjected to the same disturbance under the same conditions with the hope that the model would predict the system behaviour.

The system and model responses have been plotted in figs. 6.2.5. and 6.2.6.

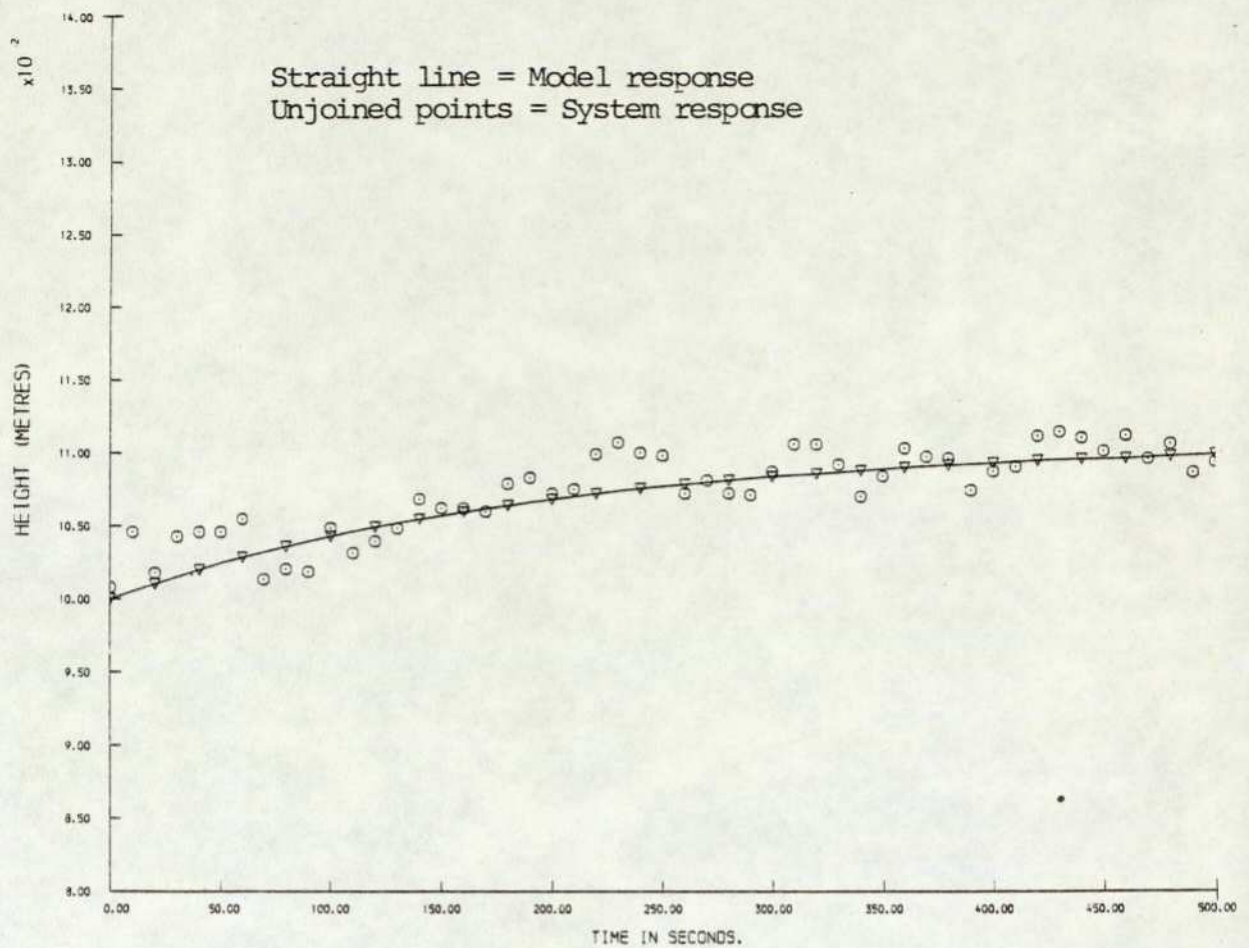


Fig.6.2.3. Open Loop Height Responses Obtained by System and Model, for a 20% Step Change in VP_1 in Case 1.

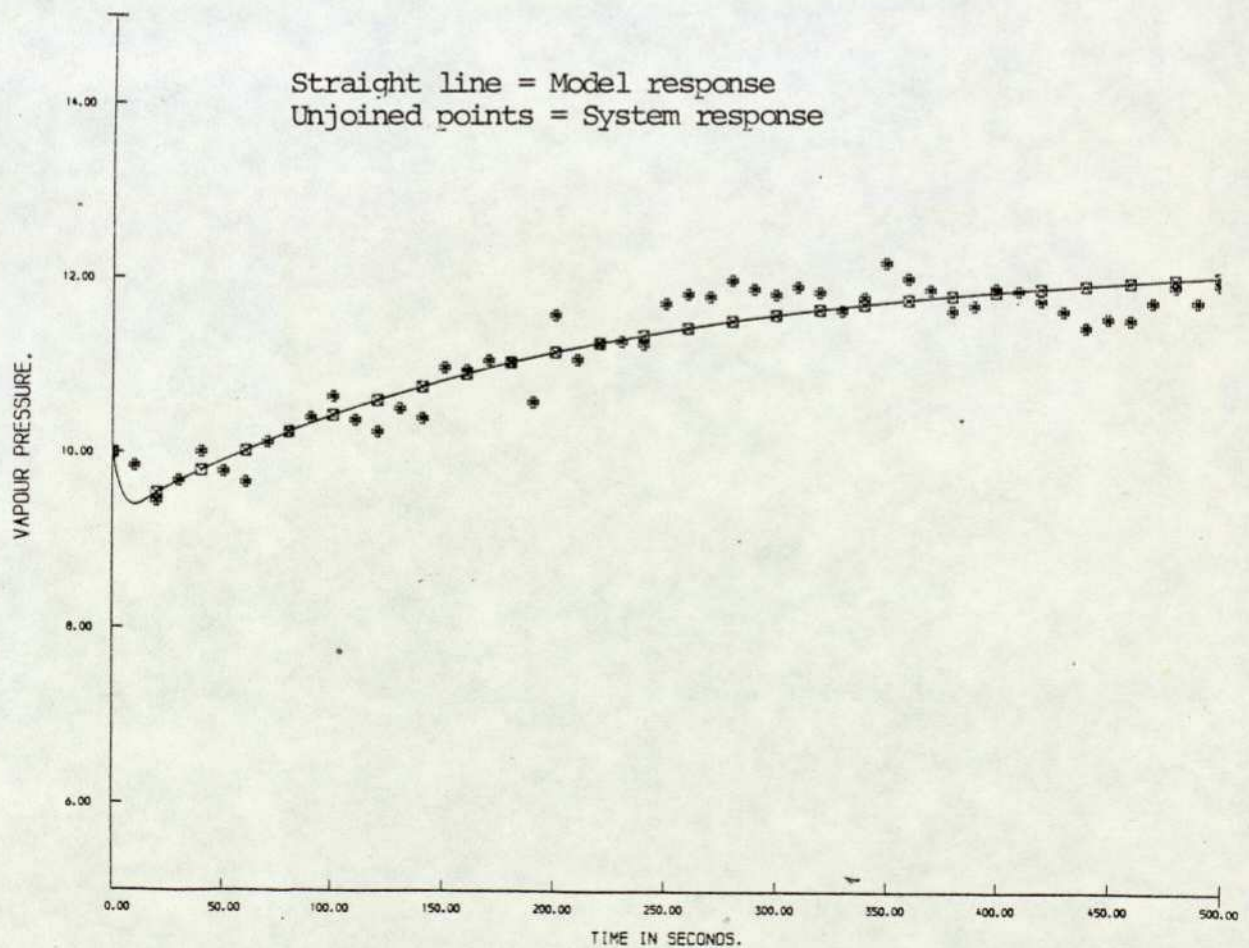


Fig.6.2.4. Open Loop Vapour Pressure Responses Obtained by System and Model for 20% Step Change in Freon Value position in Case 1.

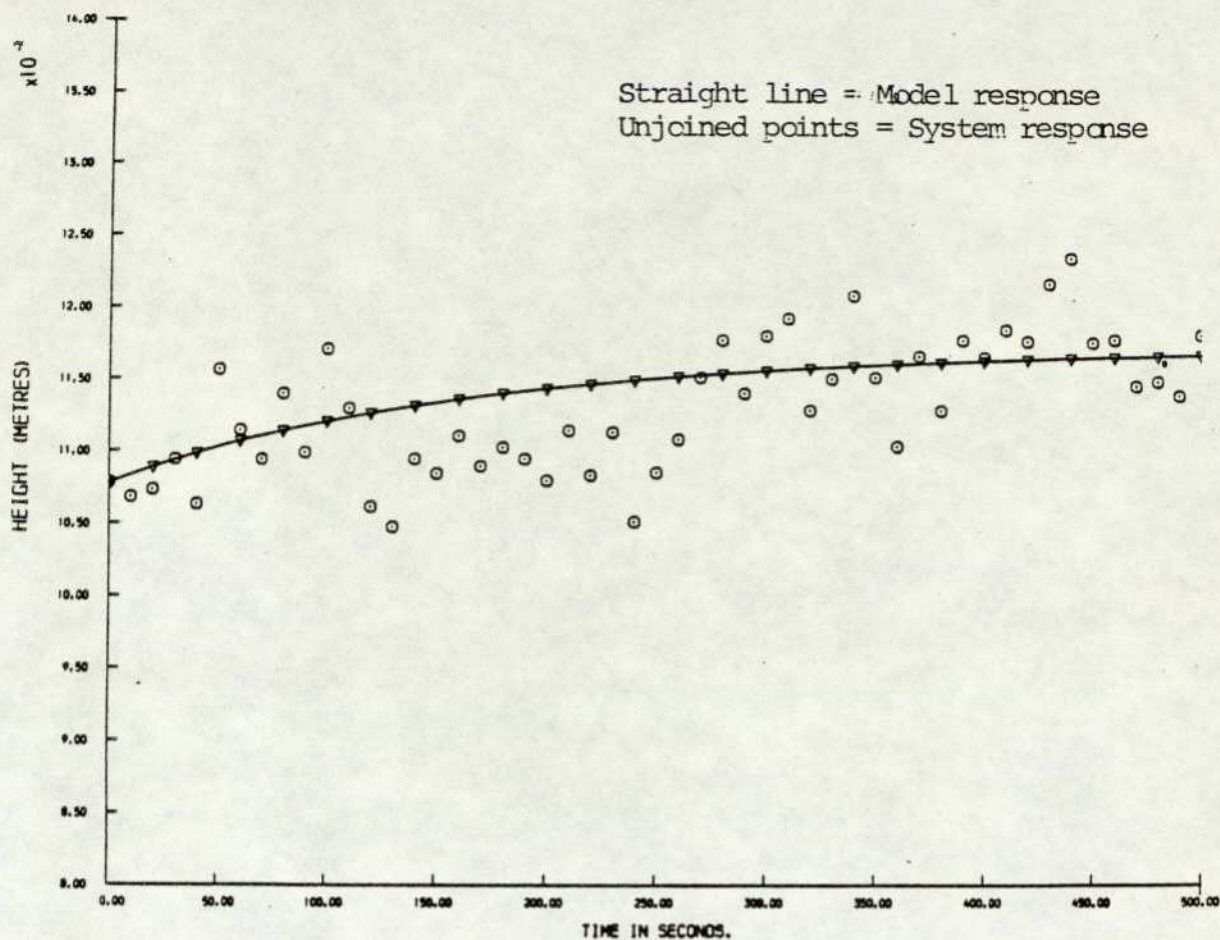


Fig.6.2.5. Open Loop Height Responses* Obtained by System and Model for a 20% Step Change in VP1 in Case 2.

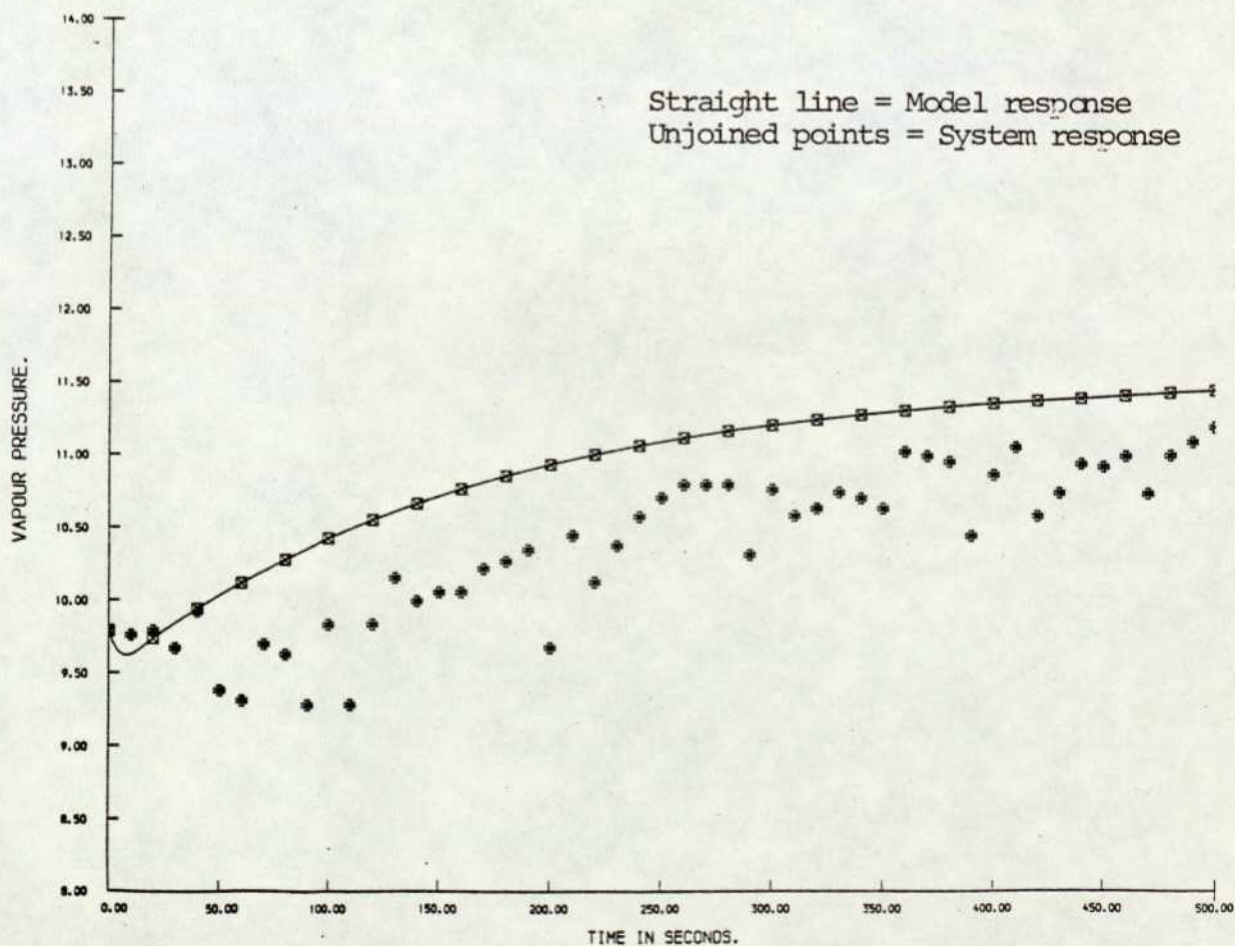


Fig. 6.2.6. Open Loop Vapour Pressure Responses Obtained by System and Model for a 20% Change in VP1 in Case 2

The H_{tc} value used is the steady state value and is equal to $2080.0 \text{ W/m}^2/\text{o}_K$ which, for identification purposes, is normalised to 1.0.

6.2.3. CASE 3

Under the same operating conditions as those in Case 2, the system was subjected to a 40% step change in the freon feed valve position, thus allowing more freon to enter the system. The resulting transient responses of H_T and P_V were observed over a 500 second period.

The model was operated under the same conditions and subjected to the same step change and the responses of H_T and P_V recorded. Both system and model responses have been plotted in figs. 6.2.7. and 6.2.8.

Again the H_{tc} value is that obtained from the steady state calculations using the information in Table 6.2. In this case, $H_{tc} = 2125 \text{ W/m}^2/\text{o}_K$ and is normalised to 1.0.

6.2.4. CASE 4

The vaporiser was operated under a new set of conditions as shown in Table 6.2. In this case, this new set of values was intended to serve two purposes: the first is that a new operating condition would be obtained which would enable investigation into whether the parameter estimate (k_o) depends on the operating conditions and the other is to operate the vaporiser under easily achievable set of conditions. The open loop responses have always been obtained in the following way: the vaporiser is first operated under multivariable closed loop control

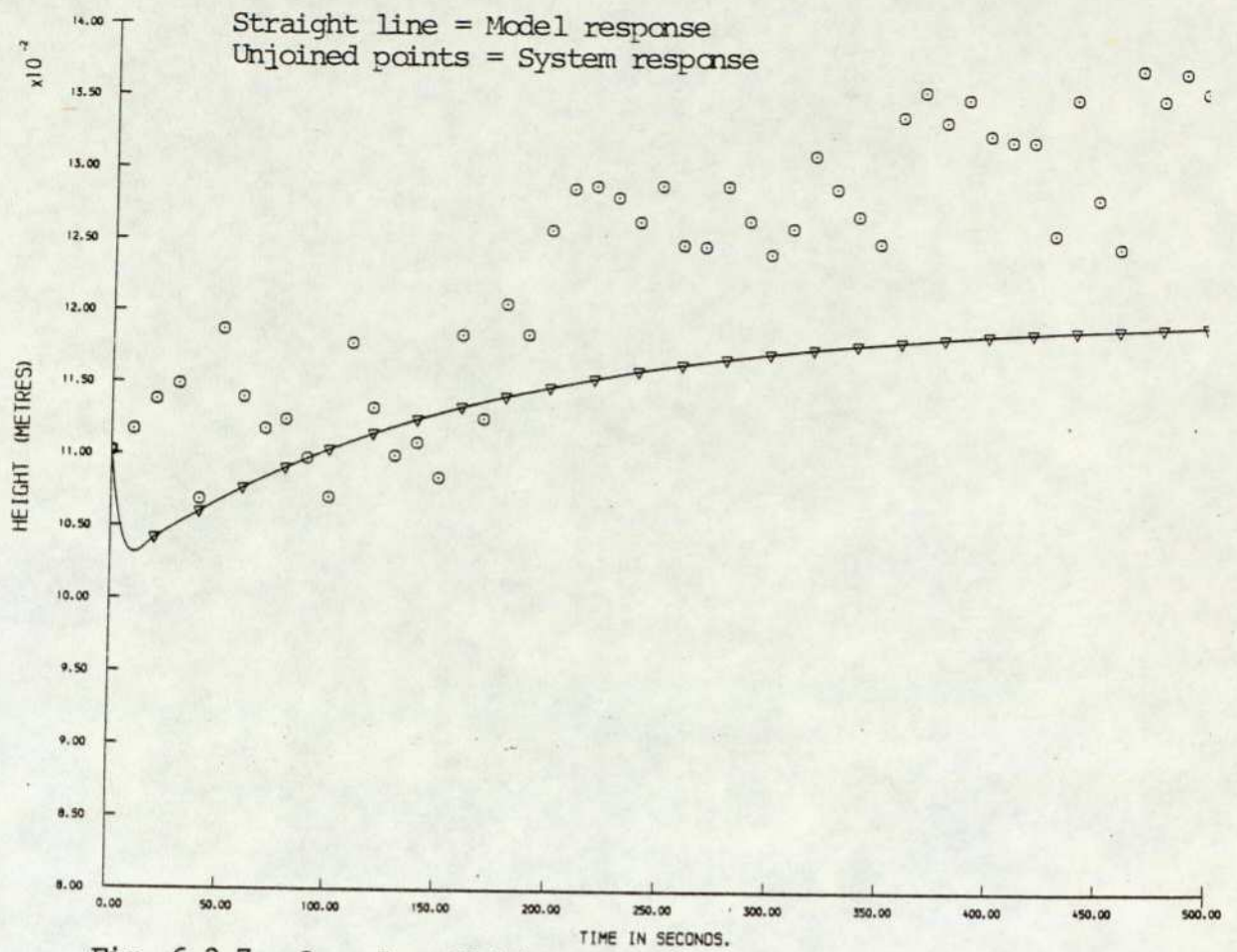


Fig. 6.2.7. Open Loop Height Responses Obtained by System and Model for a 40% Change in VP_1 in Case 3.

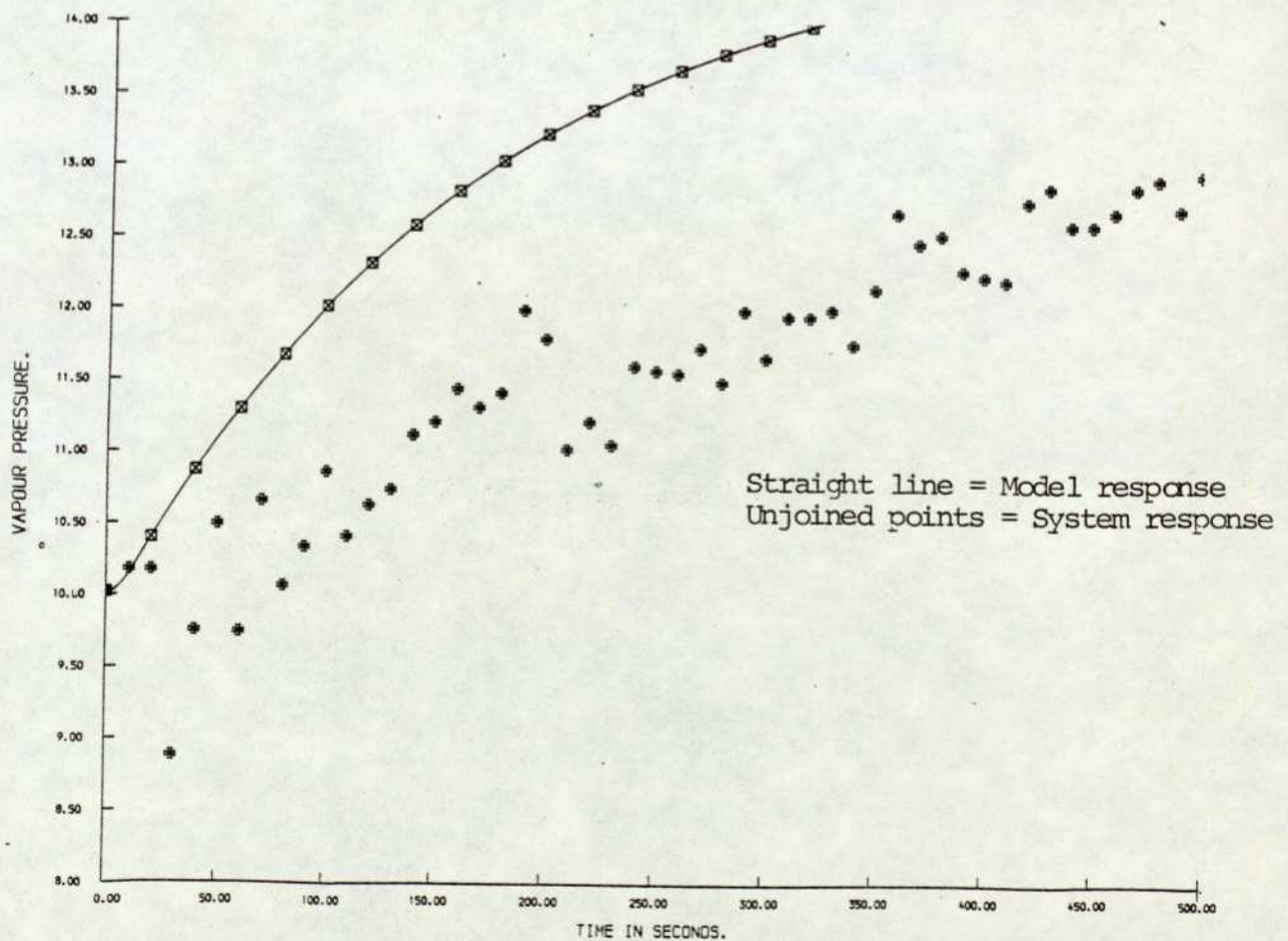


Fig. 6.2.8. Open Loop Vapour Pressure Responses of System and Model to a 40% Step Change in VP_1 in Case 3.

until the set points are achieved. The average positions of the two control valves are then calculated. The vaporiser is then operated in an open loop mode with the two valve positions fixed at the average positions obtained from closed loop operation. In this case, the vaporiser was operated in a closed loop mode with height setpoint at 0.13m and vapour pressure setpoint at 10" w.g. Certainly a higher liquid level will make the required vapour pressure of 10' w.g. easily achievable. The rig was then operated in an open loop mode, and when subjected to a 20% step change in the freon feed valve position, the system responses obtained are shown in figs. 6.2.9. and 6.2.10., together with the responses obtained when the model was operated under the same set of conditions.

The value of H_{tc} obtained from steady state calculations is equal to $1498.8 \text{ W/m}^2/\text{o}_K$ and is normalised to 1.0 when identification process is carried out.

6.2.5. CASE 5

The system was operated under the same conditions as those in Case 4. When in the steady state conditions given in table 6.2, a 20% step change was applied to the hot water valve position, thus increasing the amount of hot water flow into the system, and, consequently, the amount of heat available to the liquid freon. As expected, the system response shows a sharp rise in vapour pressure immediately after the application of the step change followed by a gradual drop. This is due to the fact that

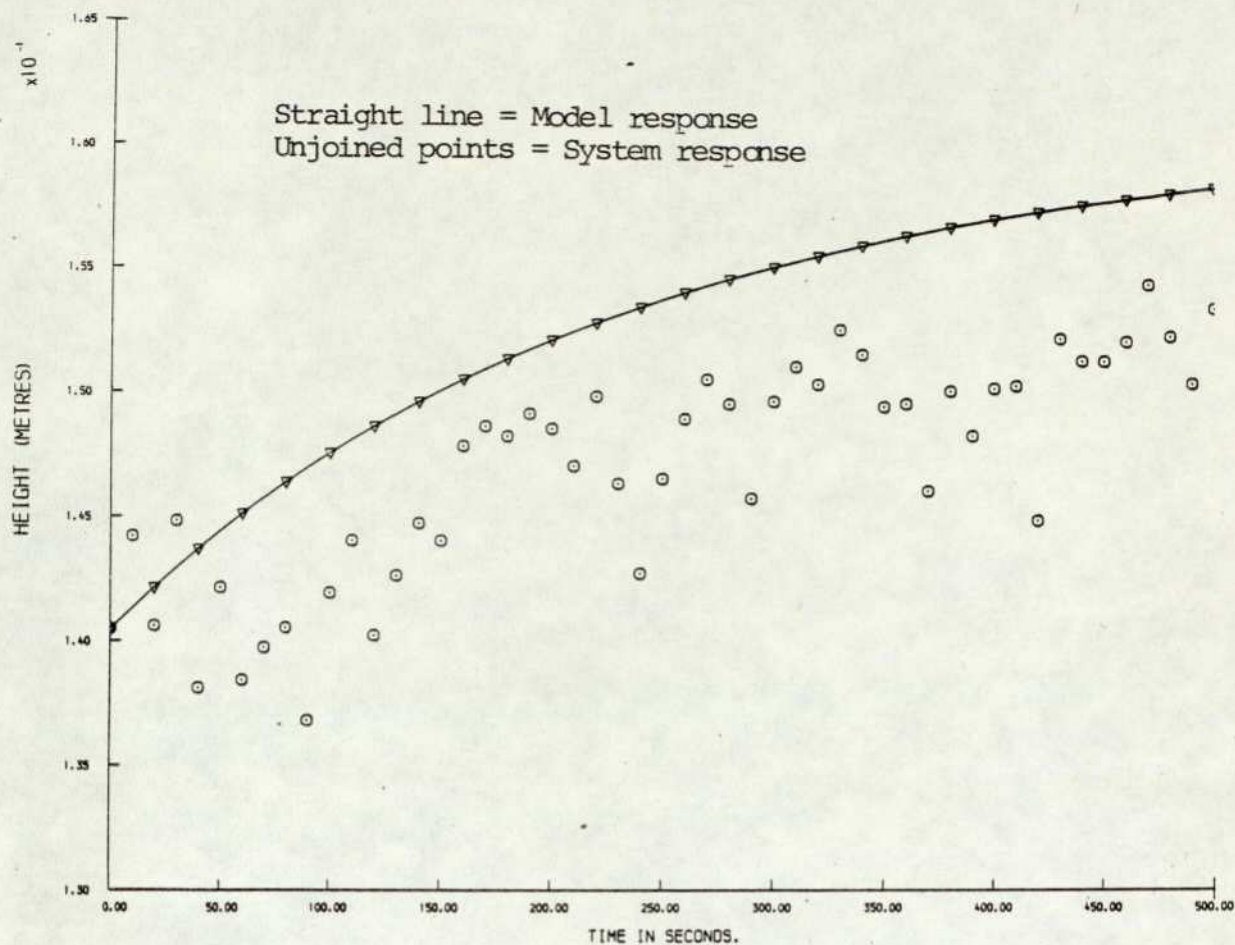


Fig.6.2.9. Open Loop Height Responses of System and Model to a 20% Step Change in VP_1 in Case 4.

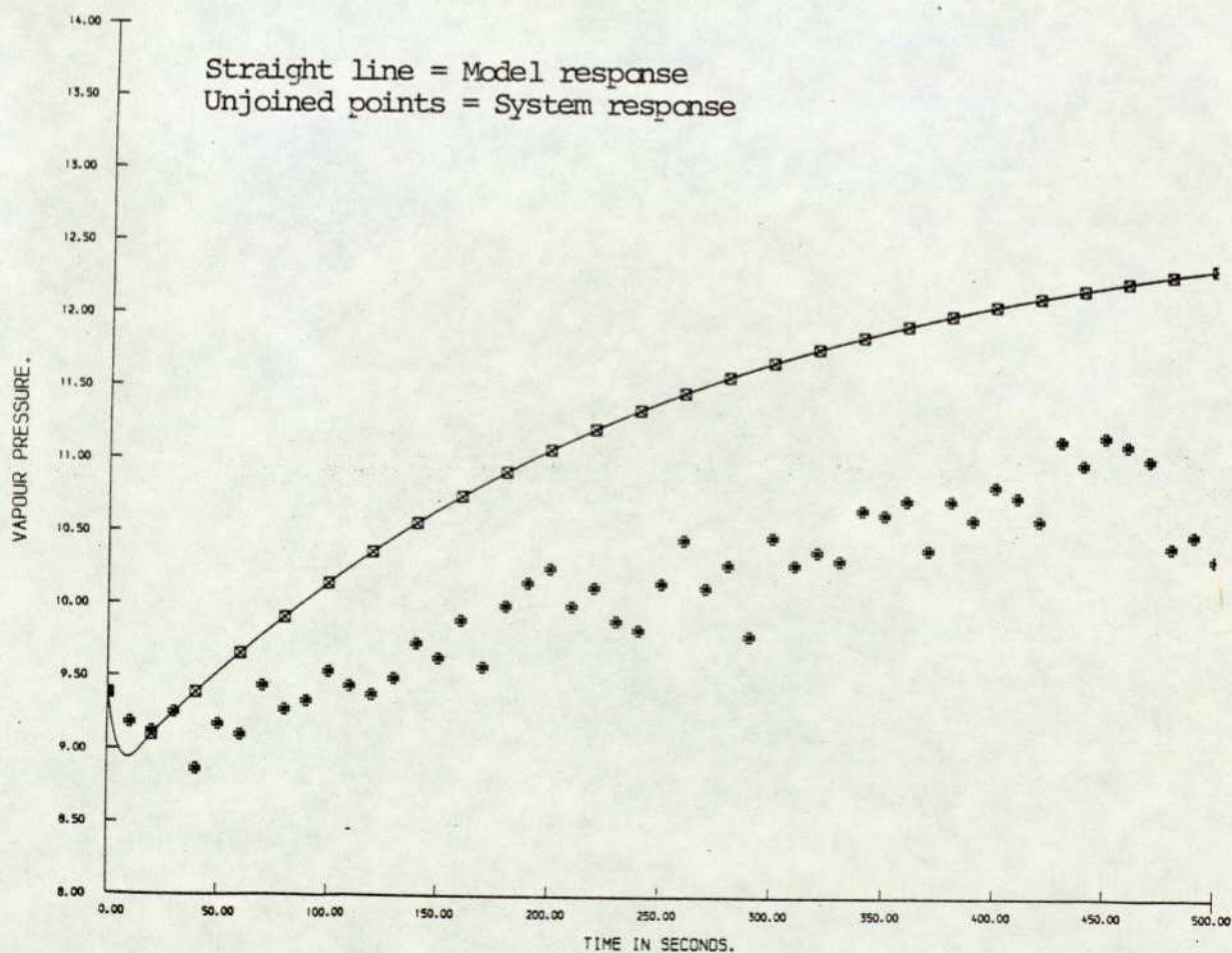


Fig.6.2.10. Open Loop Vapour Pressure Responses of System and Model to a 20% step Change in VP_1 in Case 4.

with a constant freon feed flow, an increase in the hot water flow will cause more freon boil-off causing a drop in the freon height. This results in a larger volume available to the vapour and hence lower vapour pressure. This transient behaviour continues until a state is reached whereby the incoming freon feed balances the boil-off resulting in a new steady state condition.

The model was subjected to the same step change under the same conditions. The responses show a general trend similar to that of the system but would not predict the exact behaviour.

Both the system and model responses are plotted in figs. 6.2.11 and 6.2.12. The value of H_{tc} obtained from steady state calculations is $1490.4 \text{ W/m}^2/\text{o}_K$ and in the identification process, it is normalised to 1.0.

In all the cases presented, the mathematical model when operated under the same conditions as the system, has managed to predict the general trend of the system, but has failed to predict the variations on the system observations. Although the vaporisation process is of bubbling nature, which may allow for the assumption that these variations are due to excessive noise, it remains to be seen whether accounting for such disturbances will enhance the performance of the model through improved estimates of the constant model parameters such as H_{tc} .

In the next sub-section, the identification procedure adopted for the vaporiser system will be presented and the results obtained will be evaluated.

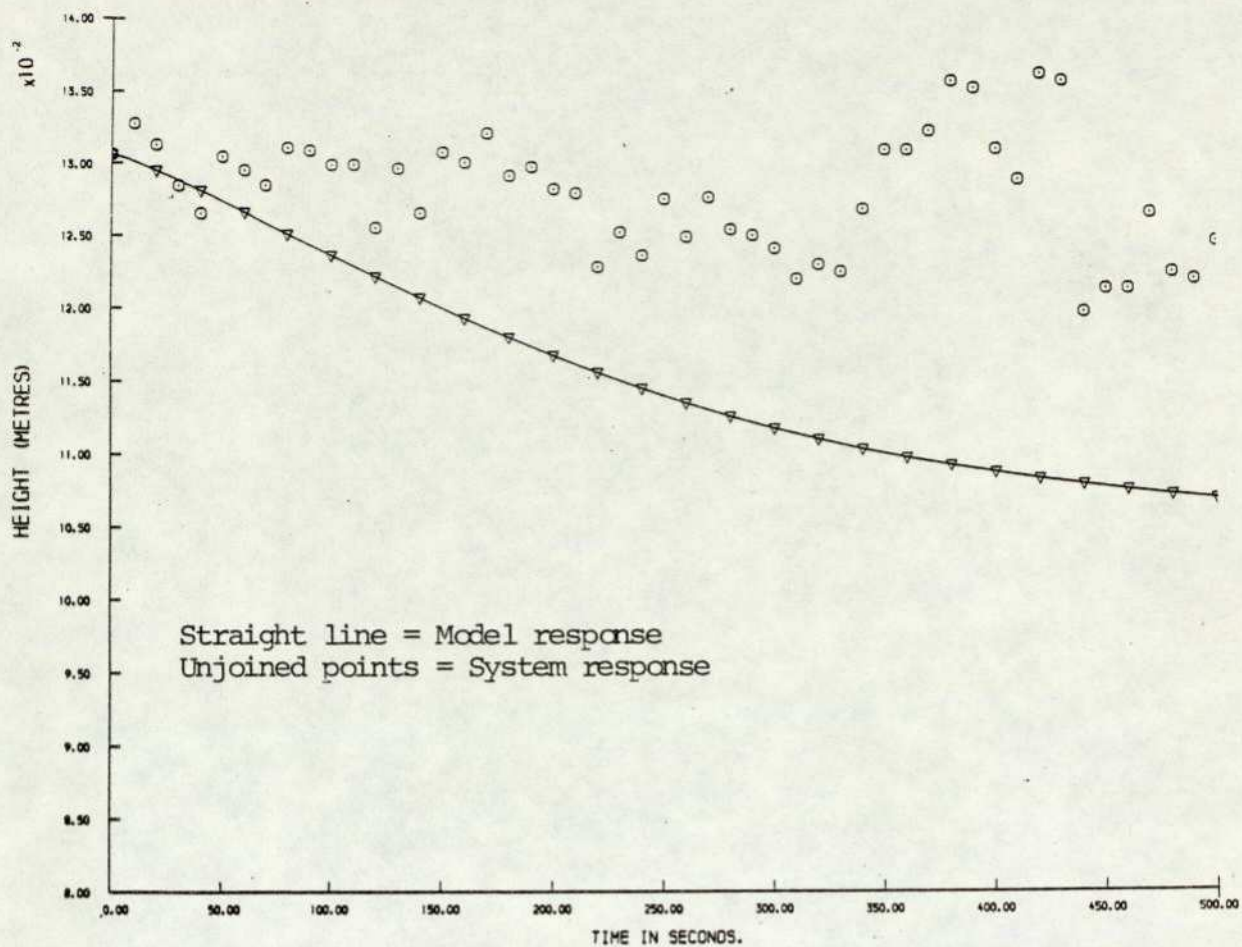


Fig.6.2.11. Open Loop Height Responses of System and Model to a 20% Step Change in Hot Water Valve Position VP_2 in Case 5.

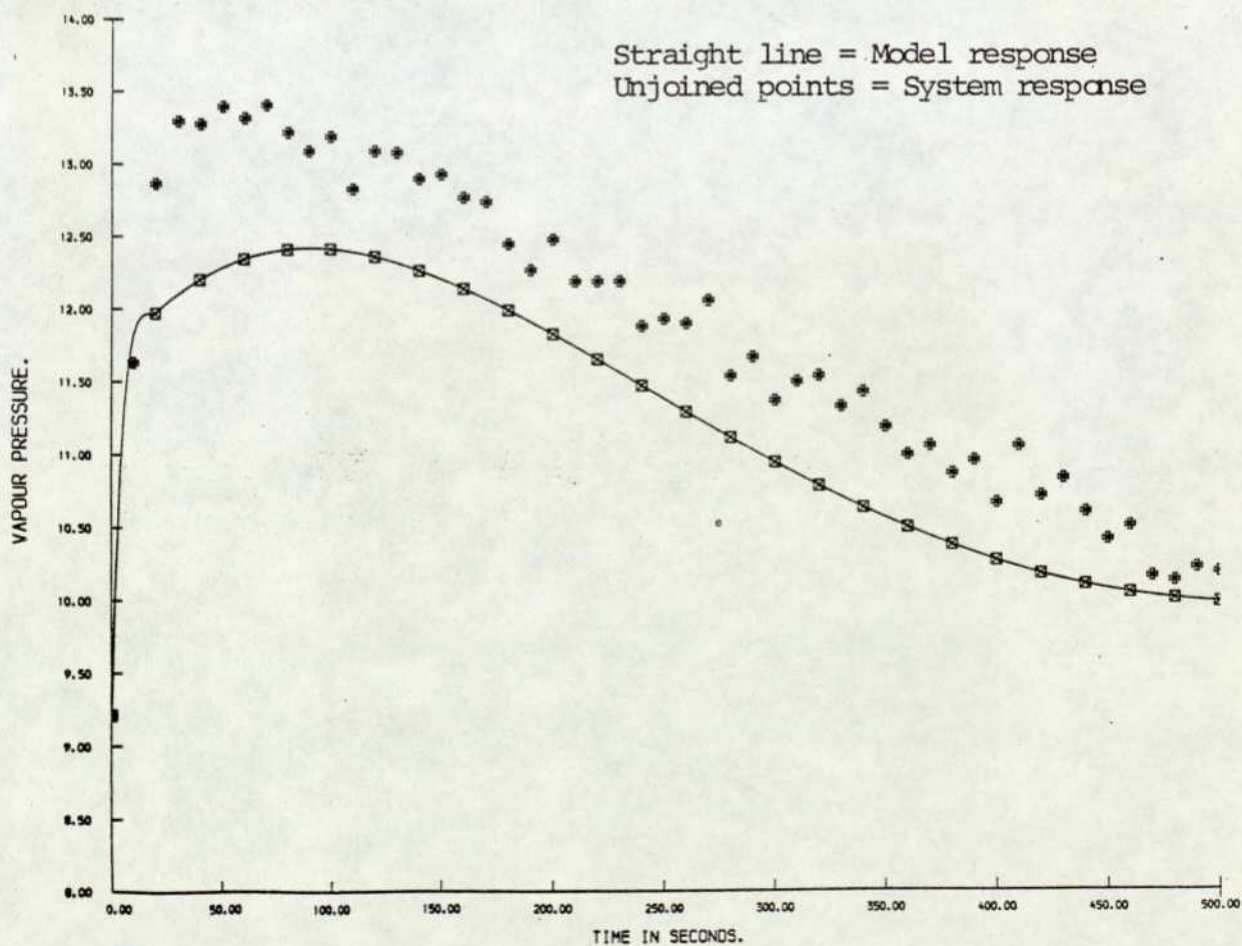


Fig.6.2.12. Open Loop Vapour Pressure Responses of System and Model to a 20% Step Change in VP_2 in Case 5.

6.3 Identification Procedure:

The comparison of model responses with corresponding real system responses reveals inadequacy in model structure suggesting unfaithful representation of the system by the mathematical model. Several questions may be raised about the model formulation ; how have the values of constant unmeasurable model parameters been calculated? Is the nature of the boiling process completely known? Have all the relevant basic laws of Physics and Chemistry relating to the boiling process and the associated structure been applied? Are all system disturbances known? Are the measuring instruments perfectly accurate ...?

Certainly the answer to the first question refers to the use of the "known" steady state equations in calculating the constant parameters of the model which cannot be measured directly. The results of these calculations will be "reasonably" accurate if all the answers to the questions above are positive. But such a positive answer to these questions can hardly be qualified. However, since all available knowledge of the vaporisation process has been applied in the modelling process, the inclination must be to compensate for the limited knowledge of the real world in a way which reduces the discrepancies between the model and the system.

In the vaporiser system, where the intention is to achieve accurate estimates of the constant model parameters, compensation must be made to overcome lack of knowledge of the vaporiser plant. The problem, thus, has two prongs: on the one hand, the structural

errors are compensated for using engineering judgement, and on the other hand, the constant model parameters can then be estimated using the modified structure. Two separate but inter-related problems have, thus, emerged, the solution of which may lead to a more faithful model.

One of the important constant model parameters whose value cannot be measured directly is the heat transfer coefficient (H_{tc}) between the heating section and the liquid freon section of the vaporiser tube. Accurate estimate of H_{tc} is essential since it determines the amount of heat transfer between the two sections which is related to the boil-off, and eventually to the vapour pressure inside the tube. The usual method of calculating the value of H_{tc} has been by the use of steady state conditions, where, using equation 5.5.12.

$$H_{tc} = \frac{Q_L \cdot \rho_L [\lambda + C_V (T_B - T_i)]}{\pi \cdot D \cdot Z (T_w - T_B)} \dots \quad 6.3.1$$

The value obtained using this equation is used as an initial guess when solving the parameter estimation problem. It must be noted here that the above equation does not involve correction to the assumed structural errors. With a corrected structure, it is anticipated that a better estimate of H_{tc} will lead to a more representative model liquid height response.

In the vaporiser system, the vapour pressure has been found to be sensitive to the inlet hot water temperature variations. Also, the inlet hot water temperature has been seen to suffer from periodical fluctuations. Incorporating these fluctuations, (if accurately known) into the model will undoubtedly result in improved vapour pressure response compatible with the

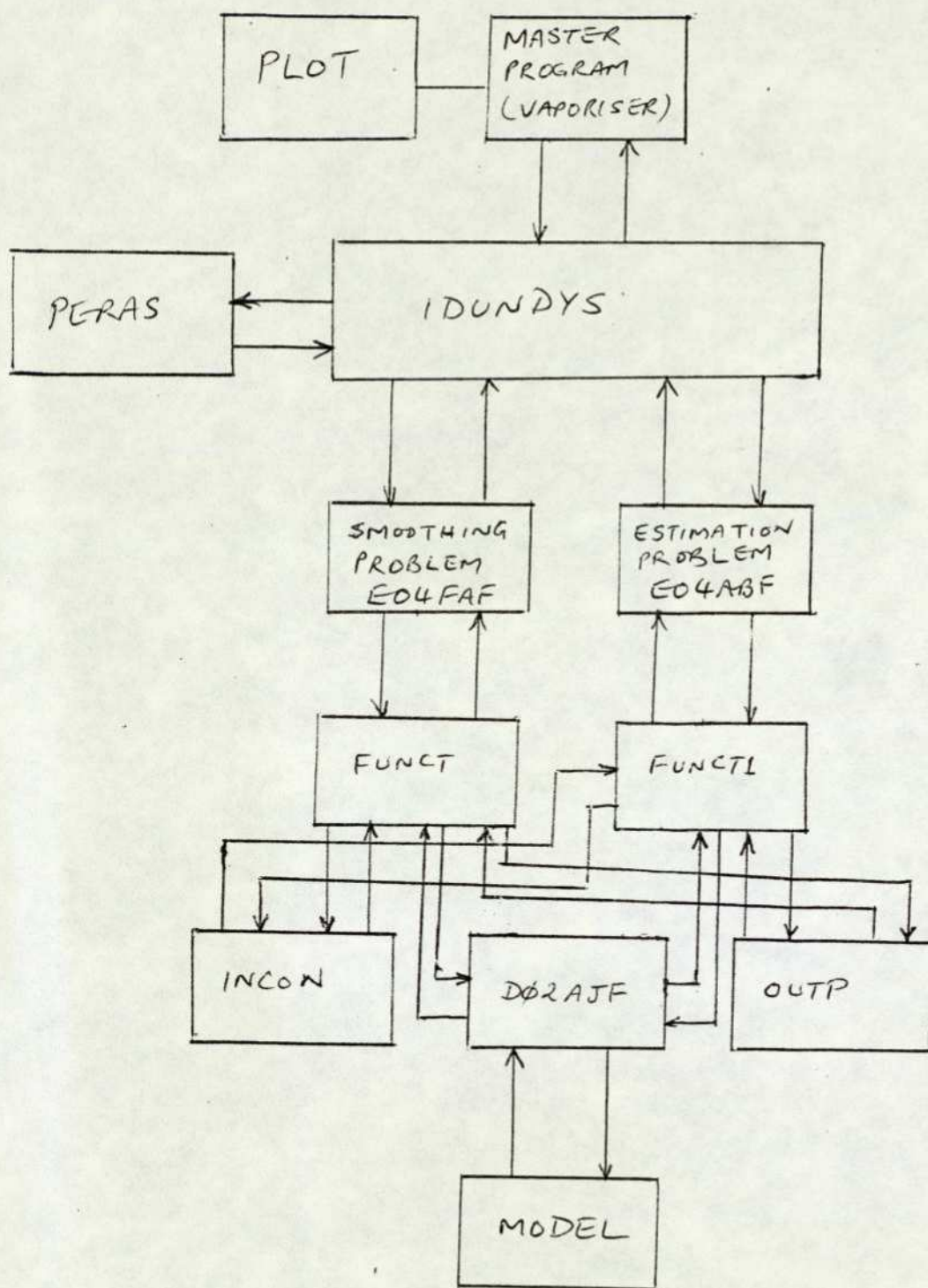


Fig. 6.3.2 Program Organisation

system response. However, due to the lack of perfect knowledge about the nature of these fluctuations and using the periodical nature of the fluctuations on the vapour pressure response, it has been decided to attach to the inlet hot water temperature (T_o) which had been found to possess periodical fluctuations (section 5.4.3.), a time-varying entity of periodic nature. Using the parameterisation concept due to Georgantzis (1977), this time-varying entity has constant parameters whose accurate values will determine the overall shape of the fluctuations. The estimates of these parameters are obtained by the solution of the smoothing problem.

Fig.6.3.2 shows the program organisation in a schematic form whilst the computer programs are shown in Appendix (4). The various parts of the program function in the same way as the corresponding ones in the identification of the mixing tank system. Besides the subroutine (INCON) concerned with calculating the initial conditions for each new estimate of H_{tc} , the system observations needed for comparison purposes by the identification process are fed into the model as data as well as the valve characteristics required by the model. In the identification of the mixing tank system, system observations were calculated from the system simulation.

The solution of the identification problem has been obtained by the use of a CDC 7600 computer. The overall structure of the process is almost the same as that used in the identification of the mixing tank system discussed in Chapter 4 with one important difference. This difference being the fact that

whilst in the mixing tank system the estimation parameter (k_o) is not included in the steady state calculations, the estimation parameter in the vaporiser model (H_{tc}) affects the steady state conditions. This means that for every new estimate of H_{tc} , the steady state conditions must be calculated so that the model responses are obtained from steady state conditions which are updated here ^{and} are those which have to be calculated and not those obtained from direct measurements on the vaporiser system. For this reason, a subroutine (INCON) to calculate these steady state conditions has been devised, tested and incorporated into the program suite.

6.4 Results:

The identification procedure has been carried out on all the five practical cases discussed in section 6.2. In each case, the identification process comprises the joint solution of the parameter estimation problem concerned with estimating the constant parameter H_{tc} , and the smoothing problem, concerned with estimating the parameter of a time-dependent uncertainty incorporated into the model to compensate for possible structural deficiencies. This time-varying uncertainty (B_{B22}) which has been attached to the inlet hot water temperature T_o is approximated to by either a sinewave or a Chebychev polynomial.

The values of the weighting matrices $\underline{W}$ and $\underline{R}$ have been varied in a way which reflects the effects of these variations on the identification process. Moreover, these matrices have been given time-dependent values which normalise the errors between the system and model responses and those between the time-varying uncertainty and its nominal trajectory. This is achieved by the use of equations:

$$W(J,I) = \frac{1}{Y_A(J,I)} \quad \dots\dots 6.4.1.$$

and

$$R = \frac{1}{Traj} \quad \dots\dots 6.4.2.$$

where

$Y_A(J,I)$ = the Ith sample of the J^{th} output signal

$Traj$ = the nominal trajectory of the time-varying uncertainty which is a constant value (equal to 1.0)

It must be noted here that the value of the estimation parameter (H_{tc}) is the normalised value, where $H_{tc} = 1.0$ is the value of H_{tc} calculated using the equation 6.3.1 which uses the steady state values of the variables involved for that particular case.

In the Fortran program used to execute the identification process, H_{tc} is given the variable name PRA and the smoothing parameters are contained in array PRB.

6.4.1. Case 1

The results obtained for the estimation parameter (H_{tc}) for different values of weighting matrices for the two forms of uncertainty are summarised in the following table:

CASE	Form of BB22	W(1)	W(2)	R	H_{tc} steady state value	H_{tc} C.L.S.	H_{tc} S.L.S.
1	SINE	10	0.5	20	1.0	0.596	0.572
2	CHEB	10	0.5	20	1.0	0.596	0.598
3	SINE	10	1.0	20	1.0	0.593	0.536
4	CHEB	10	0.1	20	1.0	0.66	0.672

Table 6.4.10: Summary of the Results obtained for Case 1

From the table, it is evident that the values of the parameter estimate H_{tc} yielded by the identification process are significantly different from those obtained from the steady state calculations. It is also clear that as $W(2)$ is increased the value of H_{tc} yielded by both techniques decreases. The smoothed least squares technique has improved over the value of H_{tc} estimated by the classical least squares. Since $W(2)$ is associated with the errors in the vapour pressure responses the estimate of H_{tc} , whose value affects the heat available within the vaporiser tube, will affect the pressure responses.

Figs. 6.4.11 and 6.4.12 show the system and model height and vapour pressure responses corresponding to case 1 in the table. The model height response does not fit very well into the system real observations and further work is necessary to investigate into the inability of the identified model to pass through the average trend of the system behaviour. On the other hand, the model pressure response seems to follow the average trend of the corresponding system response displaying the non-minimum phase behaviour. However, the periodical fluctuations on the system responses have not been predicted by the model.

The performances of the classical least squares and the smoothed least squares techniques corresponding to Case 1 are given by fig. 6.4.13. The classical least squares technique managed to yield the results corresponding to iteration 1 in the figure. Clearly, the smoothed least squares technique has improved on the value of H_{tc} (PRA) especially with the sinewave-form uncertainty with a corresponding improvement on the value of the objective function. The figure shows that whilst the value of H_{tc} (PRA) has continued to change for 12 overall iterations, the objective function has changed

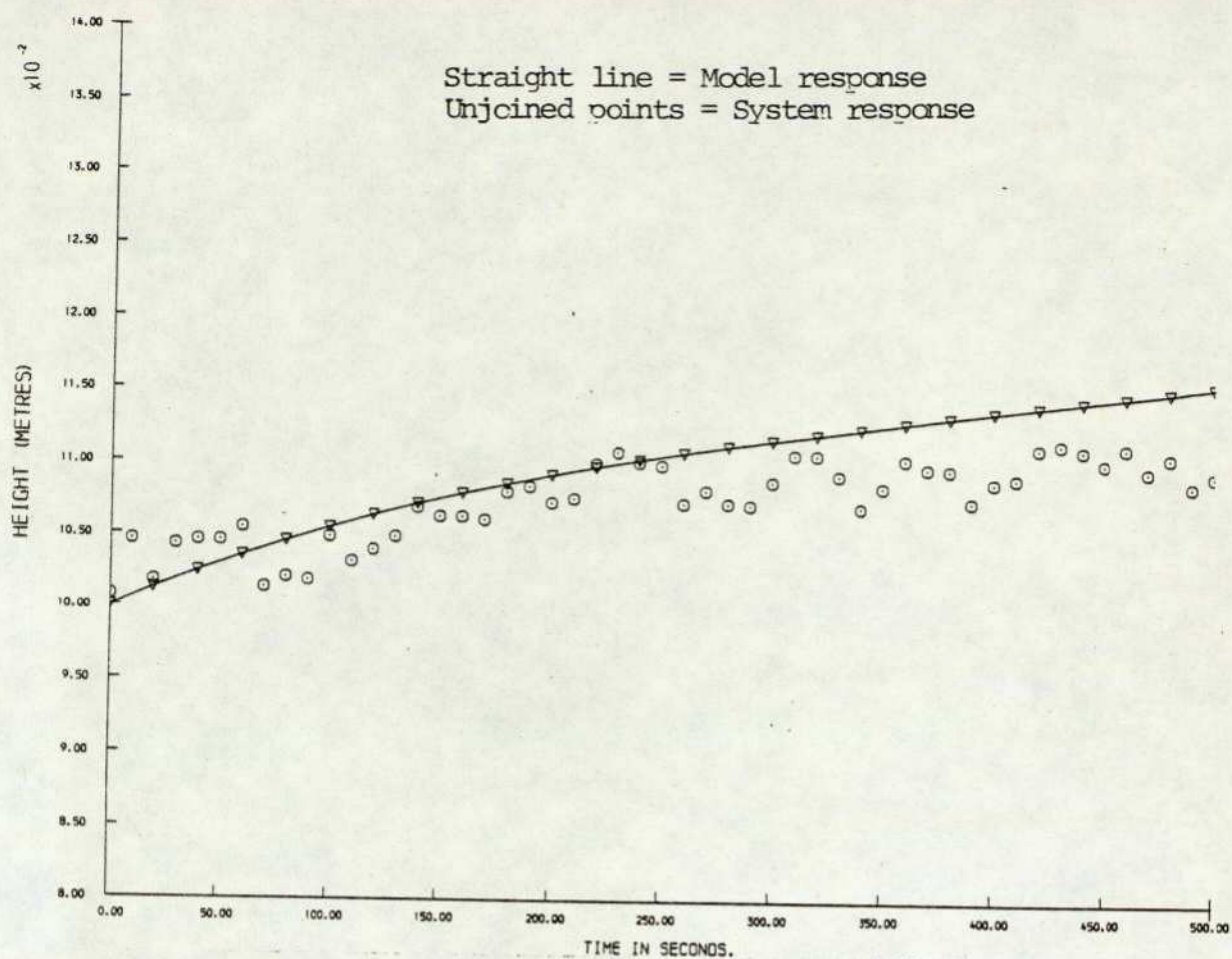


Fig.6.4.11. System and Model Height Responses Corresponding to Case 1 of Table 6.4.10 where $W(1) = 10$, $W(2) = 0.5$ and $R = 20$.

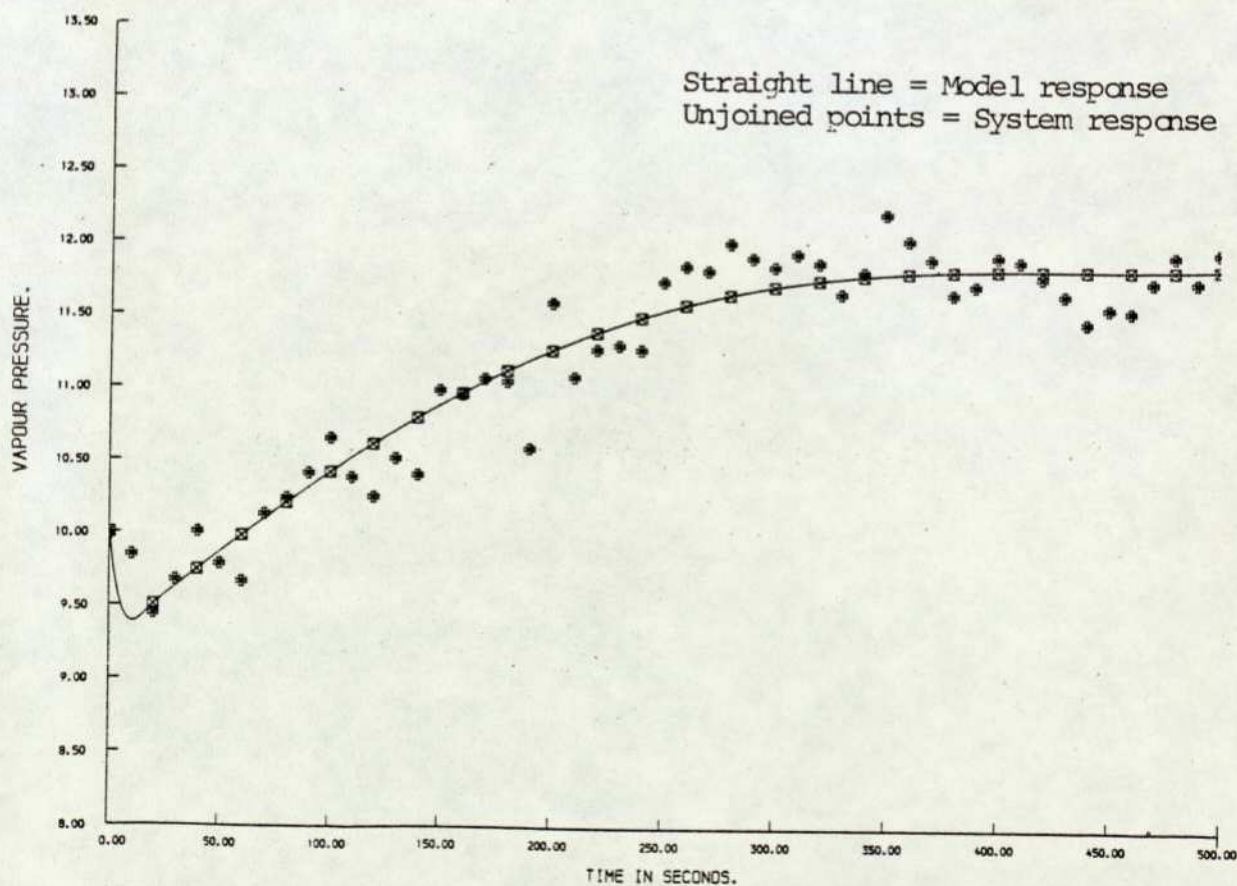
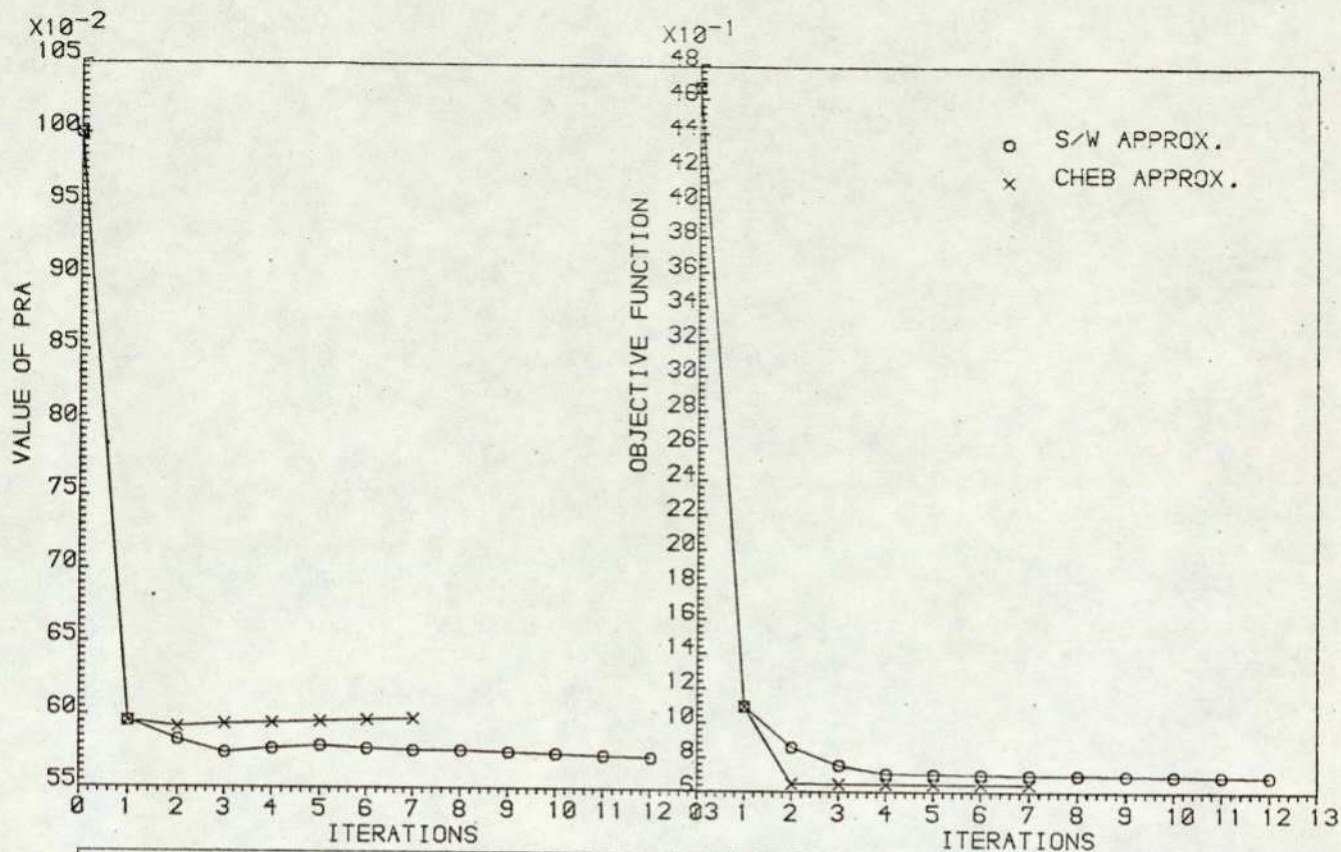


Fig.6.4.12. System and Model Vapour Pressure Responses Corresponding to Case 1 of Table 6.4.10 where $W(1)=10$, $W(2)=0.5$ and $R=20$.



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE

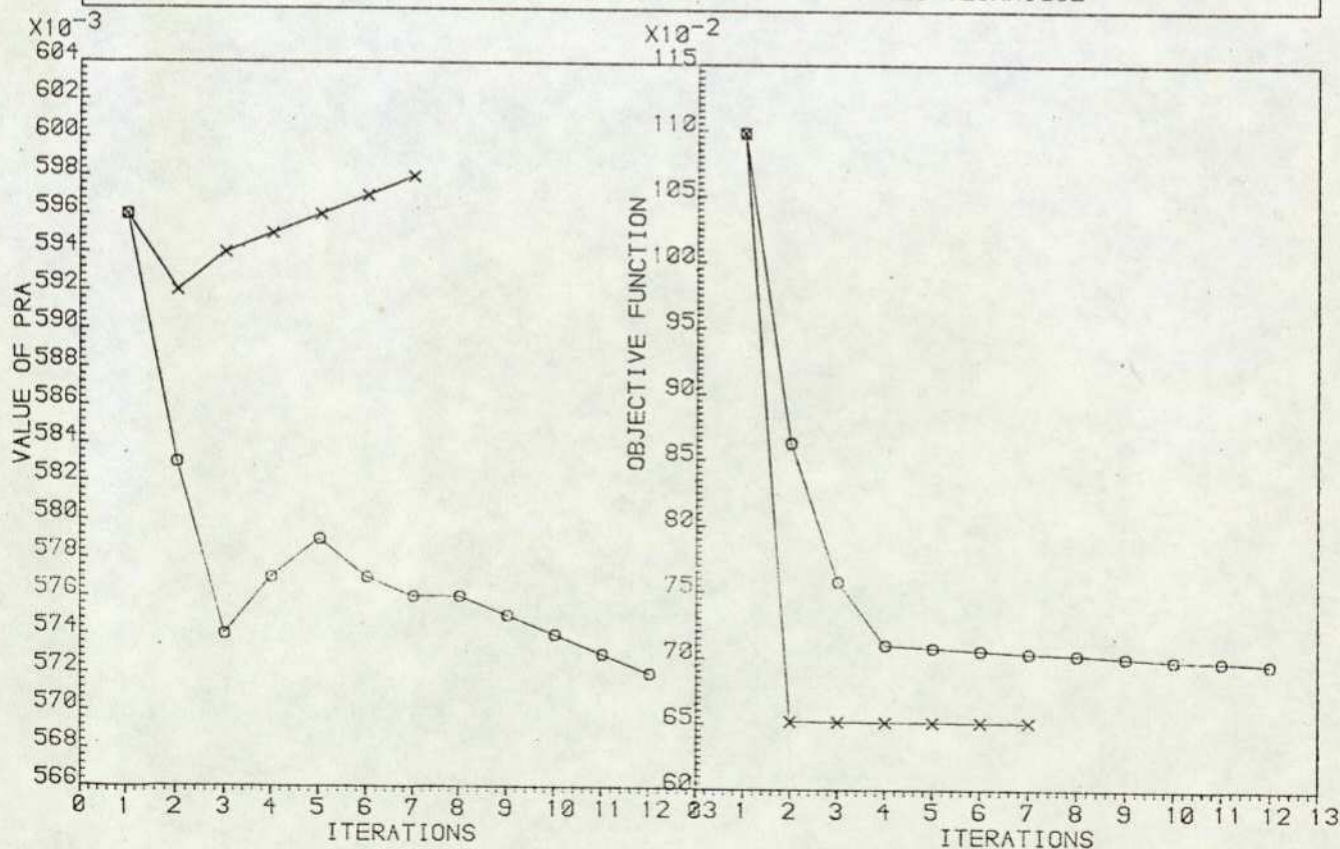
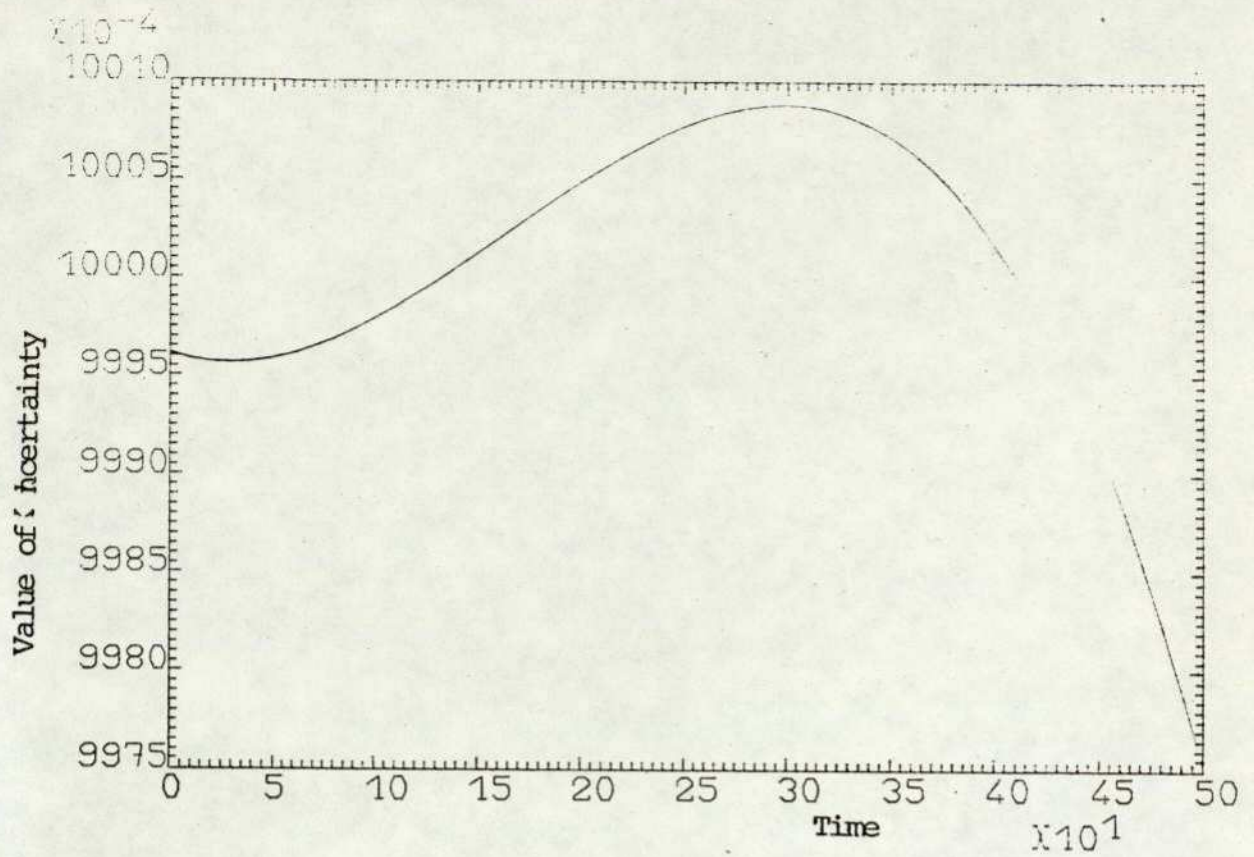


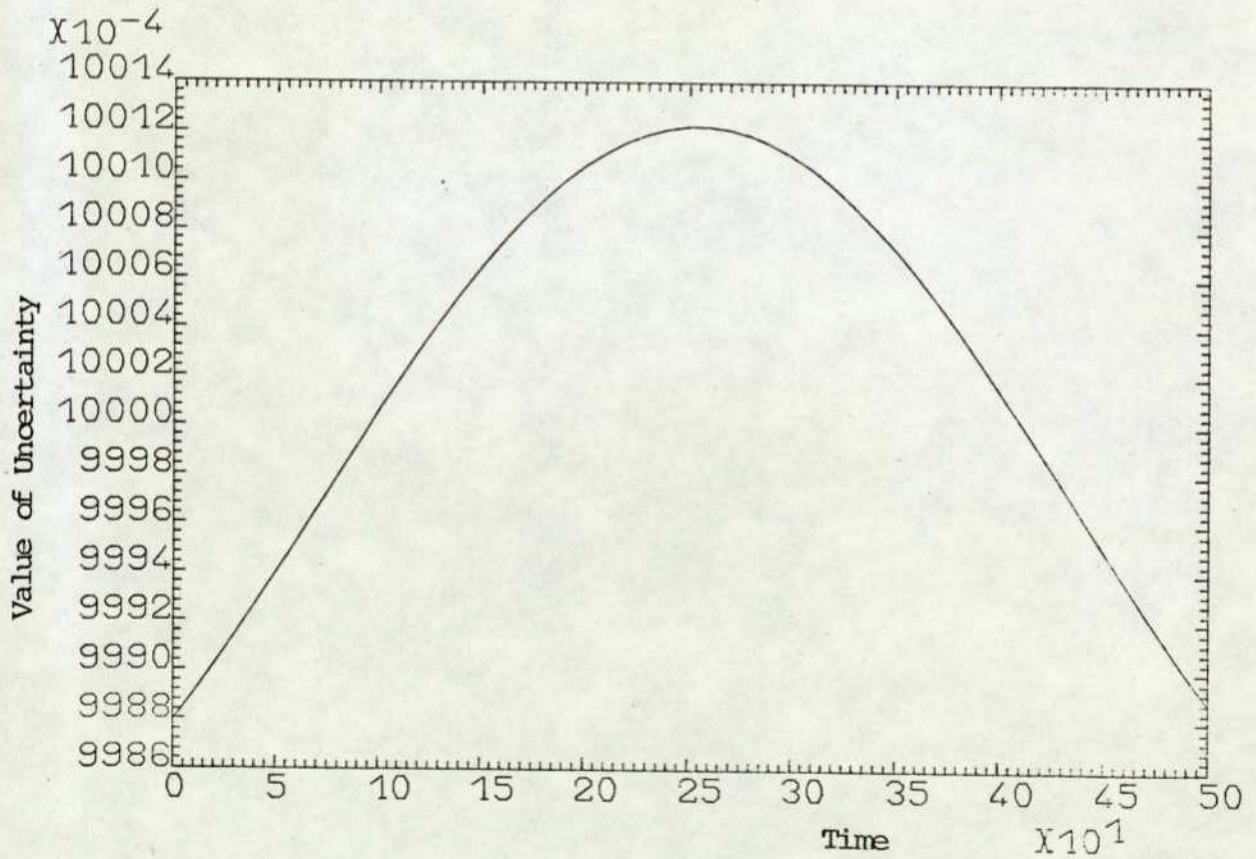
Fig. 6.4.13 The Performances of the Classical Least Squares and the Smoothed Least Squares Corresponding to Case 1 of Table 6.4.10

only slightly after the first two or three iterations. The use of Chebychev polynomial has resulted in a lower value of objective function achieved after only 7 overall iterations.

The resulting time-varying uncertainties corresponding to case 1 are shown in fig. 6.4.14.



(a) Chebychev Form



(b) Sinewave Form

Fig. 6.4.14 The Resulting Uncertainties Corresponding to Case 1 of Table 6.4.10.

6.4.2. CASE 2

In this case the effects of varying the weighting matrices on the performances of both the classical least squares and the smoothed least squares techniques have been thoroughly investigated. Using the weighting values

$$W(1) = 10.0$$

$$W(2) = 0.5$$

$$R = 20.0$$

which have been chosen to make the errors between system and model responses and the time-varying uncertainty and its nominal trajectory of similar magnitudes, as the nominal weightings, the effects of varying one of these weighting matrices keeping the other two at their nominal values, can be evaluated. As in Case 1, both forms of uncertainty (sinewave and Chebychev polynomial) have been employed and compared. The results are summarised in Tables 6.4.15, 6.4.16 and 6.4.17 for sinewave form uncertainty and Tables 6.4.18, 6.4.19 and 6.4.20 for Chebychev form uncertainty. When time-dependent weighting matrices as defined by equation 6.4.1. used, the results obtained are summarised in Table 6.4.21.

Now for the cases where sinewave-form uncertainty has been used, reference to Table 6.4.15 shows that as $W(1)$ is increased the estimate of H_{tc} increases both with the classical least squares and the smoothed least squares techniques. Fig. 6.4.22 shows the effect of $W(1)$ on the estimate of H_{tc} value.

CASE	W (1)	PRA (HTC) C.L.S.	PRA (HTC) S.L.S.	PRB (1)	PRB (2)	PRB (3)	PRB (4)	no. of overall iterations	C.P. time secs.
1	0.1	0.4116	0.4088	0.999678	-0.000974	0.01324	-0.047736	6	840
2	10	0.4188	0.4122	0.999369	0.0030183	0.000885	-0.071614	4	563
3	20	0.44	0.4342	1.00001	0.000704	-0.015064	0.280293	6	920
4	100	0.8155	0.7922	1.00082	-0.00189	-0.006304	-1.84257	4	1046

Table 6.4.15: Results obtained for Varying Values of W(1) where W(2) = 0.5 and R = 20 for a Sinewave-form Uncertainty

CASE	W (2)	PRA (HTC) C.L.S.	PRA (HTC) S.L.S.	PRB (1)	PRB (2)	PRB (3)	PRB (4)	NO OF OVERALL ITERATIONS	C.P. TIME SECS
1	0.1	0.5694	0.5694	1.0	0.0	0.0	0.0	2	355
2	0.5	0.4188	0.4122	0.999369	0.0003018	0.000885	0.071614	4	563
3	1.0	0.4135	0.4146	0.998579	0.002164	0.001926	0.039775	4	565
4	2.0	0.412	0.4047	0.999588	0.001208	0.012754	0.55894	6	900
5	5.0	0.4116	0.4039	0.999581	0.001228	0.01265	0.08377	6	982

Table 4.4.16. Results Obtained for Varying Values of W(2) where W(1) = 10, R = 20 for a Sinewave-form Uncertainty.

CASE	R	PRA (HTC) C.L.S.	PRA (HTC) S.L.S.	PRB (1)	PRB (2)	PRB (3)	PRB (4)	no. of overall iterations	C.P. time Secs.
1	0.1	0.4188	0.5154	0.999608	-0.001096	0.0134139	-0.068049	6	895
2	1.0	0.4188	0.4032	0.999793	-0.001227	0.012893	0.037899	6	965
3	20.0	0.4188	0.4122	0.999369	0.003018	0.000885	-0.071614	4	563
4	100.0	0.4188	0.4168	0.999976	-0.00023	0.013062	0.050579	4	485
5	1000.0	0.4188	0.4188	1.0	0.0	0.0	0.0	2	255

Table 4.4.17: Results Obtained for Varying Values of R, where $W(1) = 10$ and $W(2) = 0.5$ for a Sinewave-form uncertainty.

CASE	W(1)	PRA (HTC) C.L.S	PRA (HTC) S.L.S.	RBB (1)	PRB (2)	PRB (3)	PRB (4)	no. of overall iterations	C.P. time Secs
1	0.1	0.4116	0.4089	0.999747	0.000358	0.000221	-0.000780	3	575
2	10.0	0.4188	0.4183	0.999769	0.000239	0.000206	-0.00076	3	614
3	20.0	0.44	0.4372	0.999985	-0.000016	0.000206	-0.000705	3	585
4	100.0	0.8155	0.82	1.00047	-0.002417	0.00038	-0.000705	4	700

Table 6.4.18: Results Obtained for Varying Values of W(1) where W(2) = 0.5 and R = 20 for a Chebychev-form uncertainty.

CASE	W (2)	PRA (HTC) C.L.S.	PRA (HTC) S.L.S	PRB (I)	PRB (2)	PRB(3)	PRB (4)	NO OF OVERALL ITERATIONS	C.P. TIME Secs.
1	0.1	0.5694	0.5694	1.0	0.0	0.0	0.0	2	488
2	0.5	0.4188	0.4183	0.4183	0.999769	0.000239	0.00076	3	614
3	1.0	0.4135	0.4133	0.999639	0.000413	0.000256	0.000864	2	400
4	2.0	0.412	0.4122	0.999572	0.000449	0.000272	0.000907	2	386
5	5.0	0.4116	0.4119	0.99955	0.000459	0.000274	0.000918	2	404

Table 6.4.19 Results Obtained for Varying Values of W (2) Where W(1) = 10 and R = 20 for a
Chebychev - Form Uncertainty.

CASE	R	PRA (HTC) C.L.S.	PRA (HTC) S.L.S	PRB (I)	PRB (2)	PRB (3)	PRB (4)	NO OF OVERALL ITERATIONS	C.P. TIME SECS
1	0.1	0.4186	0.999675	0.000306	0.000306	0.000262	0.000913	2	367
2	1.0	0.4188	0.4184	0.999676	0.000304	0.000258	0.000912	2	360
3	20.0	0.4183	0.4183	0.999769	0.000239	0.000206	0.000762	3	614
4	100.0	0.4188	0.4189	0.999997	0.000016	0.000049	0.000122	2	675
5	1000.0	0.4188	0.4188	1.0	0.0	0.0	0.0	2	855

Table 6.4.20. Results Obtained for Varying Values of R where $W(1) = 10$ and $W(2) = 0.5$ for a Chebychev-form Uncertainty.

CASE	form of BB22	PRA (HTC) C.L.S.	PRA (HTC) S.L.S.	PRB (1)	PRB (2)	PRB (3)	PRB (4)	no. of overall iterations	C.P. time
1	sine	0.5405	0.5405	1.0	0.0	0.0	0.0	2	280
2	Cheb	0.5405	0.5406	1.00043	-0.001290	0.000283	-0.000735	3	520
3	$WT(2)=\frac{10}{Y_A(2)}$ sine	0.4022	0.3926	0.999659	-0.001406	0.012788	0.056001	6	955
4	$WT(2)=\frac{10}{Y_A(2)}$ Cheb	0.4022	0.4022	0.999611	0.000521	0.000286	-0.001057	2	410

Table 6.4.21: Results Obtained for Time-Varying Weighting Matrices for both Forms of Uncertainty.

Comparing the computer time needed to achieve the smoothed least squares solution as given by Table 6.4.15 with the improvement in H_{tc} value, it can be said that much effort is spent for little improvement.

Table 6.4.16 which gives the effects of the value of $W(2)$ on H_{tc} shows that as $W(2)$ is increased the value of H_{tc} decreases with a greater demand for smoothing (though the amount of smoothing is not significant). Fig. 6.4.23 shows how the value of H_{tc} changes with the value of $W(2)$ under the classical least squares and the smoothed least squares techniques. Here again, the changes in H_{tc} due to the smoothed least squares technique are small.

Table 6.4.17 which gives the effects of R on H_{tc} values shows that as R is increased, the classical least squares solution remains the same over the whole range of R , whilst the smoothed least squares produces very small changes, giving the impression that the value of H_{tc} is insensitive to R .

Tables 6.4.18, 6.4.19 and 6.4.20 which give the corresponding information to that given by the first three tables but for Chebychev-form time-varying uncertainty give almost the same information with only slight differences in the classical least squares solutions, and a tendency towards quicker convergence as indicated by lower central processor (CP) times in most of the cases.

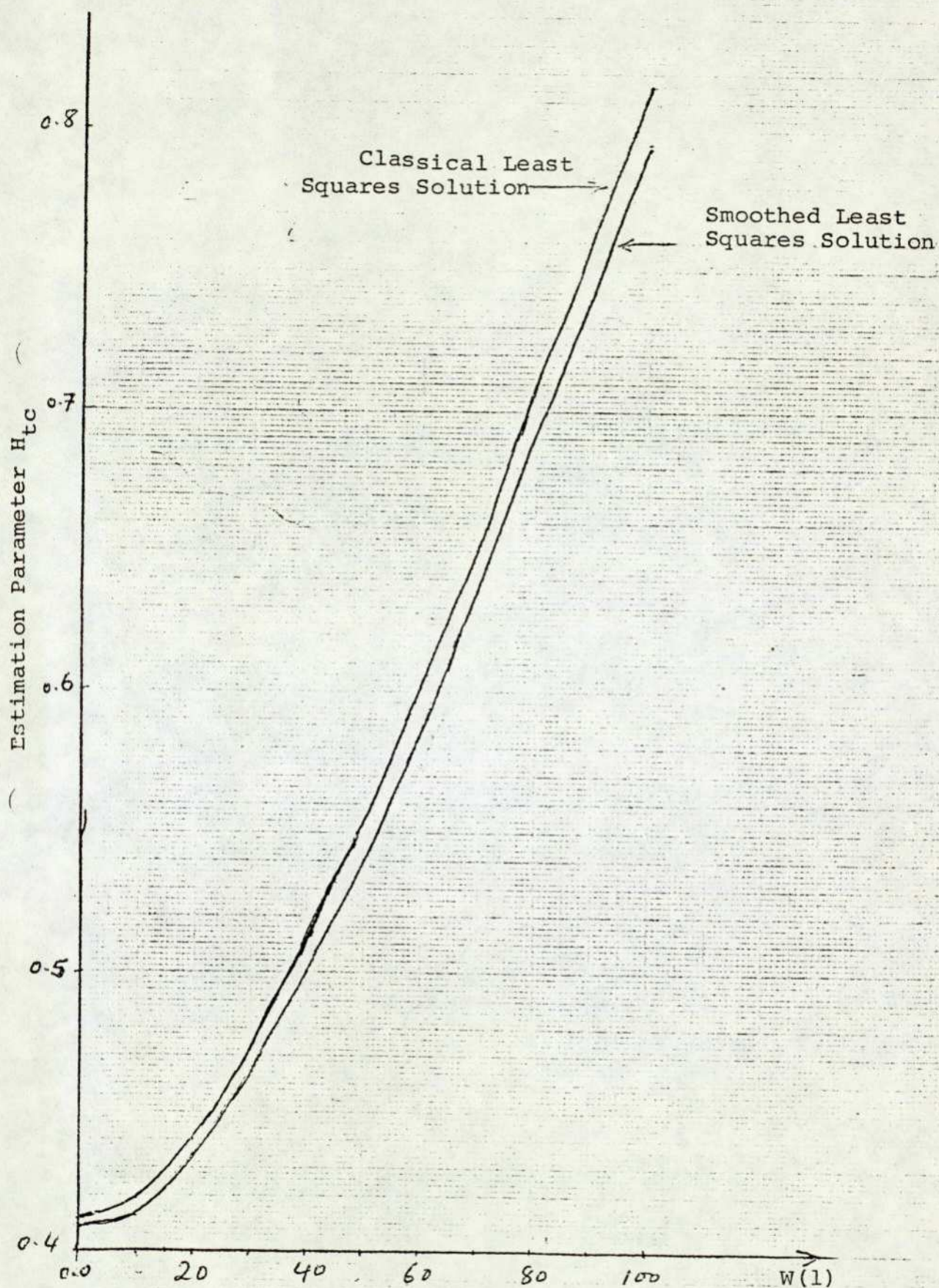


Fig.6.4.22. The Effect of $W(1)$ on the Estimation Parameter H_{tc}

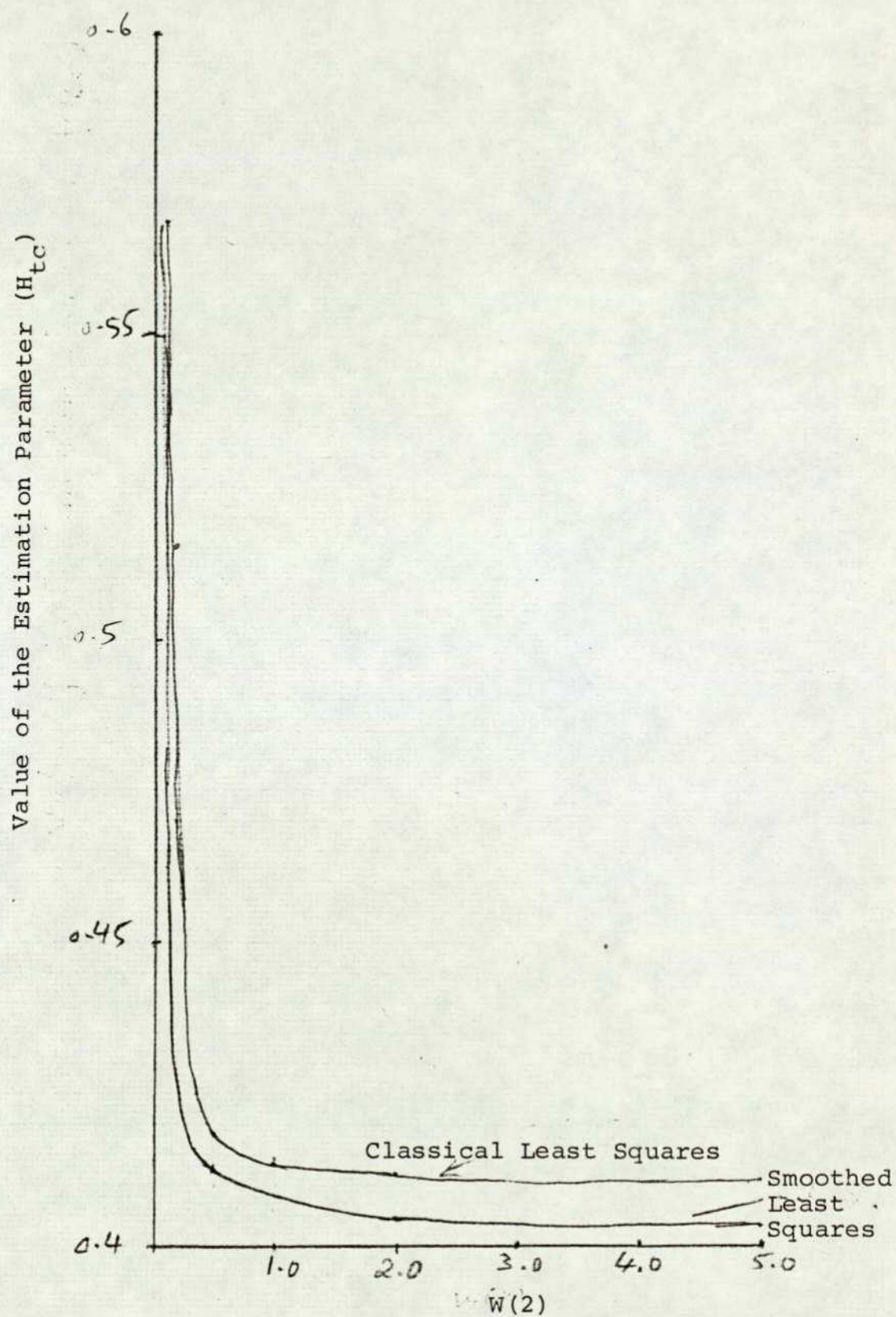


Fig.6.4.23. The Effect of $W(2)$ on the Estimation Parameter H_{tc}

Table 6.4.21 shows the effects of using time-varying weighting matrices given by equations 6.4 and 6.5 which are the inverse of the system samples. The solutions obtained by the two techniques are the same, resulting in a constant uncertainty equal to its nominal value. When the time-varying weighting matrix $W(2)$ is increased by a factor of 10.0, the value of H_{tc} obtained by the smoothed least squares technique differs by about 2.5% from the classical least squares solution in the case of sinewave-form uncertainty, whilst no change in the smoothed least squares occurred for the Chebychev-type uncertainty.

Typical responses yielded by the model are given by figs. 6.4.24 and 6.4.25. These responses correspond to case 1 in Table 6.4.15 where $W(1) = 10.0$, $W(2) = 0.1$ and $R = 20.0$. Whereas the model vapour pressure response fits nicely into the average trend of the real system response, the model height response does not have good agreement with that of the system. The vapour pressure response exhibits the non-minimum phase behaviour but could not follow the fluctuations on the system response.

When the weighting of the errors in the height responses has been increased to 100 as in Case 4 of table 6.4.16 the responses yielded by the model are shown in figs. 6.4.26 and 6.4.27. In this case the model height response follows the average trend of that of the system whereas the model vapour pressure response becomes unable to follow that of the system to the extent that it does not exhibit the non-minimum phase behaviour.

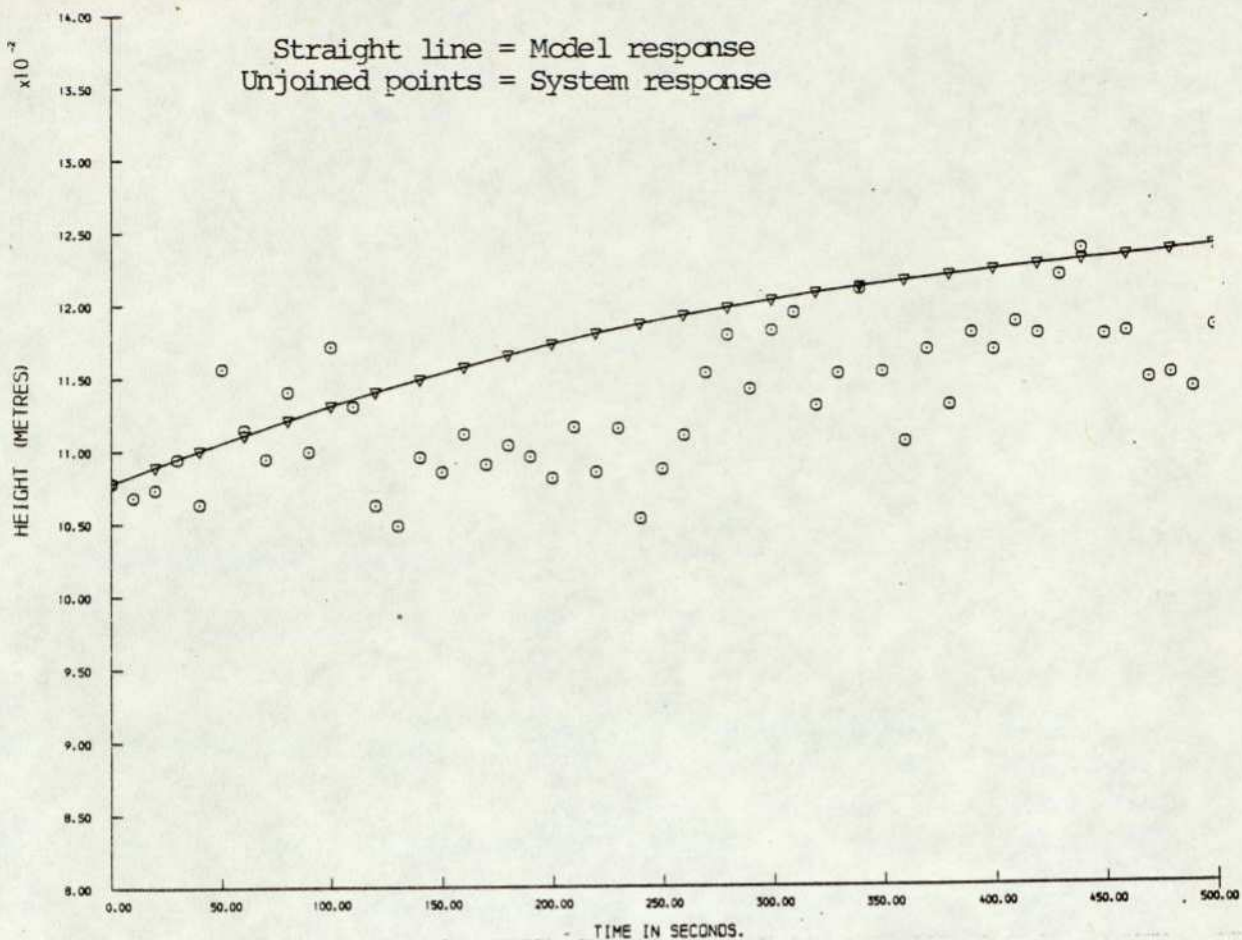


Fig.6.4.24 System and Model Height Responses Corresponding to Case 1 of Table 6.4.16.

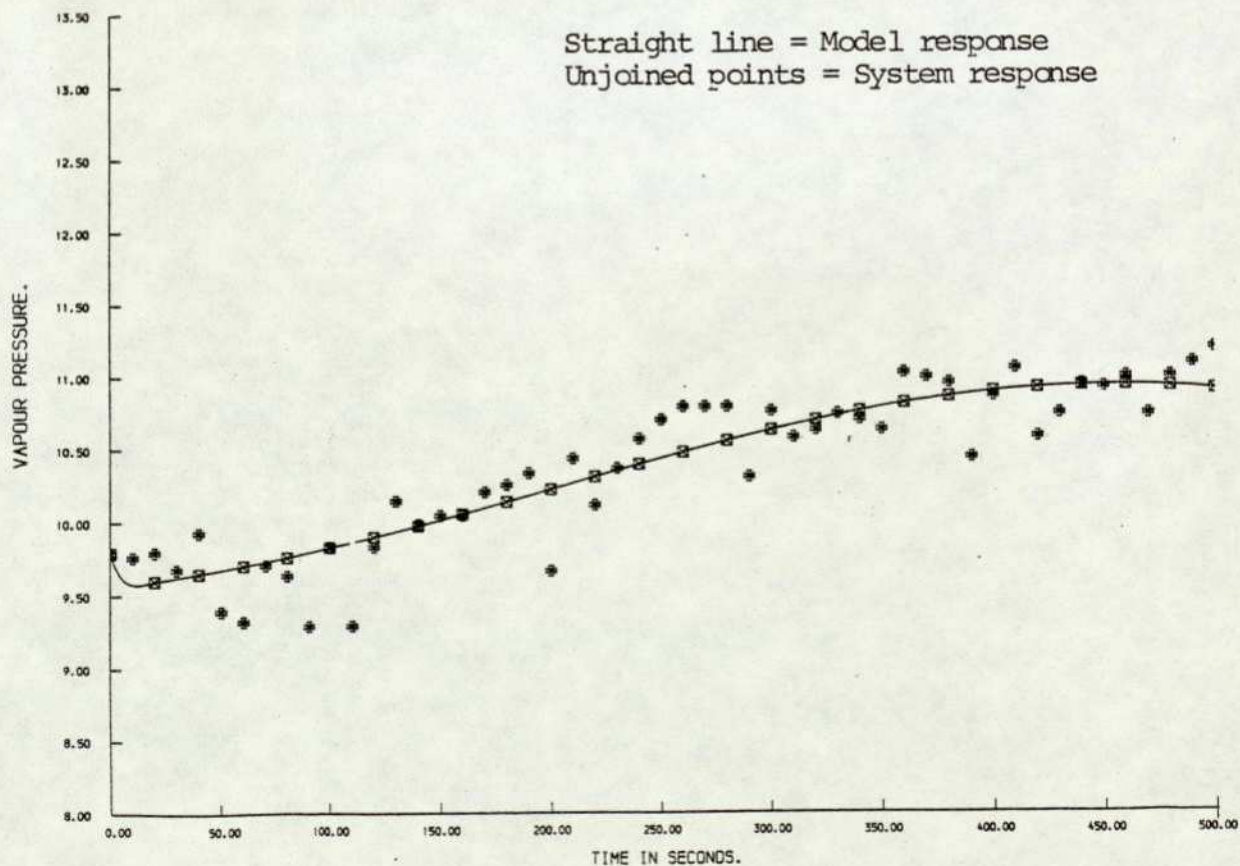


Fig.6.4.25 System and Model Vapour Pressure Responses Corresponding to Case 1 of Table 6.4.16.

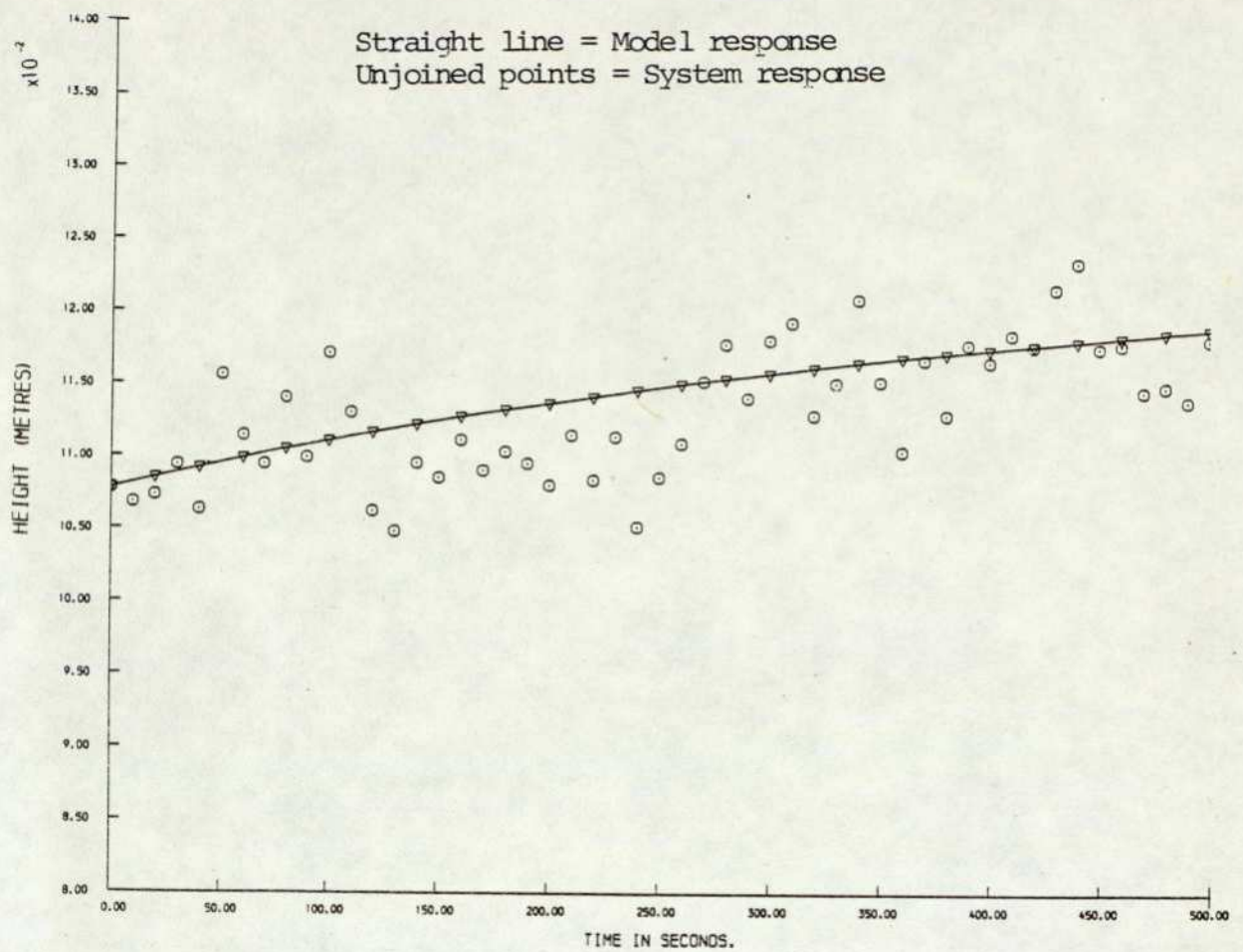


Fig.6.4.26 System and Model Height Responses Corresponding to Case 4 of Table 6.4.15.

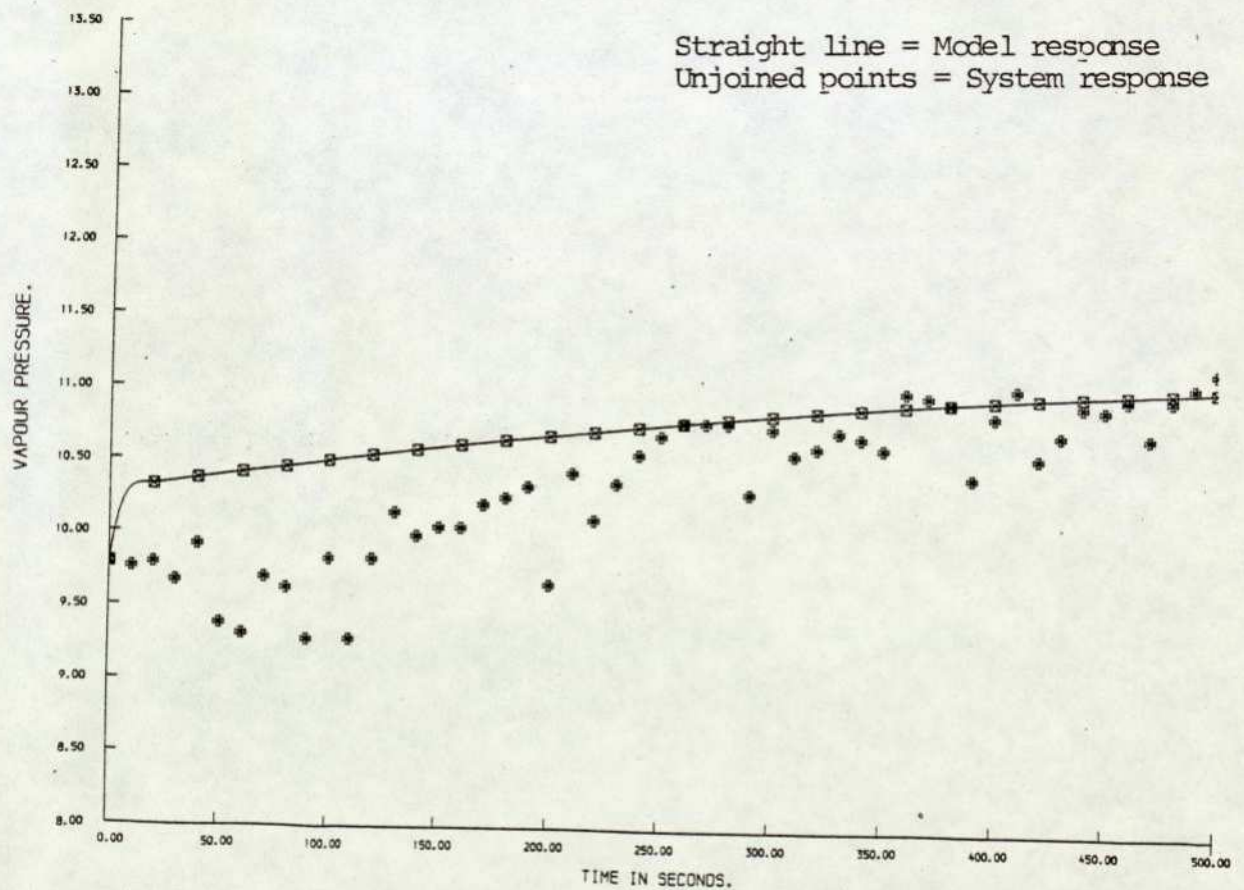
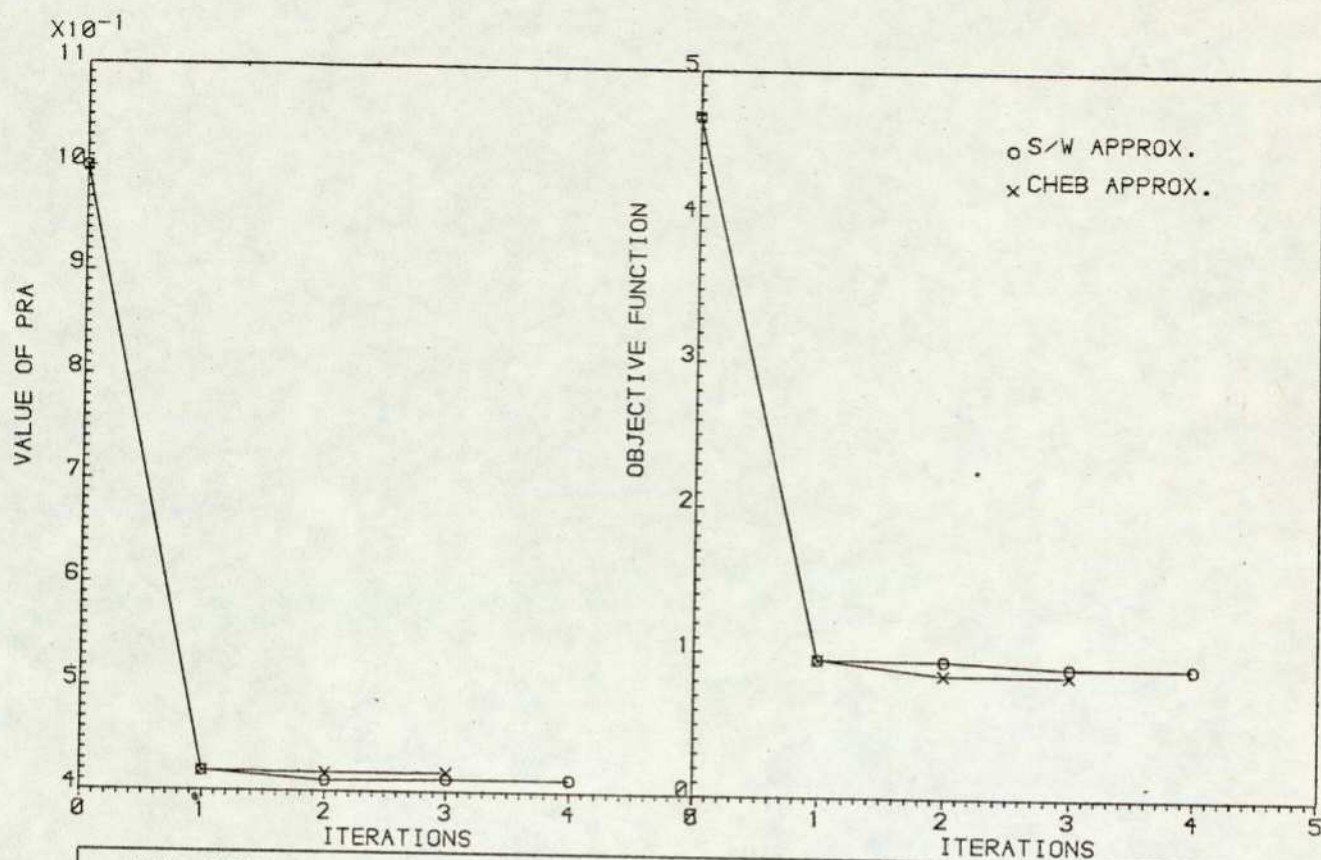


Fig.6.4.27 System and Model Vapour Pressure Responses Corresponding to Case 4 of Table 6.4.15.

The performance of the classical least squares and the smoothed least squares techniques with regards to the estimation parameter H_{tc} and the objective function are plotted in figs. 6.4.28 for the nominal weightings in Cases 2, 2 and 3 of Tables 6.4.15, 6.4.16 and 6.4.17 respectively and the corresponding three tables for the Chebychev case. These graphs give the overall performances of the two techniques and an enlarged version of that to closely compare the performances of the two techniques. The classical least squares solution is given by the solution at iteration 1, while subsequent solutions are those of the smoothed least squares technique. The classical least squares solution is obtained by setting the time-varying uncertainty incorporated by the model at its nominal value (1.0). From these graphs it can be seen that the classical least squares technique effects a big change in the value of H_{tc} leading to a big drop in the objective function. The smoothed least squares then affects small changes in the value of H_{tc} and objective function after several overall iterations. In this case, changes of 1.6% in H_{tc} and 10% in objective function over the classical least squares values have been achieved.

Figs. 6.4.29 and 6.4. 30 refer to the cases of Table 6.4.21 in which time-varying weighting matrices are used. The graphs also compare the performances of the classical least squares and the smoothed least squares techniques, and point to the idea that, for the particular system concerned, the introduction of smoothing into the identification problem affects little change on the performance of the classical least squares technique.



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE

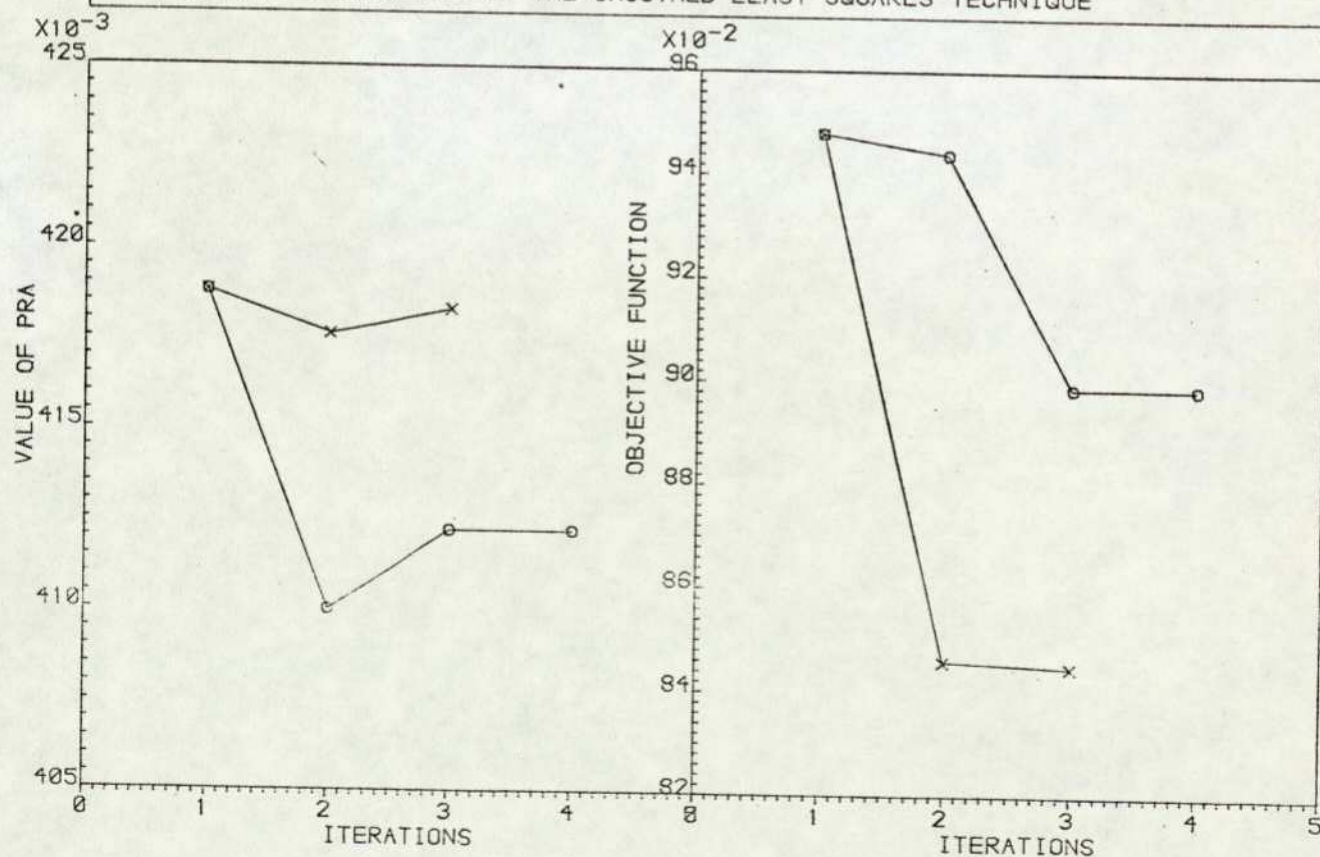
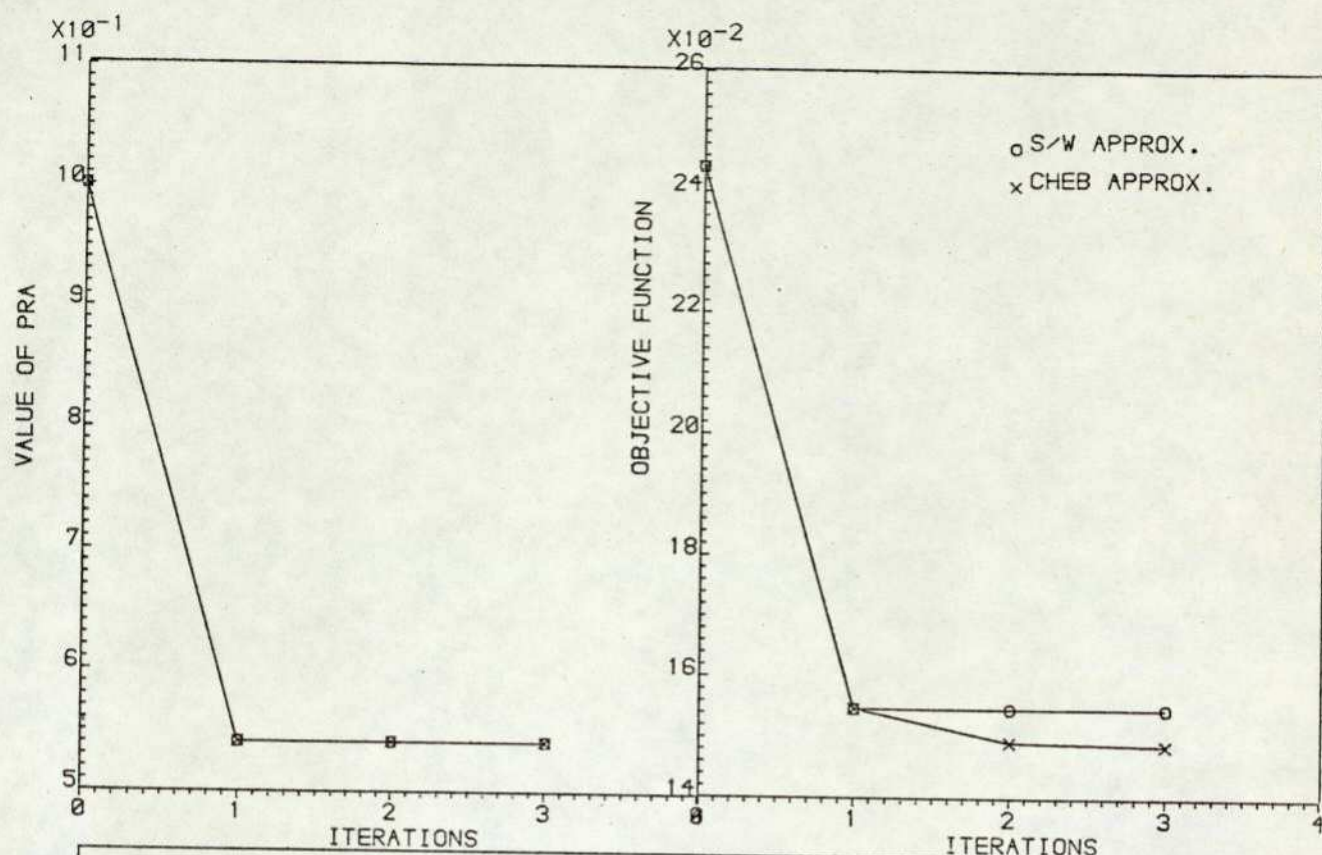


Fig. 6.4.28: The Performance of the Classical Least Squares and the Smoothed Least Square where $W(1) = 10$, $W(2) = 0.5$ and $R = 20$ for Case 2 of Table 6.4.15.



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE

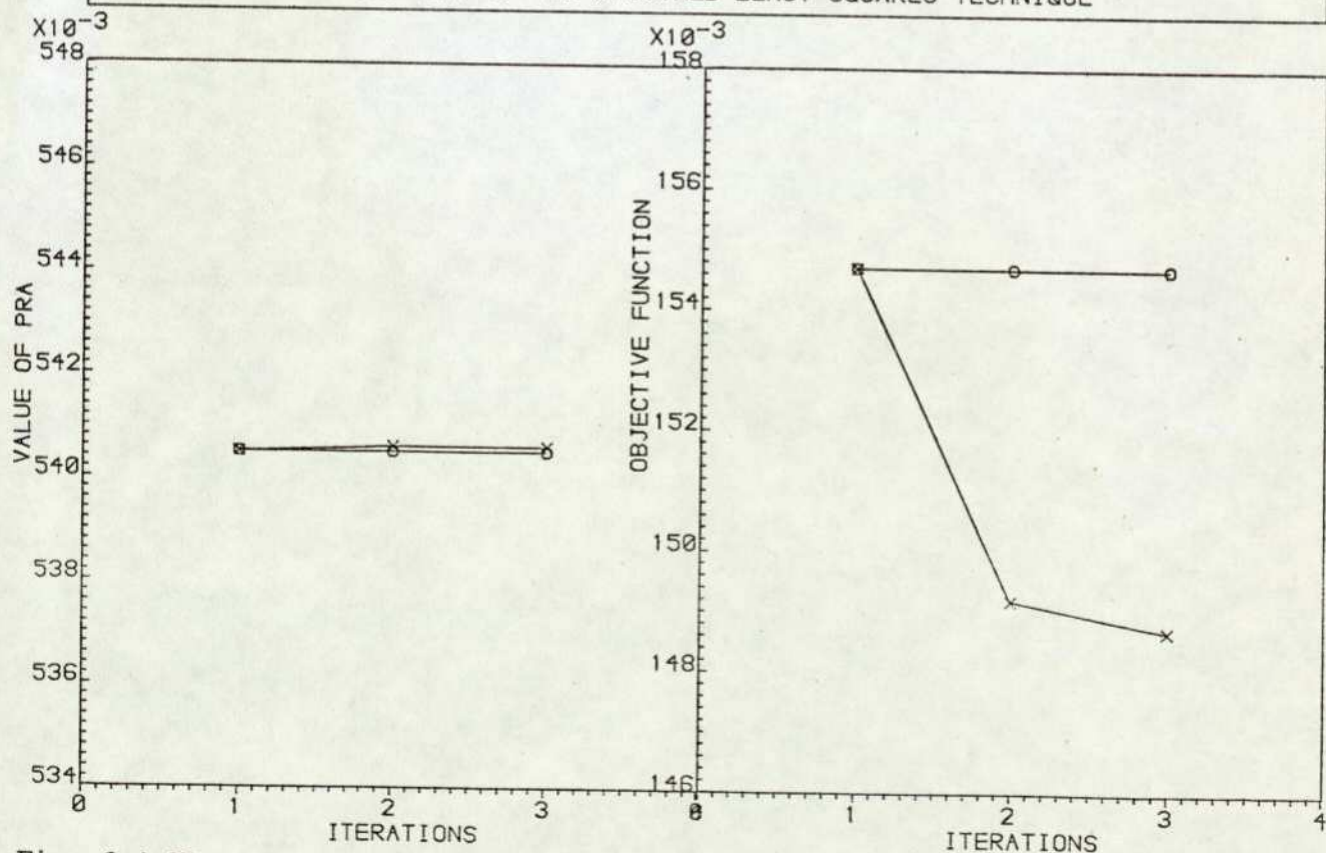
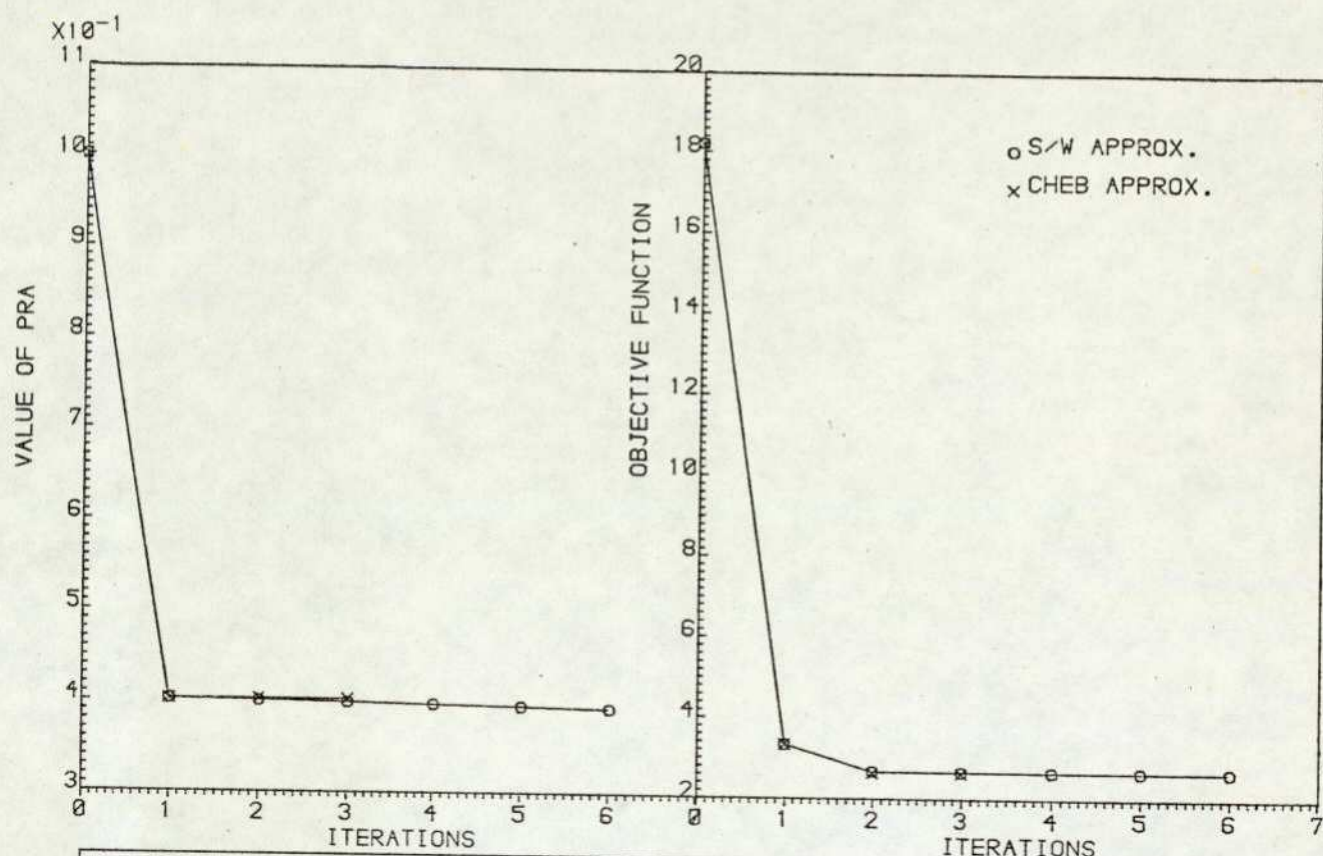


Fig. 6.4.29: The Performance of Classical Least Squares and the Smoothed Least Squares for time varying weighting matrices corresponding to Case 1 and 2 of table 6.4.21



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE

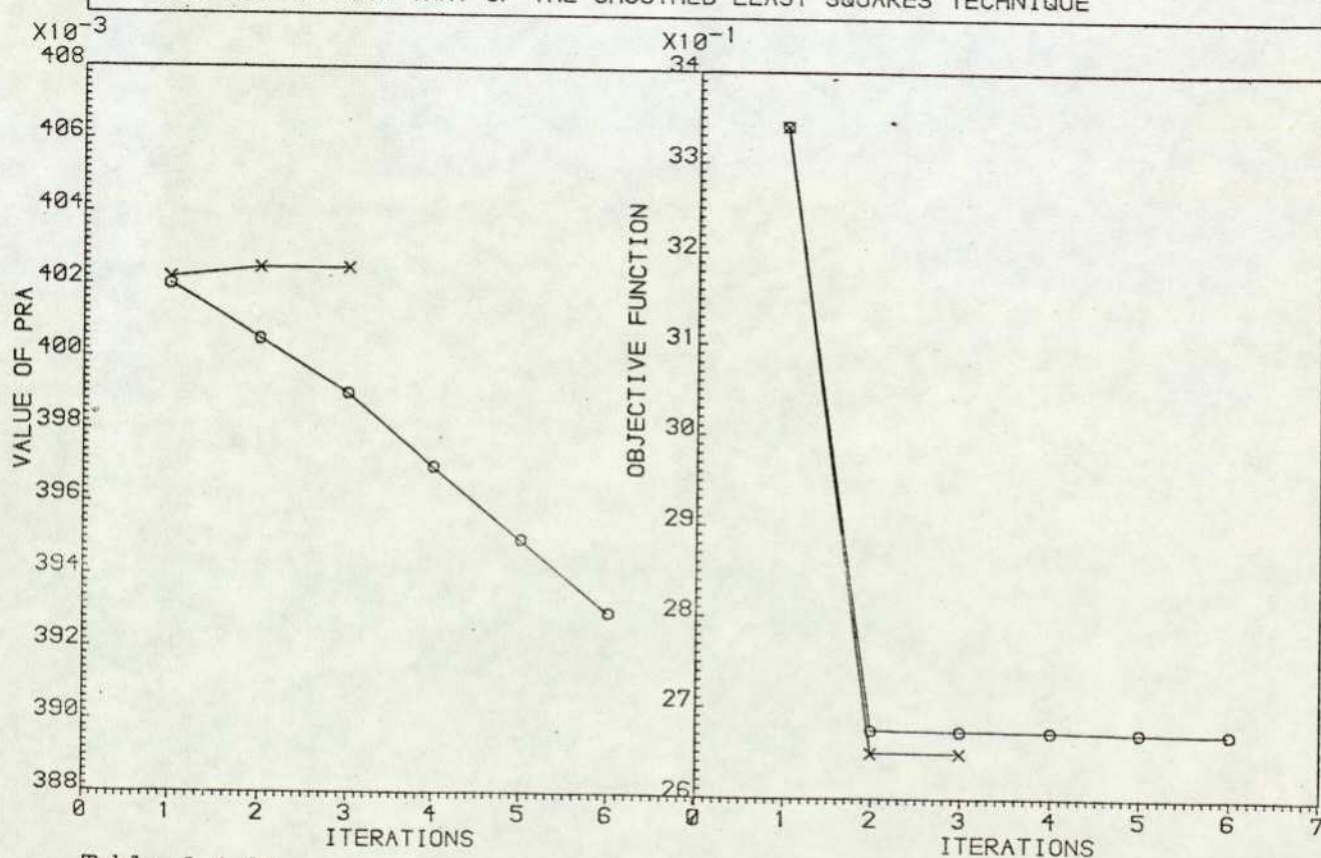


Table 6.4.30

The Performance of the Classical Least Squares and the Smoothed Least Squares techniques using time varying weighting matrices corresponding to Cases 3 and 4 of table 6.4.21.

6.4.3. CASE 3

The results obtained for the estimation parameter obtained by the classical least squares and the smoothed least squares techniques using the two forms of the time-varying uncertainty are summarised in the following table:

CASE	FORM OF BB22	W(1)	W(2)	R	PRA (HTC) C.L.S.	PRA (HTC) S.L.S.	NO. OF OVERALL ITERS.	CP TIME secs.
1	SINE	10	0.5	20	0.4342	0.4358	6	875
2	CHEB	10	0.5	20	0.4342	0.4348	2	382
3	SINE	$\frac{1}{YA(1)}$	$\frac{1}{YA(2)}$	$\frac{1}{TRAJ}$	0.480	0.492	6	760
4	CHEB	$\frac{1}{YA(1)}$	$\frac{1}{YA(2)}$	$\frac{1}{TRAJ}$	0.480	0.479	4	675

Table 6.4.31. Summary of the Results of Case 3.

The table shows that the smoothed least squares estimate hardly differs from that obtained by the classical least squares technique in all the cases shown. The improvements range from 0.122% in Case 2 to about 2.5% in Case 3. The time needed to achieve this minimal improvement is so large that unless this improvement is critically needed, the smoothing procedure may be considered unnecessary. The table also shows that the use of time varying matrices yields a higher value of parameter estimate. This estimate may be considered more accurate because it is the result of an averaging process performed by the identification algorithm

due to the use of the time-varying weighting matrices.

Responses obtained for the case of time-varying weightings are shown in Figs. 6.4.32 and 6.4.33. As can be seen from the height response, the system response is too oscillatory and the model response could not follow the system behaviour. On the other hand, the vapour pressure system response is less oscillatory and the model has produced a response which has managed to follow the general trend of the system response passing through the average values. However, the model has not reproduced the fluctuations of the system response.

A comparison between the performances of the two techniques is given by Fig. 6.4.34 for Cases 1 and 2 and Fig. 6.4.35 for Cases 3 and 4. In both figures, the performance of the classical least squares technique outweighs that of the smoothed least squares technique since it carries out most of the work in reducing the objective ^{function} value from its initial value (which is always relatively high) to a much smaller value depending on the change in the parameter estimate. The contribution of subsequent smoothing iterations (which lead to updating of the parameter estimates) is relatively small. It is also apparent from the graphs that the use of the Chebychev form of approximation to the time-varying uncertainty results in a lower value of objective function with a smaller number of overall iterations.

The resulting forms of the uncertainties corresponding to these two graphs are shown in Figs. 6.4.36 and 6.4.37. Although these uncertainties appear to possess certain shapes, due to the scaling of the Y axis of the graph, the fact is that when these are compared with the values of the variables to which they are attached (T_0), they will appear as almost a constant value near to their nominal trajectory (1.0).

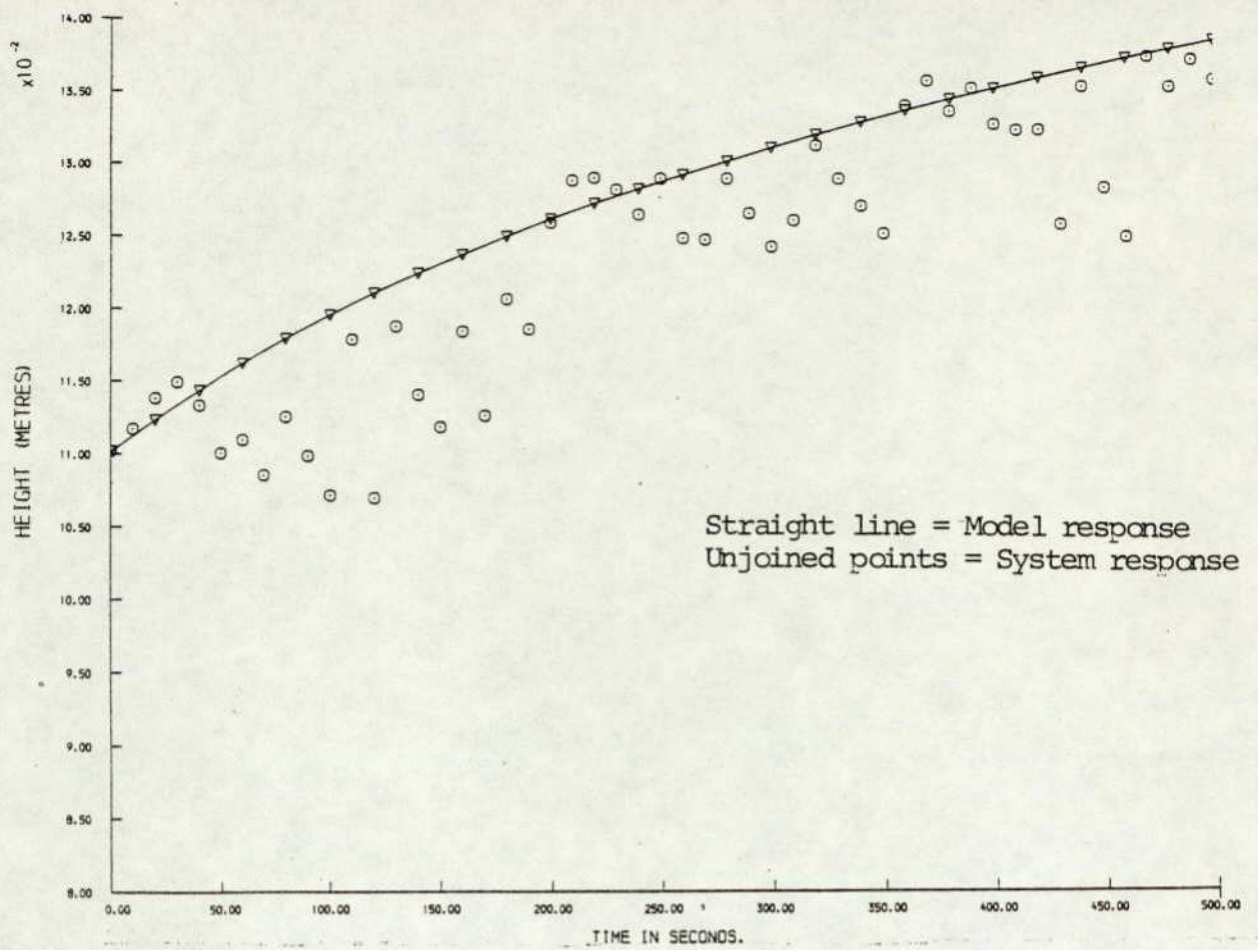


Fig.6.4.32 System and Model Height Responses Corresponding to Case 3 of Table 6.4.31.

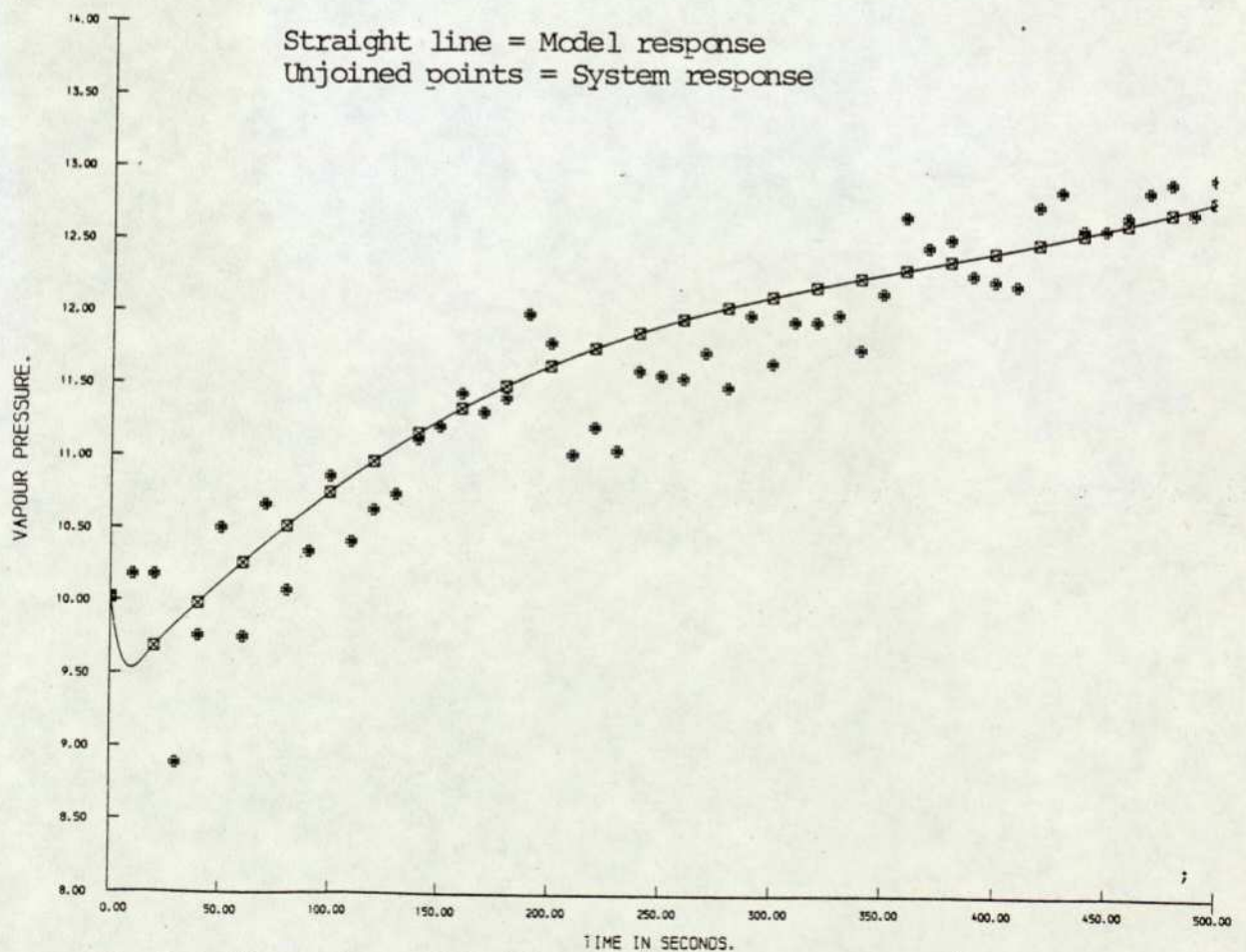
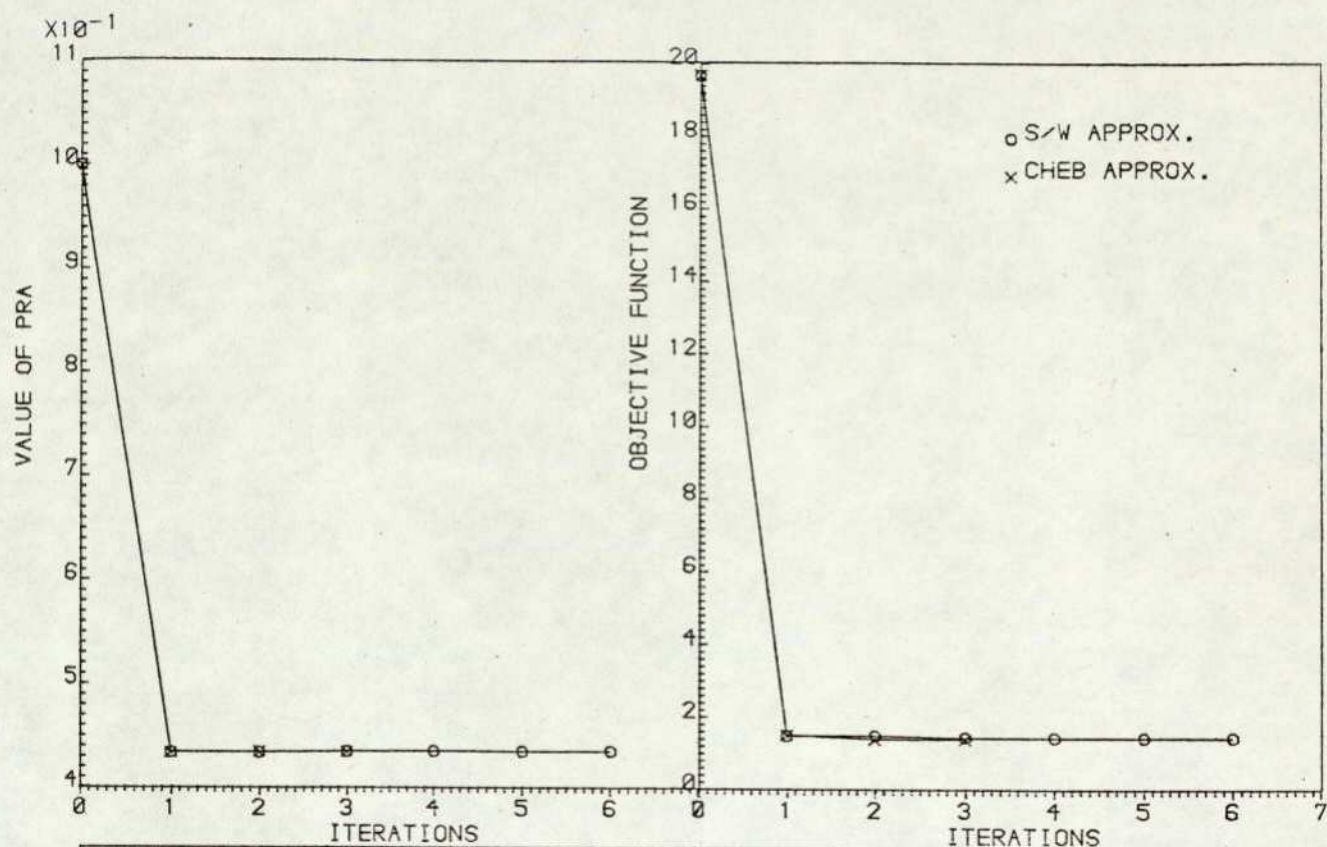


Fig.6.4.33 System and Model Vapour Pressure Responses Corresponding to Case 3 of Table 6.4.31.



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE

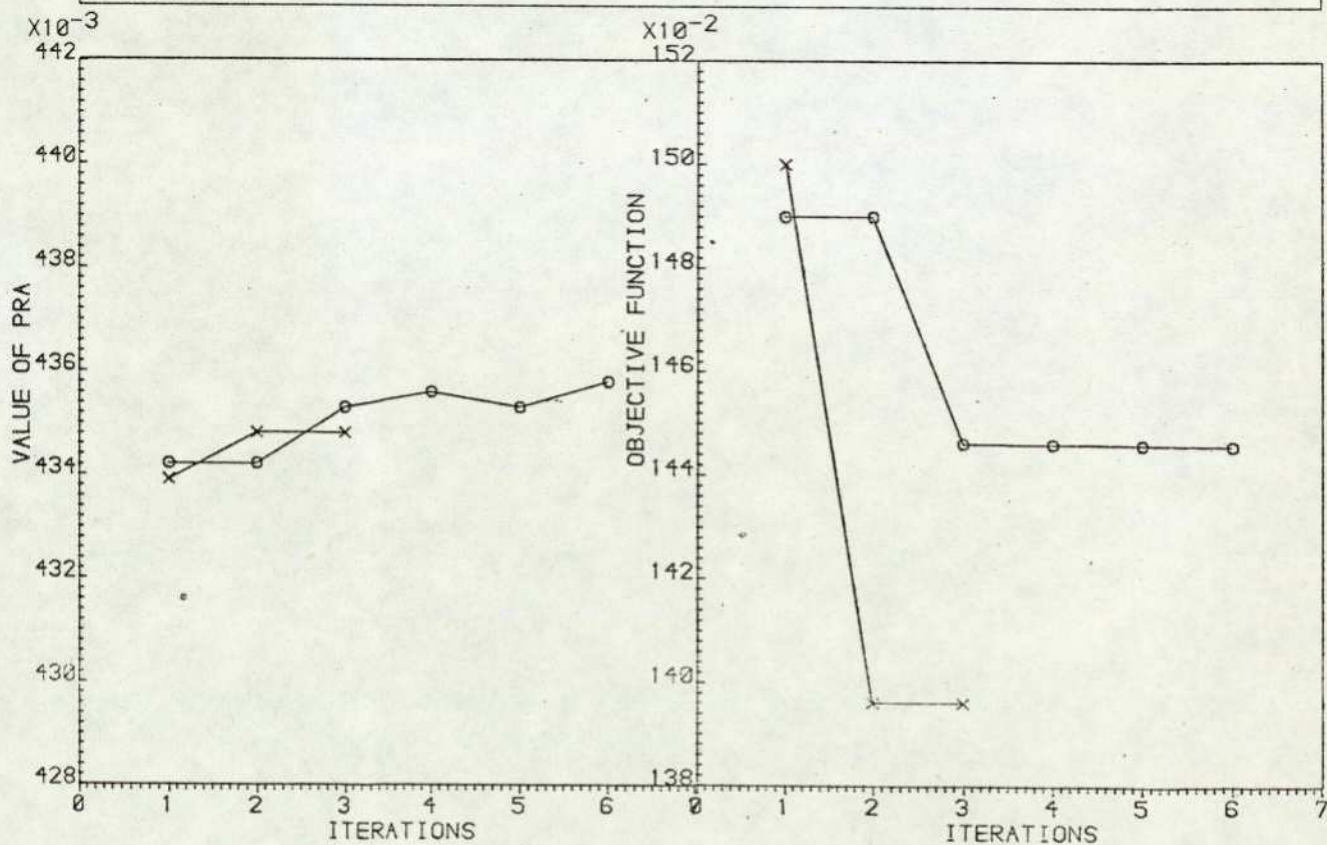
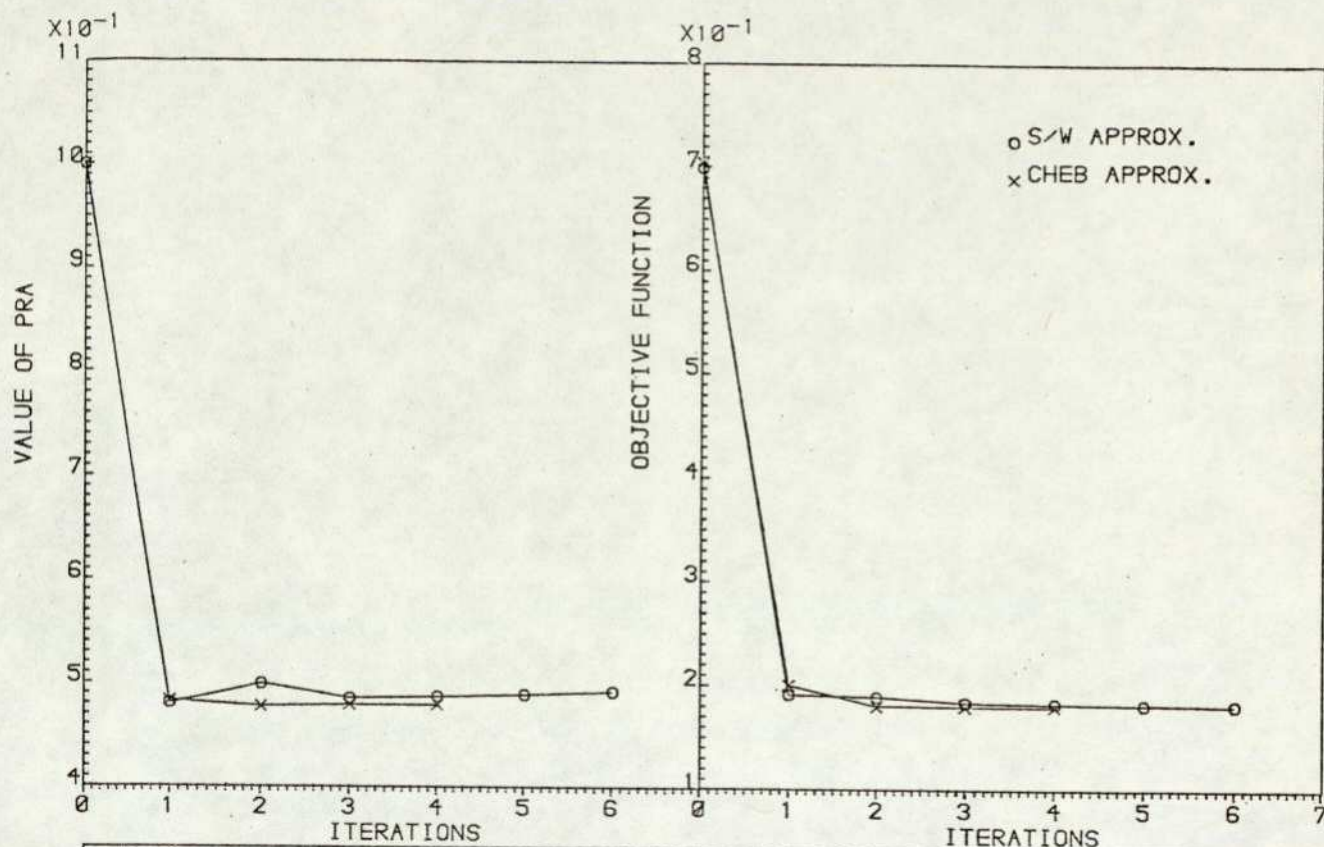


Fig. 6.4.34 The performances of the classical least squares and the smoothed least squares techniques corresponding to Cases 1 & 2 of Table 6.4.31.



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE

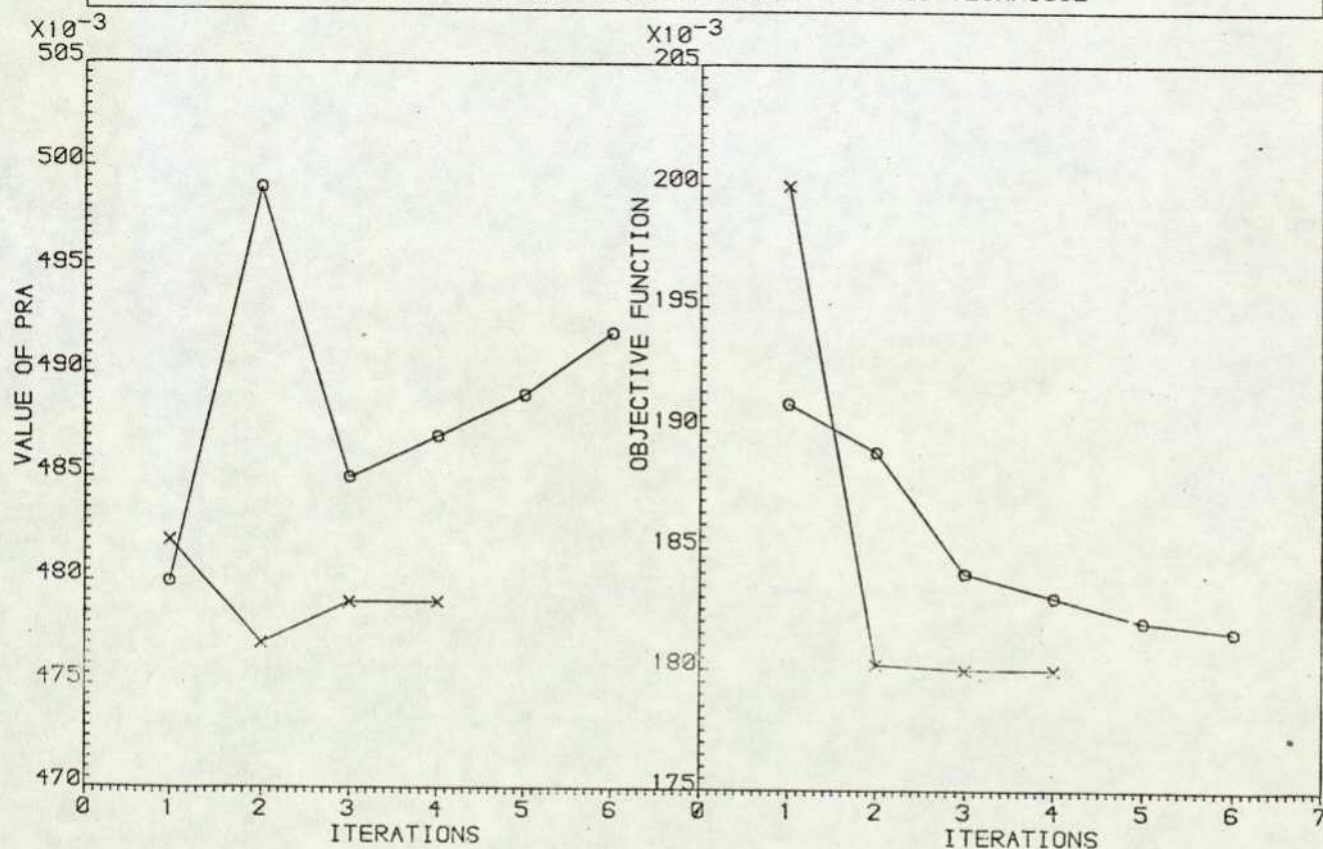


Fig. 6.4.35 The performances of the classical least squares and the smoothed least squares techniques corresponding to Cases 3 & 4 of Table 6.4.31.

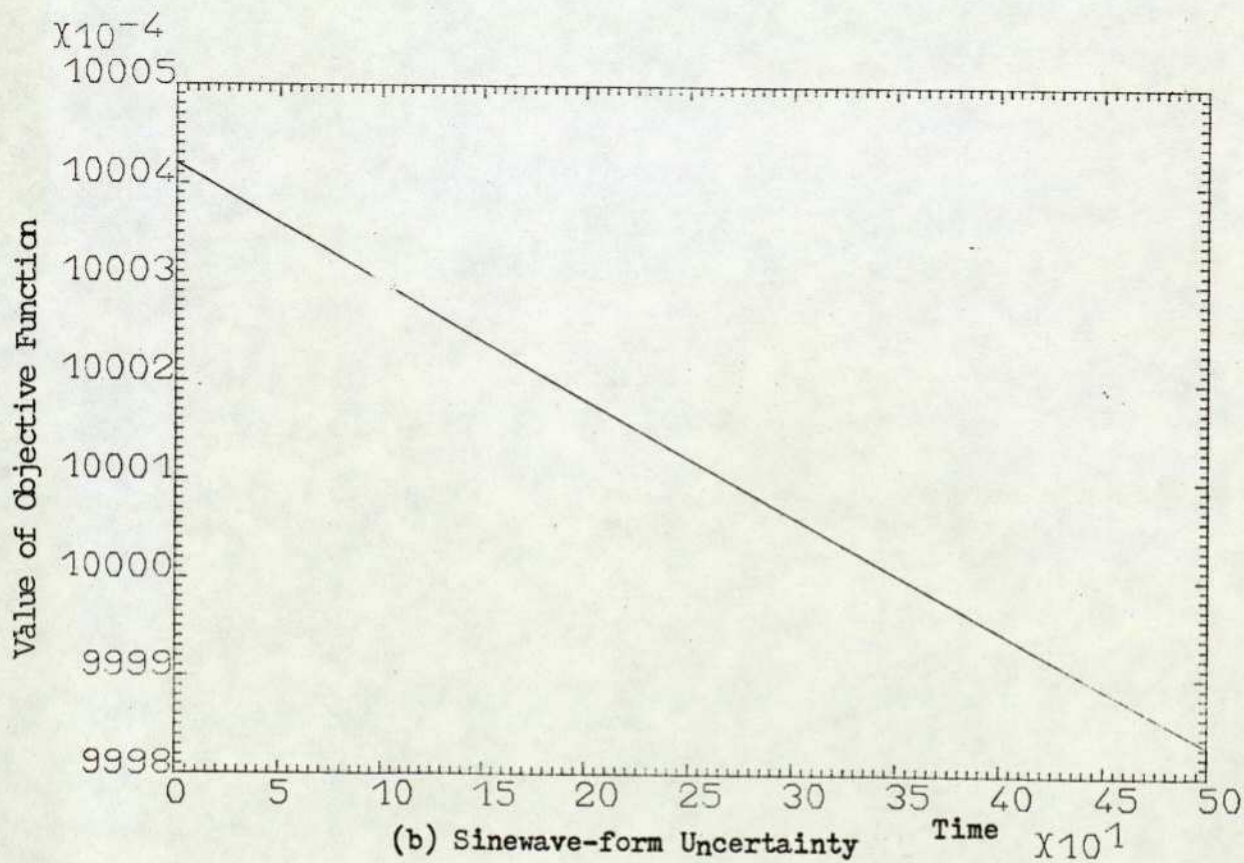
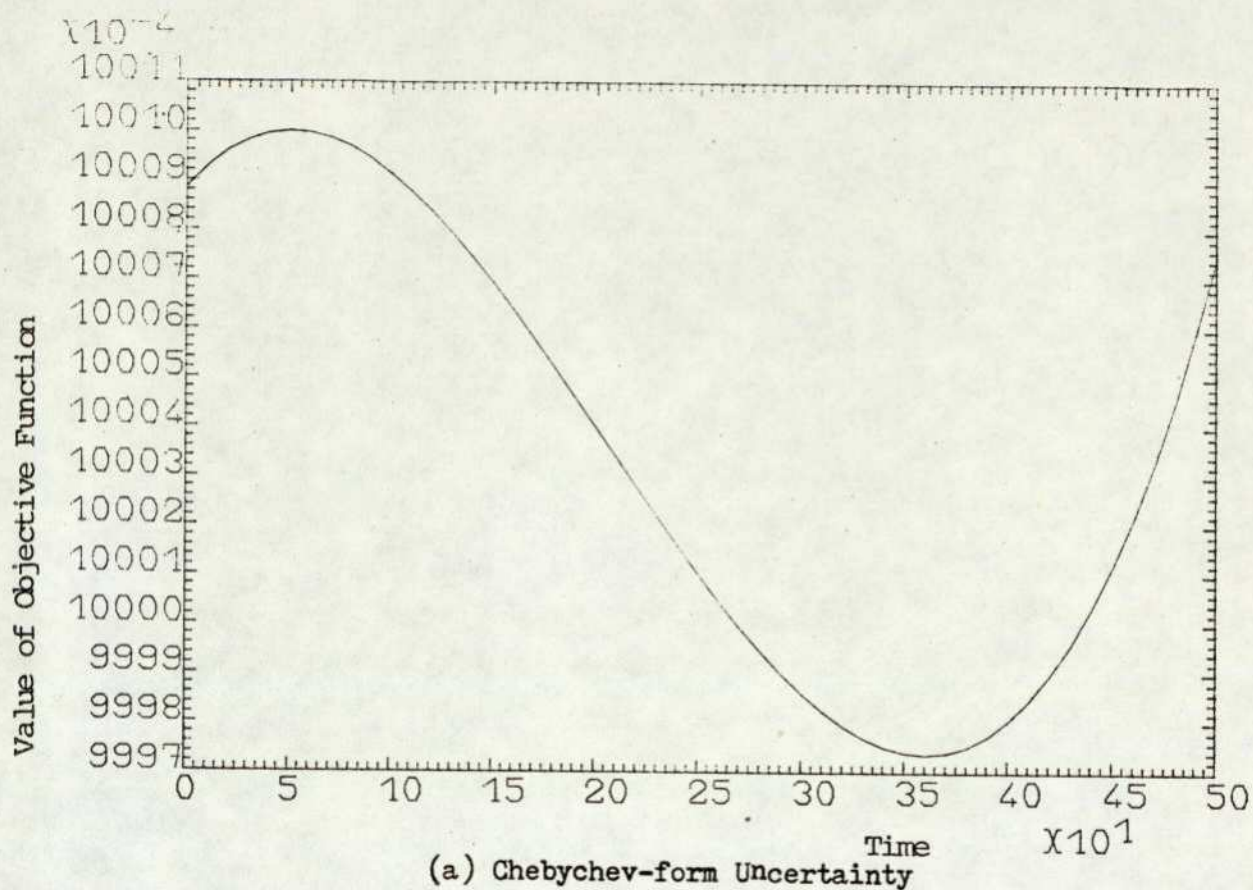
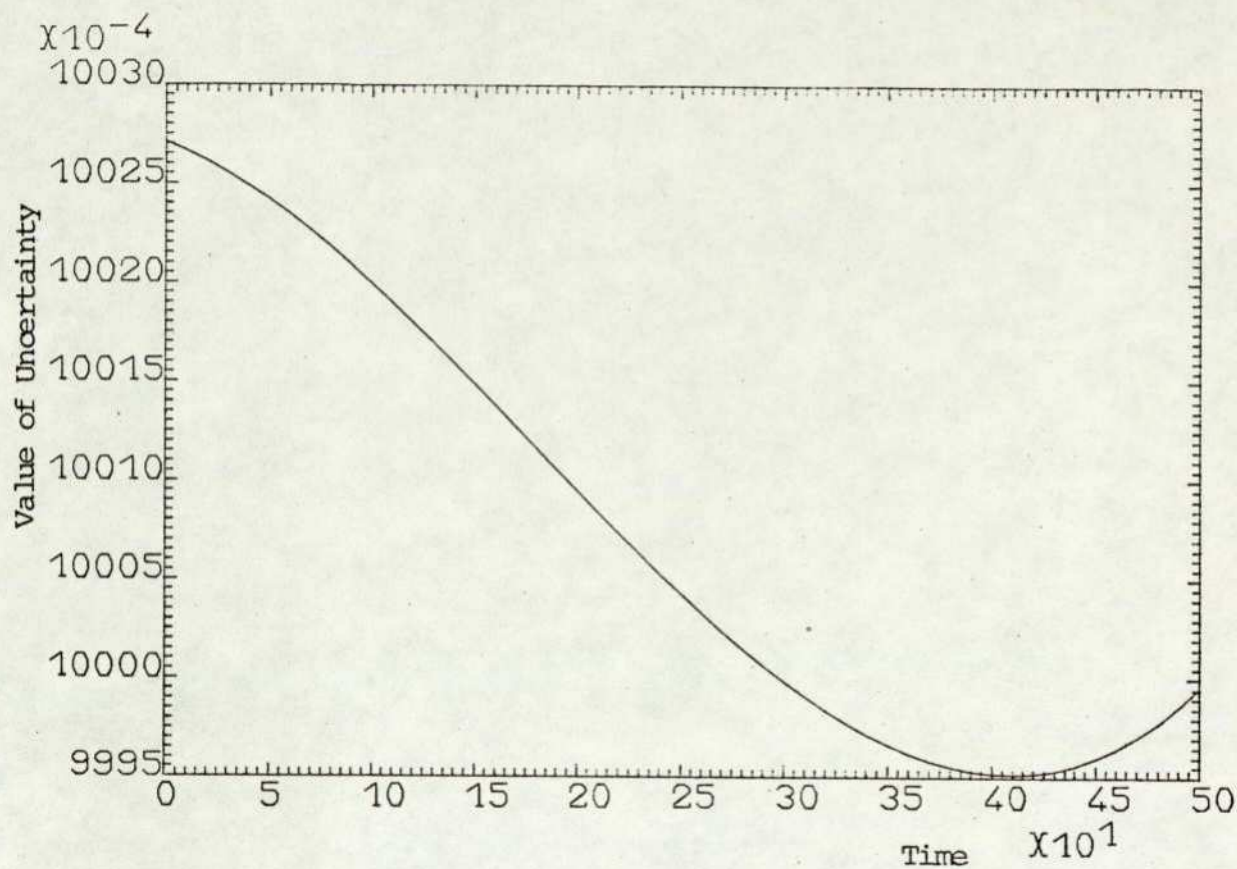
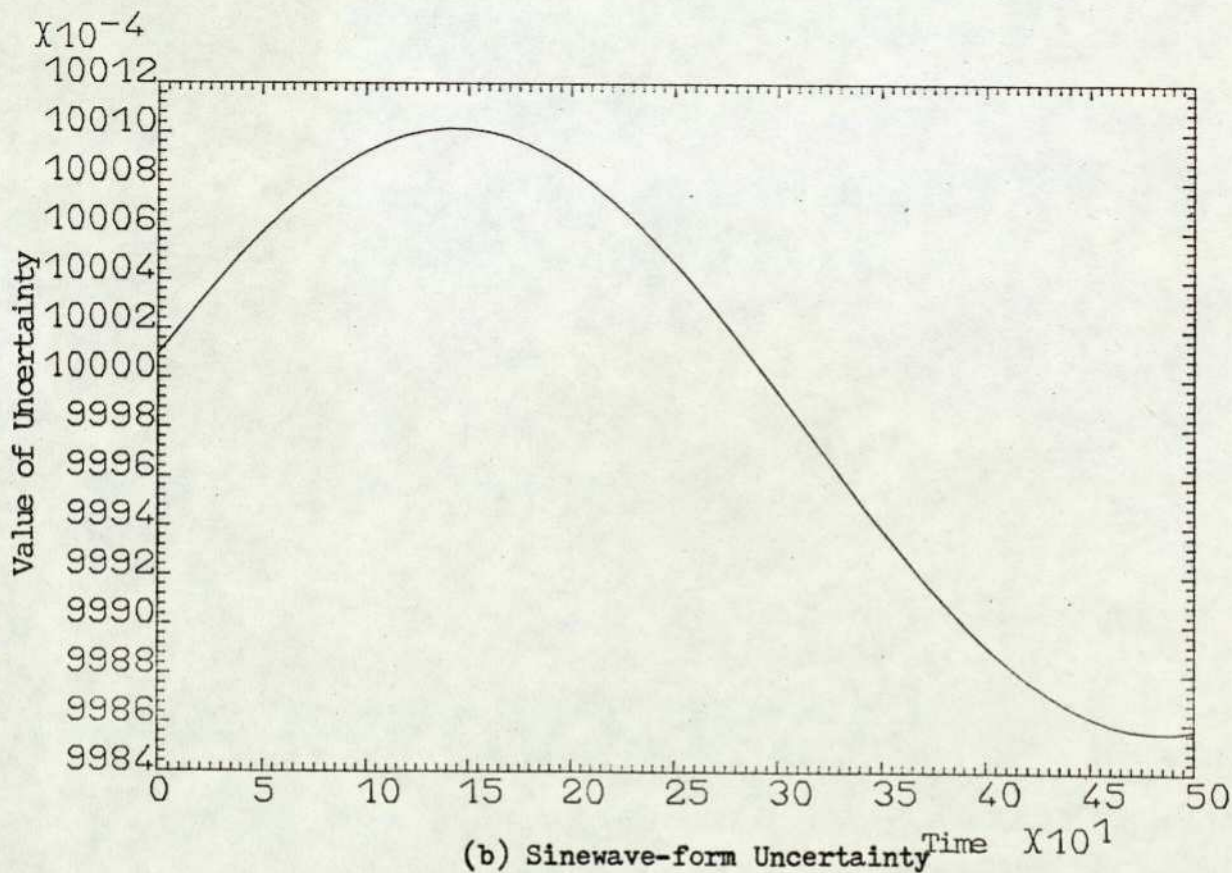


Fig. 6.4.36 The resulting time-varying uncertainties corresponding to Fig. 6.3.34.



(a) Chebychev-form Uncertainty



(b) Sinewave-form Uncertainty

Fig. 6.4.37 The resulting time-varying uncertainties corresponding to Fig. 6.4.35.

In addition to these results, an attempt had been made to attach the time-varying uncertainty to the equation of $\dot{M}_{vp}$ to compensate for the seemingly periodical variations on the vapour pressure response, thus

$$\dot{M}_{vp} = 2.0 (P_{vw} - X(6)) + B_{B22}$$

This kind of compensation for the uncertainties in model structure was mentioned by Leal (1977). The results obtained are summarised in the following table:

CASE	FORM OF BB22	W(1)	W(2)	R	PRA (HTC) C.L.S.	PRA (HTC) S.L.S.	NO.OF OVERALL ITTERS.	C.P. TIME SECS
1	SINE	10	0.5	20.0	0.31	0.31	2	315
2	CHEB	10	0.5	20.0	0.31	0.31	2	1145
3	SINE	$\frac{1}{YA(1)}$	$\frac{1}{YA(2)}$	$\frac{1}{TRAJ}$	0.3085	0.3085	2	185

Table 6.4.38 Summary of the Results when B_{B22} is attached to $\dot{M}_{vp}$

From the table it is evident that the identification process rejected, altogether, the existence of the uncertainty in the vapour pressure derivative as manifested by the fact that the smoothed least squares solution resulted in a parameter estimate equal to that obtained by the classical least squares. Indeed this was achieved in only two overall iterations with smoothing parameters given their nominal values. A further attempt (which is not listed in the table) was made by starting the identification process with smoothing parameters set at values other than their nominal values.

The process converged to the classical least squares solution thereby supporting these results.

Responses which correspond to Case 1 in table 6.4.38 are given by Figs. 6.4.39 and 6.4.40. An important feature of the height response is the fact that the response has exhibited a behaviour similar to that of the non-minimum phase concept. This may be explained on the basis that the introduction of a time-varying uncertainty to the height differential equation (which was originally set to its nominal value of 1.0) has caused a constant shift in the response which has made the whole model response follow the average trend of the system response. This result can be made use of in further experimentation on the subject and may yield more accurate results.

The vapour pressure response is similar to that of Fig. 6.4.33 except for the non-minimum phase behaviour which is not exhibited clearly here. This may be due to the shift which has occurred in the height response.

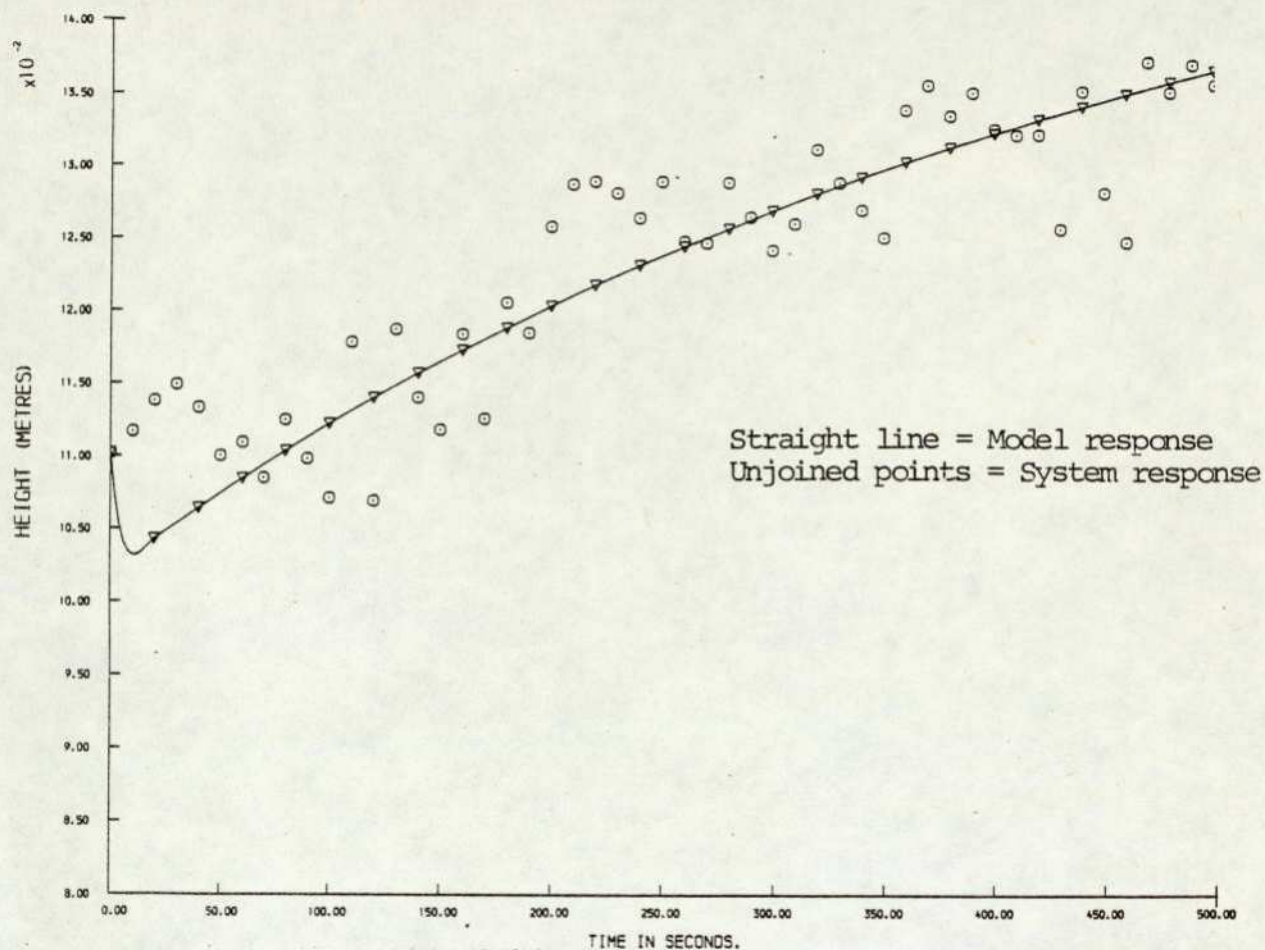


Fig.6.3.39. System and Model Height Responses Corresponding to Case 1 of Table 6.4.38.

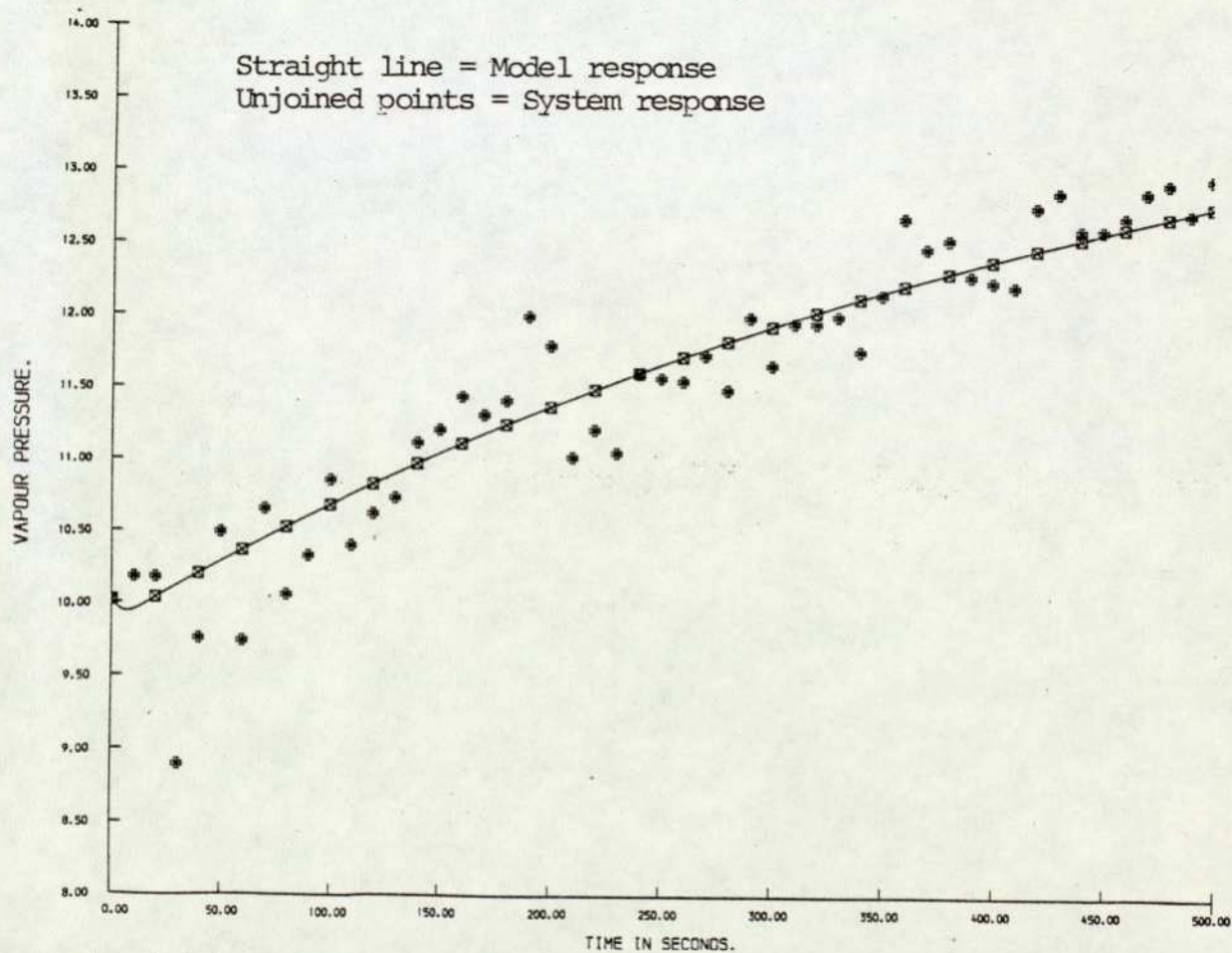


Fig.6.4.40 System and Model Vapour Pressure Responses Corresponding to Case 1 of Table 6.4.38.

6.4.4. Case 4

The results obtained using the nominal weightings and the time-varying weightings for both forms of the time-varying uncertainty are summarised in the following table:

CASE	FORM OF BB22	W(1)	W(2)	R	PRA(HTC) C.L.S.	PRA(HTC) S.L.S.	NO.OF OVER- ALL ITERS	C.P. TIME SECS
1	SINE	10	0.5	20.0	0.386	0.381	6	700
2	CHEB (4terms)	10	0.5	20.0	0.386	0.391	3	745
3	CHEB (6terms)	10	0.5	20.0	0.386	0.394	6	1900
4	SINE	$\frac{1}{YA(1)}$	$\frac{1}{YA(2)}$	$\frac{1}{TRAJ}$	0.465	0.430	6	770
5	CHEB	$\frac{1}{YA(1)}$	$\frac{1}{YA(2)}$	$\frac{1}{TRAJ}$	0.465	0.465	2	365
6	SINE	$\frac{1}{YA(1)}$	$\frac{1}{YA(2)}$	$\frac{1}{TRAJ}$	0.465	0.490	6	720
7	CHEB	$\frac{1}{YA(1)}$	$\frac{1}{YA(2)}$	$\frac{1}{TRAJ}$	0.465	0.460	15	2000

Table 6.4.41. Summary of the results of Case 4.

In the first three cases where nominal weightings are used, the classical least squares solutions are the same whereas the smoothed least squares solutions differ slightly. The improvements achieved by the use of the smoothed least squares technique are very small (about 1.4% in Cases 1 and 2 and 2.1% in Case 3).

The use of a six-term Chebychev polynomial with the accompanying large increase in computing time has contributed only little to the improvement on the parameter estimate achieved by the use of the classical least squares technique.

The use of time-varying weighting matrices in cases 4-7 resulted in slightly different results. The parameter estimates obtained by the classical least squares technique are larger than the corresponding values obtained by the use of the nominal weighting matrices. The smoothed least squares solution of cases 4 and 6 differ slightly from those of cases 5 and 7 which are almost indifferent from the classical least squares solutions.

Increasing the weighting matrix associated with the time-varying uncertainty (R) by a factor of 10 has only little effect on the smoothed least squares solution and no effect on the classical least squares solution indicating to the insensitivity of the classical least squares solution to R, which is perceivable since the classical least squares solution is obtained by setting the term with which R is associated to zero.

Now, responses corresponding to Cases 2 and 3 of table 6.4.41 are given by Figs. 6.4.42 and 6.4.43 respectively. Although the use of six-term Chebychev polynomial has contributed only little to the improvement on the parameter estimate (H_{tc}), compared with that obtained by the use of four-term Chebychev polynomial, the vapour pressure response has improved to the extent of being able to follow major changes in the system response. However, the pressure response obtained by

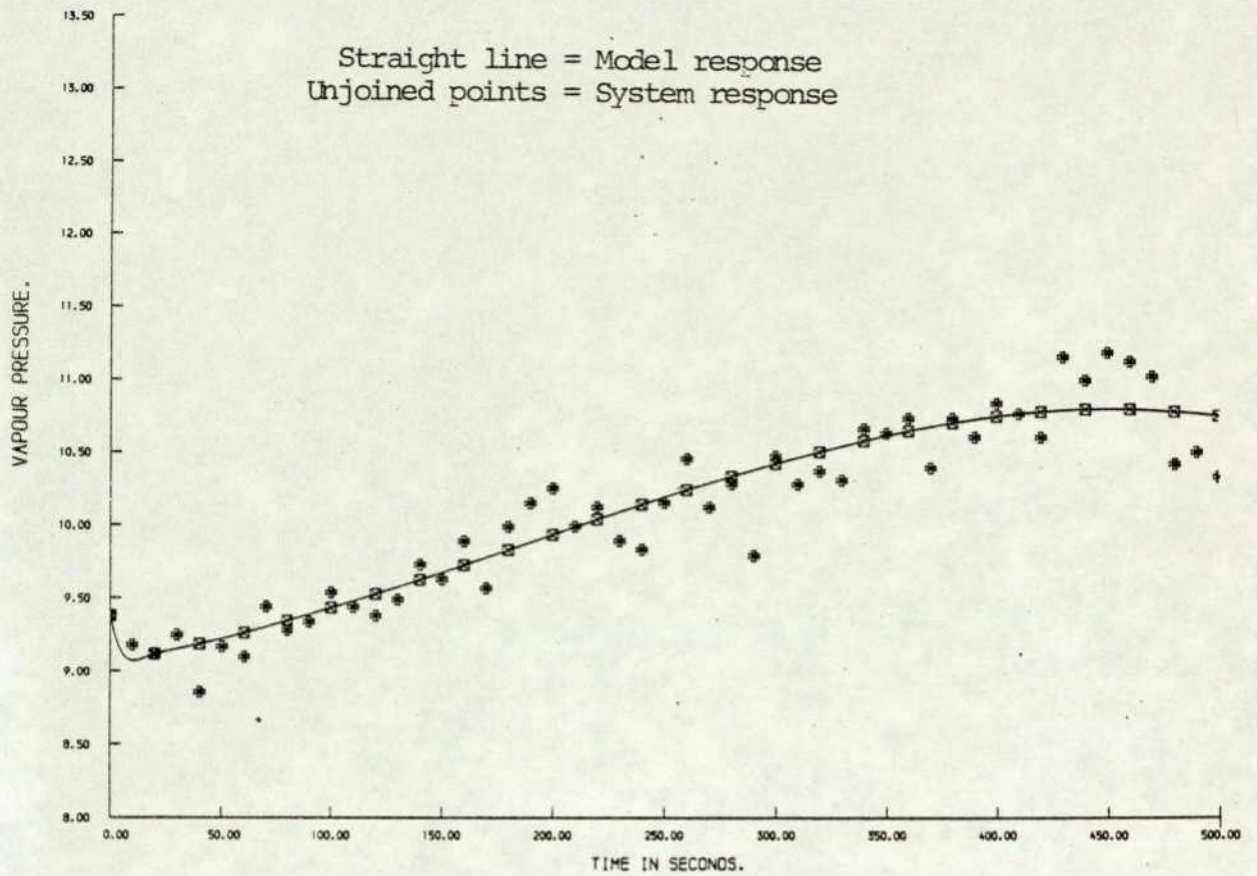


Fig. 6.4.42 System and Model Vapour Pressure Responses Corresponding to Case 2 of Table 6.4.41.

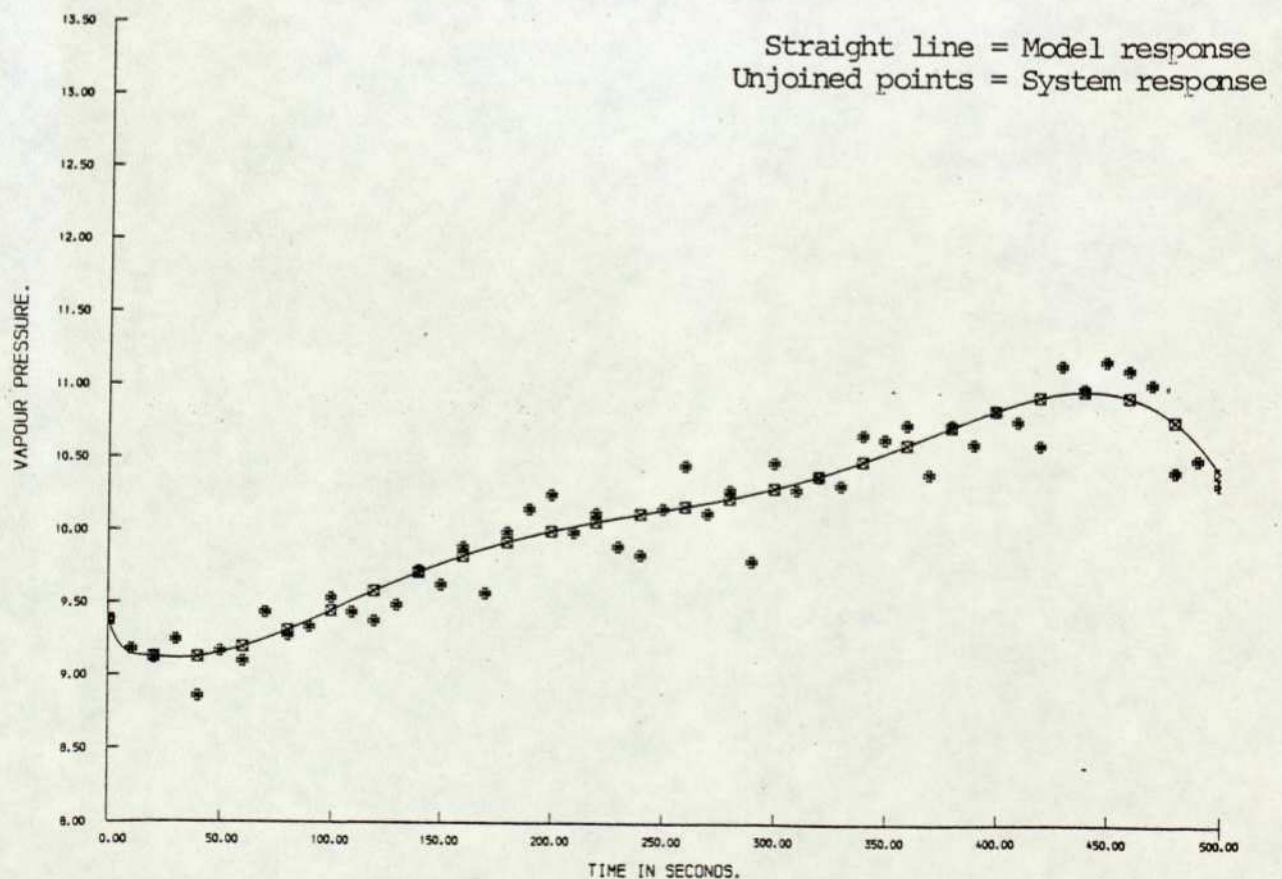
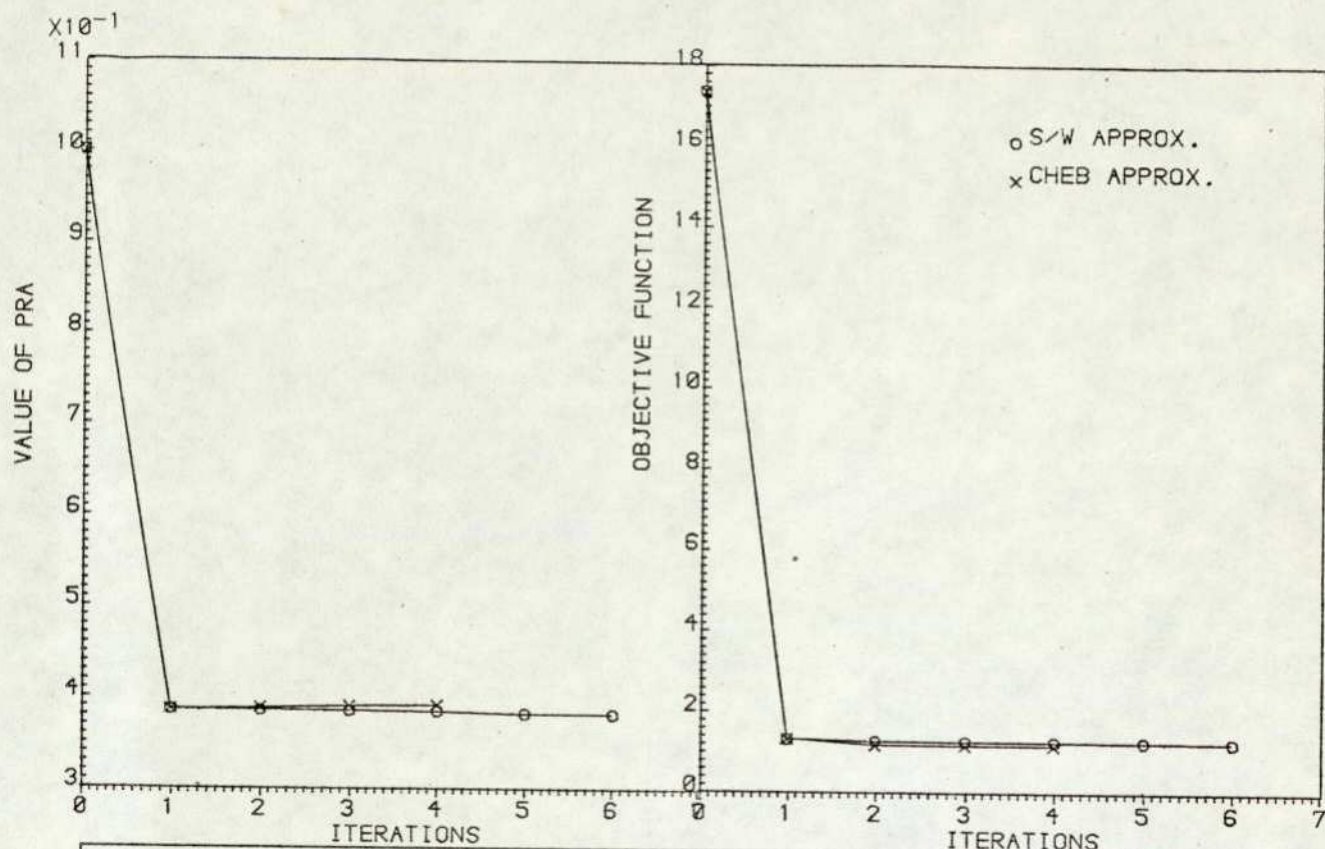


Fig.6.4.43. System and Model Vapour Pressure Responses Corresponding to Case 3 of Table 6.4.41.

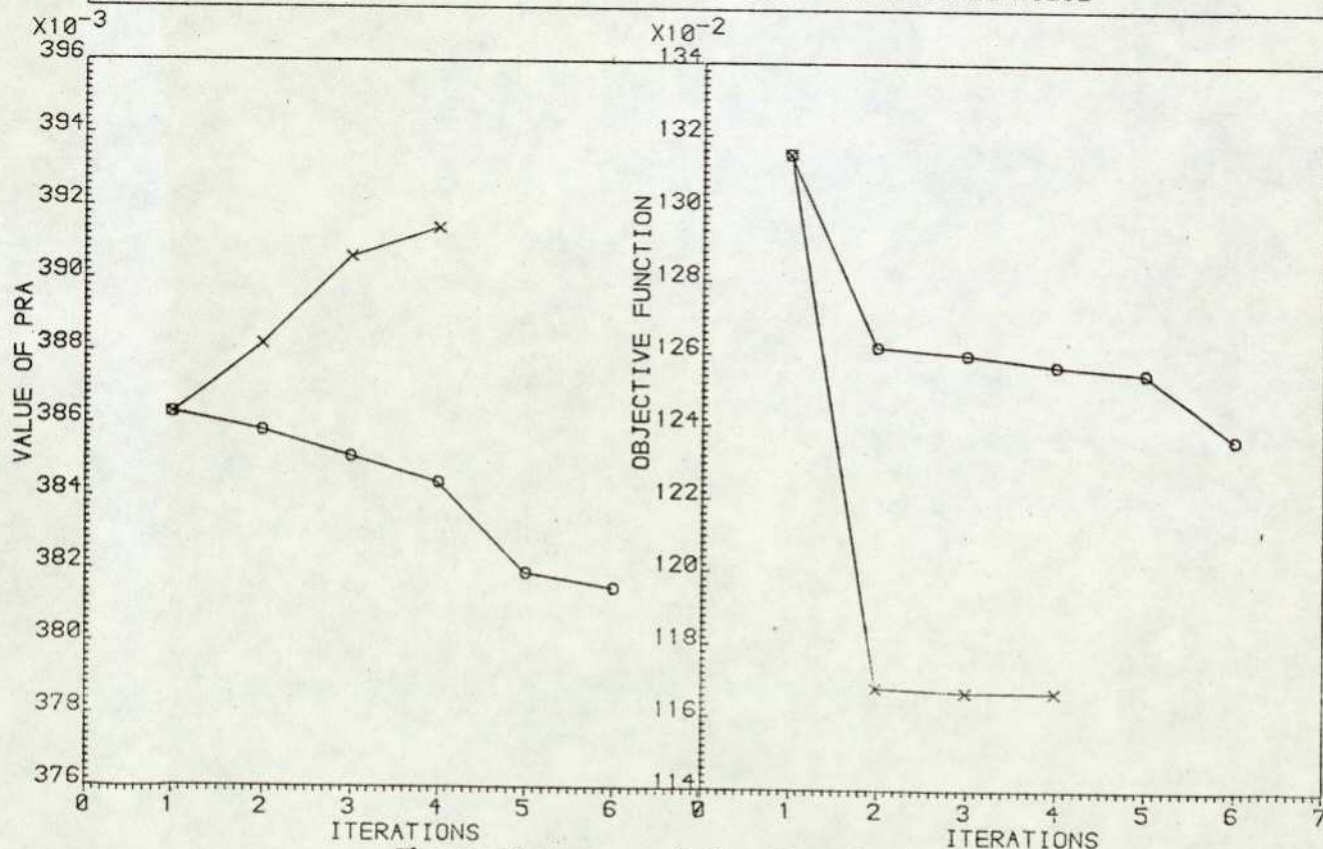
the use of only four-terms Chebychev polynomial has followed the general trend of the system response and fitted into its average values. The improvement yielded by the use of six-terms Chebychev polynomial opens the door for further experimentation on the effect of the number of Chebychev terms on the parameter estimates and on the ability of the technique to predict unknown system variations.

The performances of the classical least squares and the smoothed least squares technique are given by Fig. 6.4.44 for Cases 1 and 2 and Fig. 6.4.45 for Cases 4 and 5. Both sets of graphs have the same trend whereby the classical least squares technique plays the major part in reducing the objective function whereas the smoothed least squares technique yields only a little improvement at a much higher cost in terms of computing time. As before, the Chebychev type approximation to the time-varying uncertainty results in a lower objective function than the sinewave type.

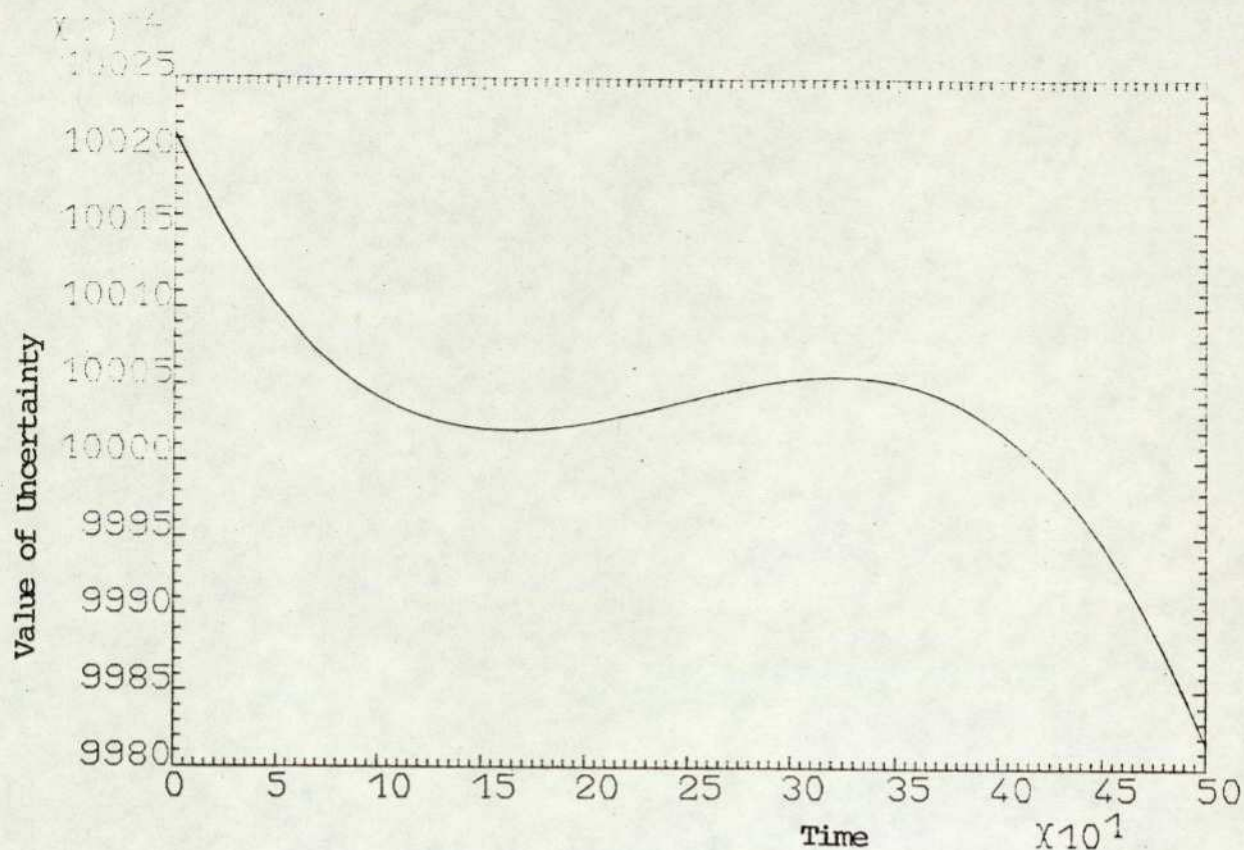
The forms of the uncertainties corresponding to Figs. 6.4.44 and 6.4.45 are shown in Figs. 6.4.46 and 6.4.47 respectively. As before the scaling of the Y-axis has made the shapes of the uncertainties show out whilst in reality, they differ only slightly from their constant nominal trajectory (1.0). However, it is due to these uncertainties however small, that the smoothed least squares technique has managed to improve, though only slightly, over the performance of the classical least squares technique.



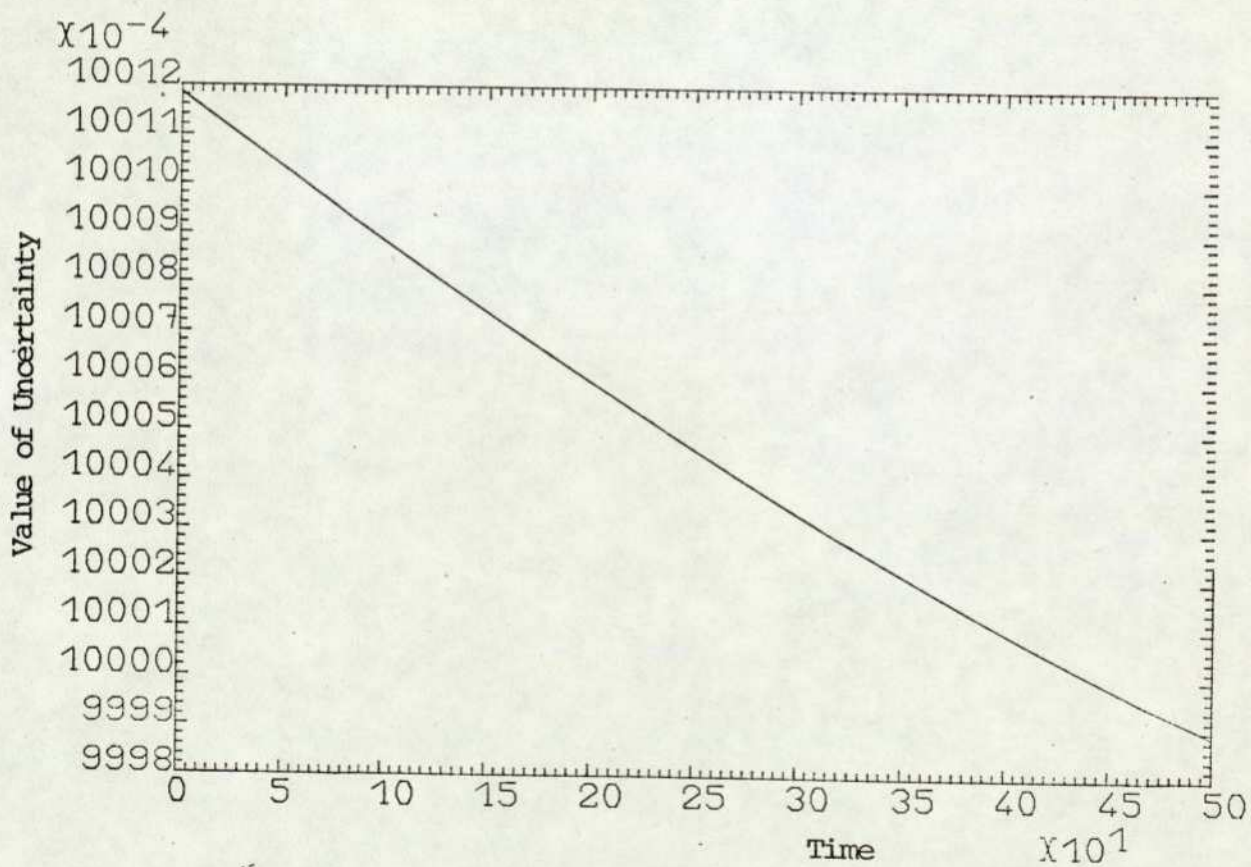
THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE



The Performance of the Classical Least Squares and the Smoothed Least Squares which Correspond to Cases 1 & 2 of Table 6.4.41.

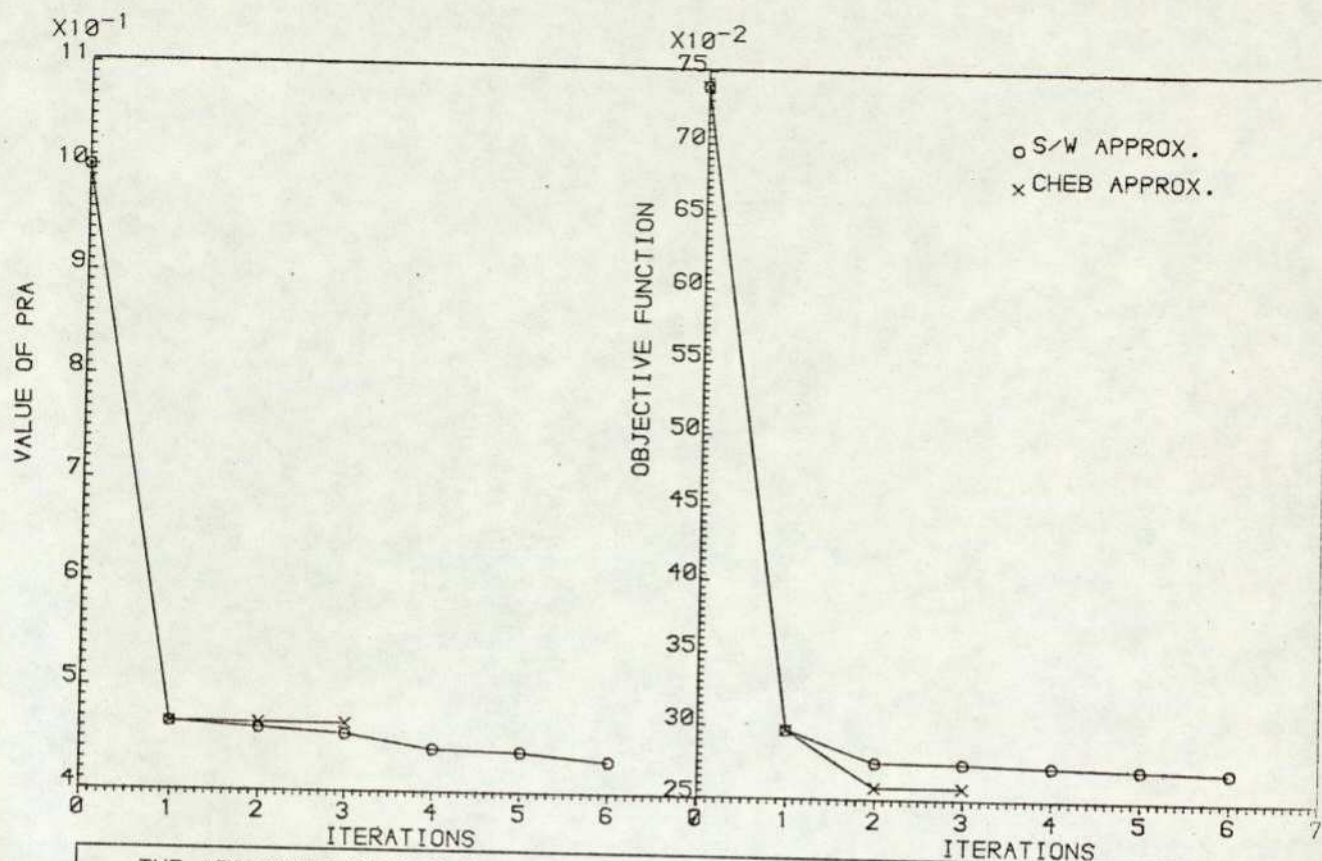


(a) Chebychev form



(b) Sinewave form

Fig. 6.4.45 The Resulting Uncertainty Forms which Correspond to Fig. 6.4.44.



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE

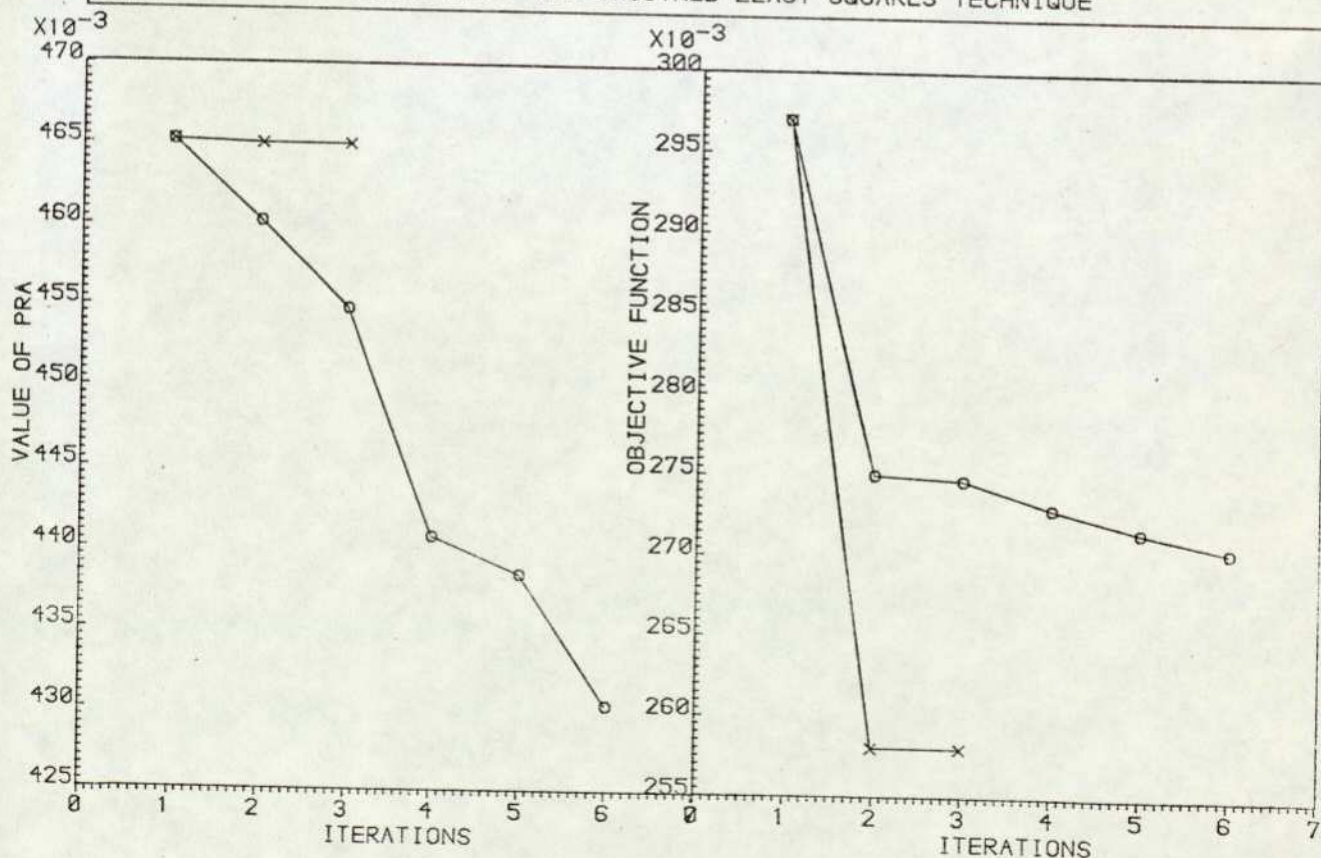


Fig. 6.4.46

The Performance of the Classical Least Squares and the Smoothed Least Squares techniques which Correspond to Cases 4 & 5 of Table 6.4.41.

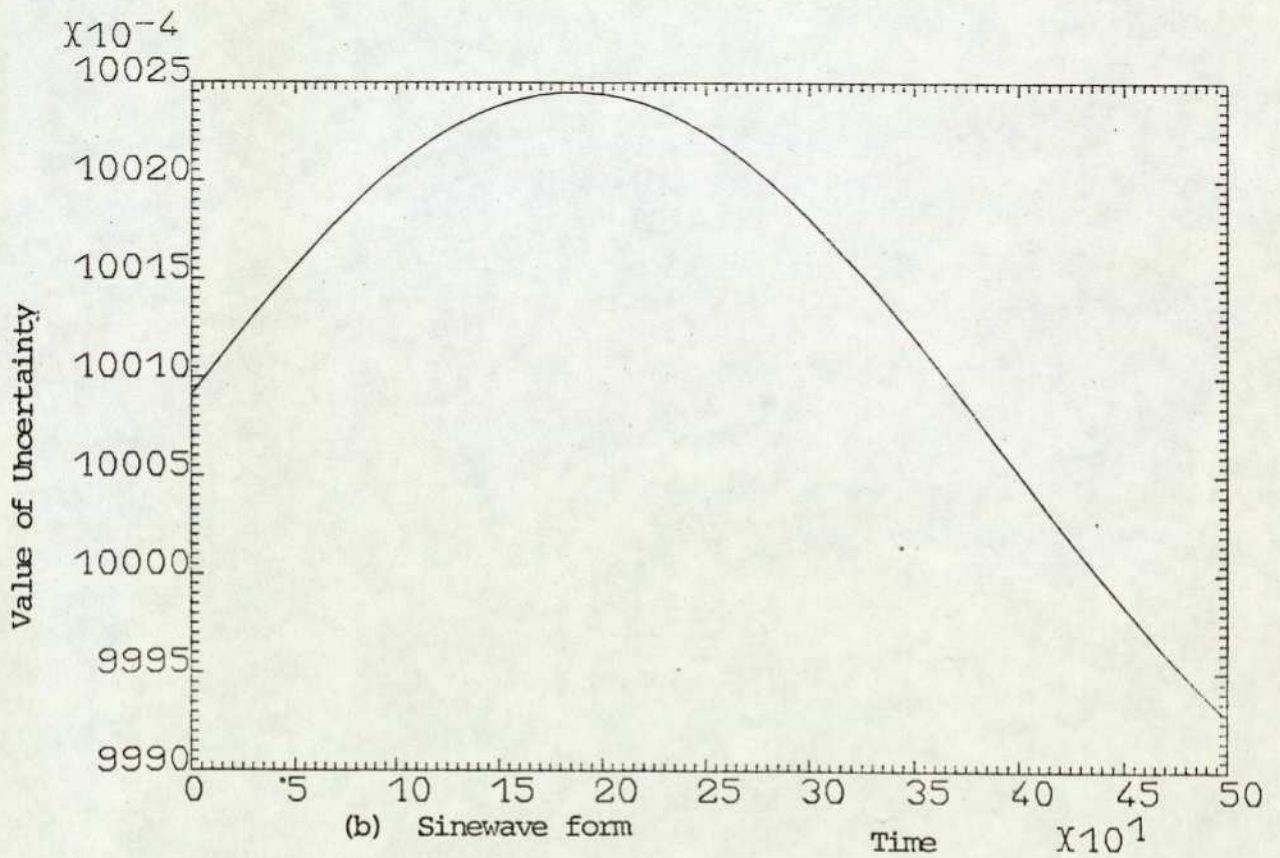
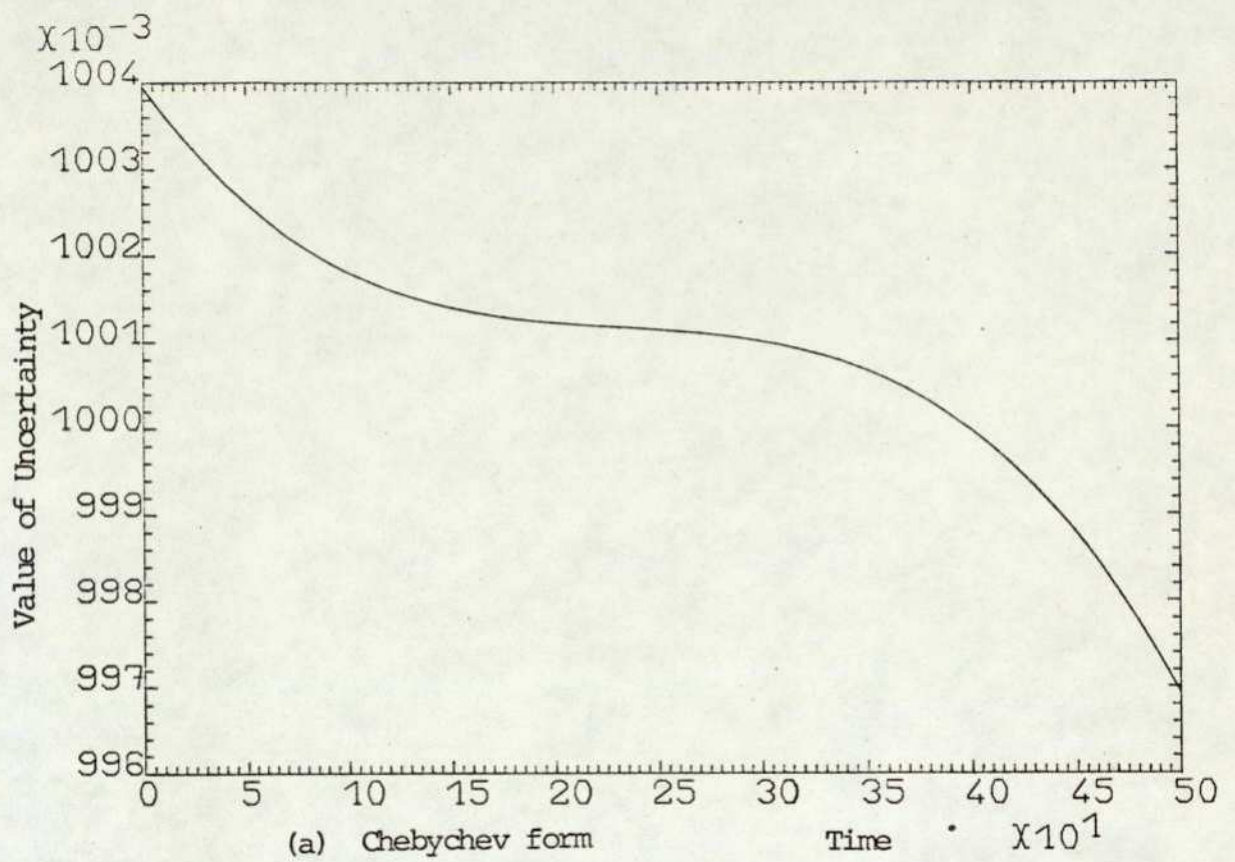


Fig. 6.4.47 The Resulting Uncertainty Forms which Correspond to Fig. 6.4.46.

6.4.5. CASE 5

In this case, where a 20% step change has been applied to the hot water valve position, the parameter estimation results obtained are summarised in the following table:

CASE	form of BB22	W(1)	W(2)	R	PRA(H_{TC}) C.L.S.	PRA(H_{TC}) S.L.S.	no. of overall iters	C.P. time Secs
1	Sine	10.0	0.5	20.0	0.591	1.0699	16	3200
2	Cheb	10.0	0.5	20.0	0.591	1.157	5	3750
3	Sine	$\frac{1}{YA(1)}$	$\frac{1}{YA(2)}$	$\frac{1}{TRAJ}$	0.591	0.679	11	1850
4	Cheb	$\frac{1}{YA(1)}$	$\frac{1}{YA(2)}$	$\frac{1}{TRAJ}$	0.591	0.564	4	920

Table 6.4.51: Summary of the Results obtained for Case 5

Unlike previous cases, the smoothing problem has contributed a great deal in bringing down the value of the objective function by its contribution to enhancing the value of the estimation parameter H_{tc} . The open loop responses of this case have been obtained by the application of a 20% step change to the hot water valve position (V_{p2}) causing more heat to enter the system.

The system and the model open loop responses which correspond to case 2 in table 6.4.51 are shown in figs. 6.4.52 and 6.4.53. Both model responses do not have good agreement with corresponding system responses.

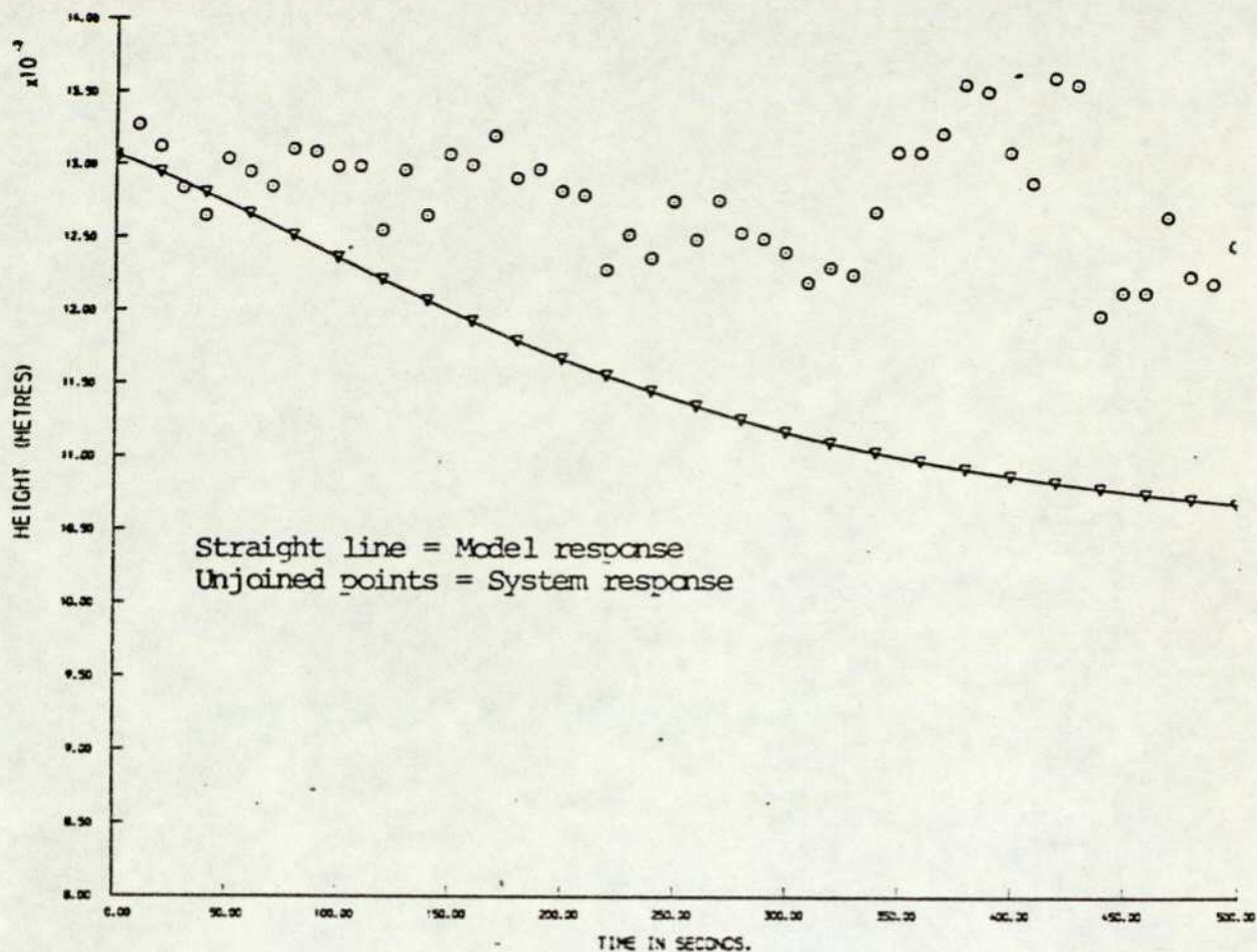


Fig.6.4.52 System and Model Open Loop Height Response to a 20% Step Change in Hot Water Valve Position Corresponding to Case 2 of Table 6.3.51.

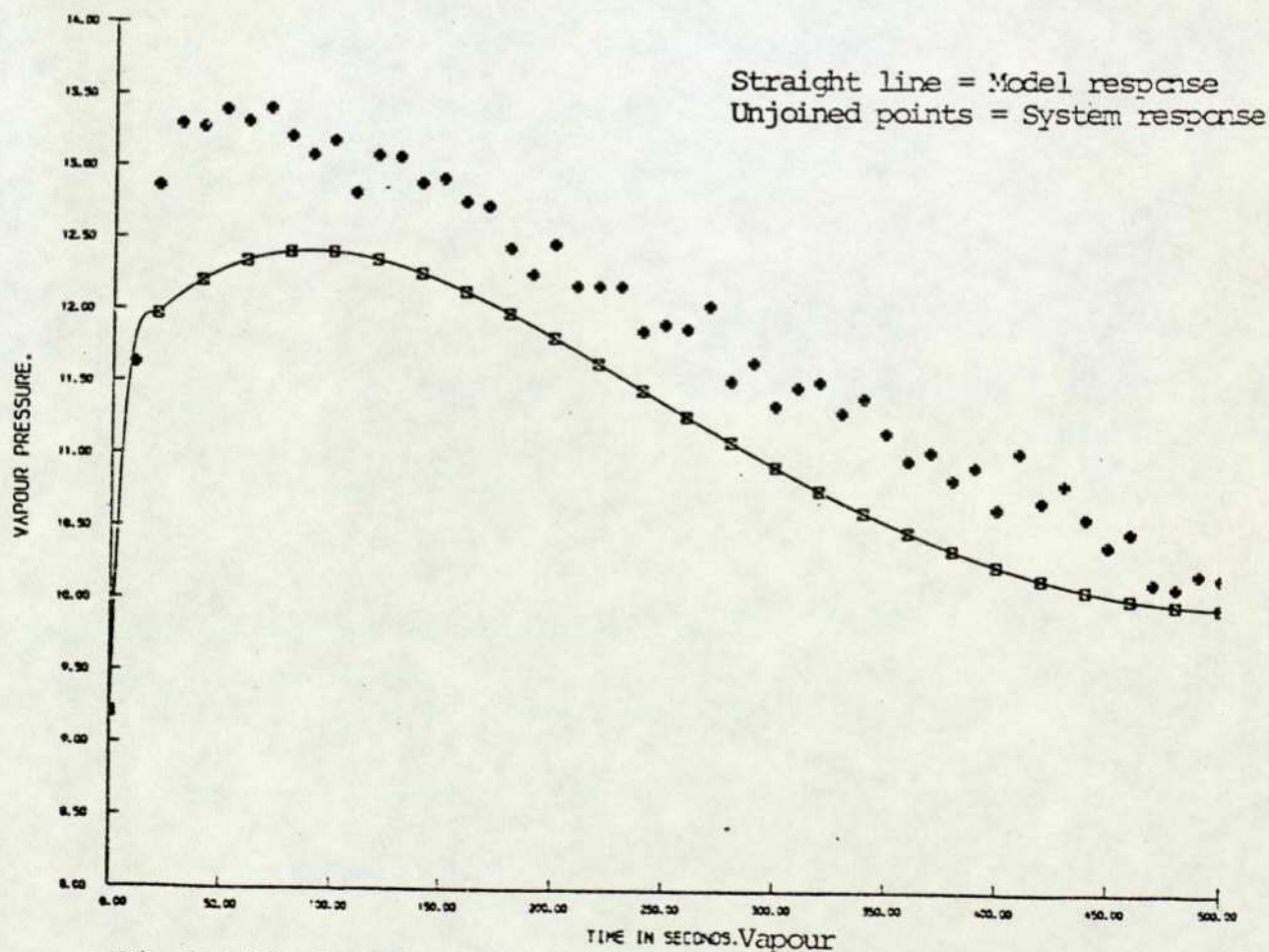


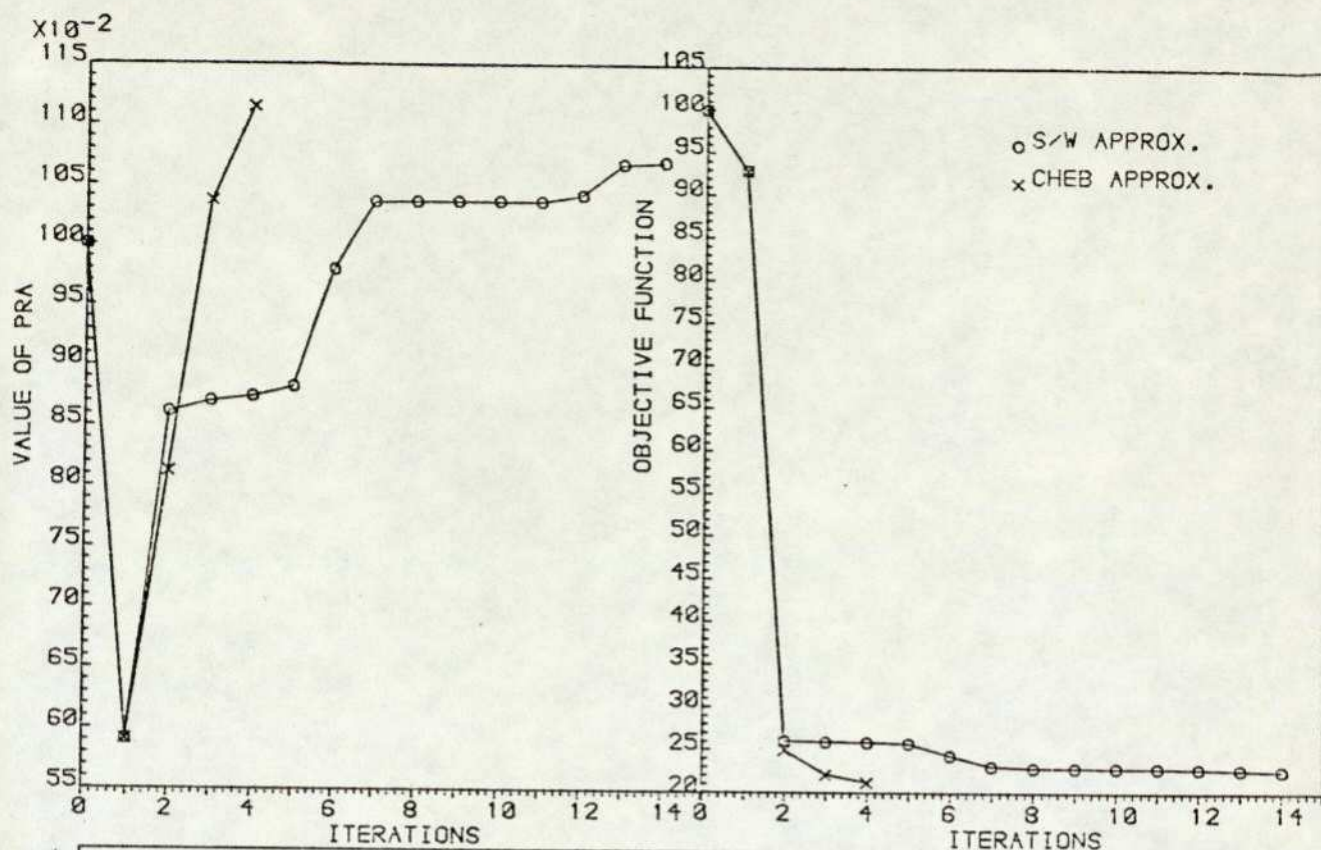
Fig.6.4.53 System and Model Open Loop/Pressure Responses to a 20% Step Change in Hot Water Valve Position Corresponding to Case 2 Table 6.4.51.

Although the assumption that inaccurate estimate of H_{tc} is behind the lack of agreement between the system and model responses has been made, other parameters and, more importantly, system variables may be in error. It has been hoped that the smoothing will make the model insensitive to such inaccuracies, but as reflected by these responses this is not so, and thus further investigation needs to be carried out in order to overcome the inability of the model to predict system behaviour. Clearly, the vapour pressure response needs a constant shift in order to pass through the average values of system response.

The computing time given in the table reflects the amount of work done by the identification procedure. The overall iterative process between the solution of the parameter estimation problem and the smoothing problem has helped in obtaining the parameter estimates in the table though at a high cost of computer time.

The use of time-varying weighting matrices resulted in the same classical least squares solutions but different smoothed least squares solutions.

The performance of the two techniques can be visualised in fig. 6.4.54 for cases 1 and 2 and fig. 6.4.55 for cases 3 and 4. From these graphs it can be seen that although the classical least squares technique has not taken the major part in reducing the objective function, one solution of the smoothing problem managed to bring down the objective function drastically. The subsequent iterations helped, but only slightly in reducing the value of the objective function, but the parameter estimate H_{tc} continued to improve though at a smaller pace.



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE

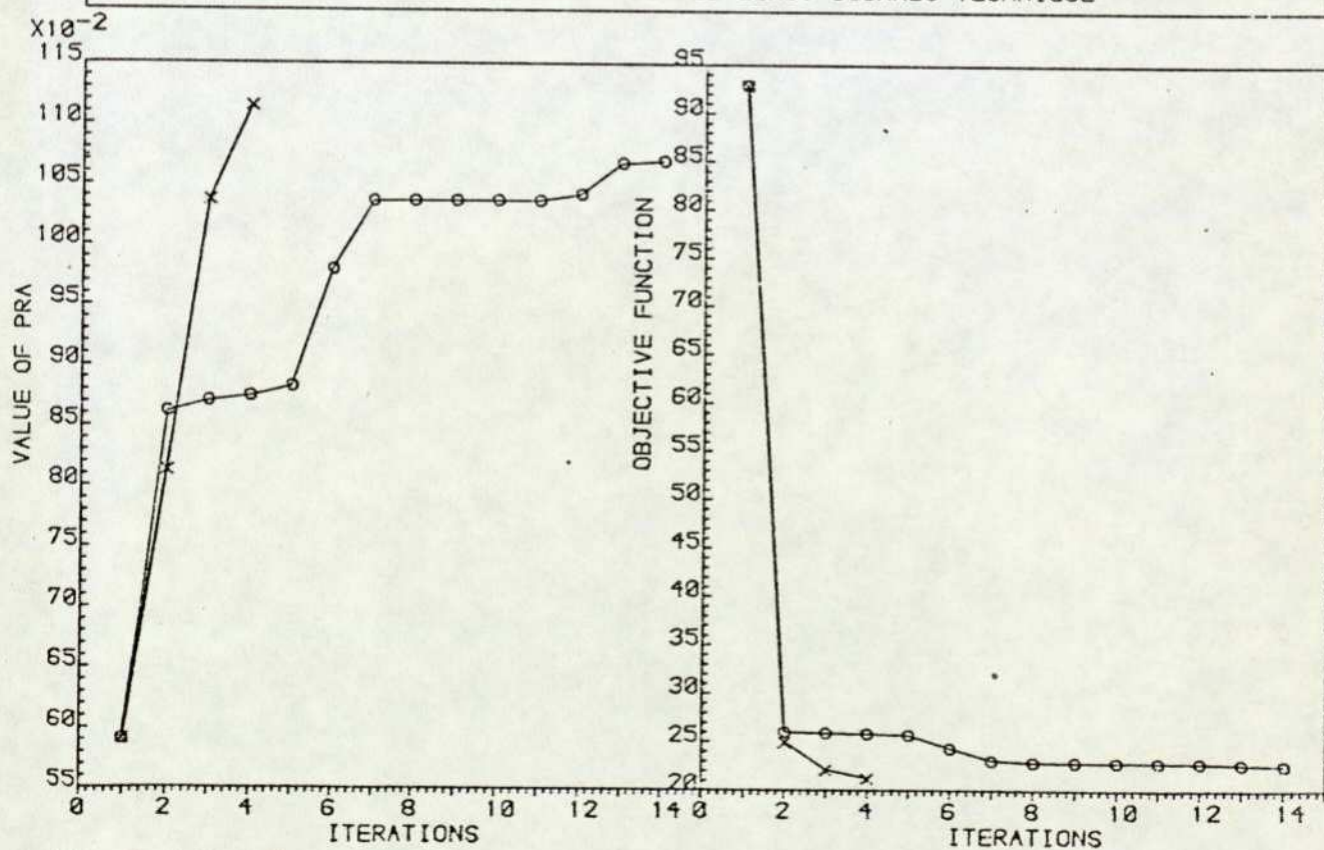
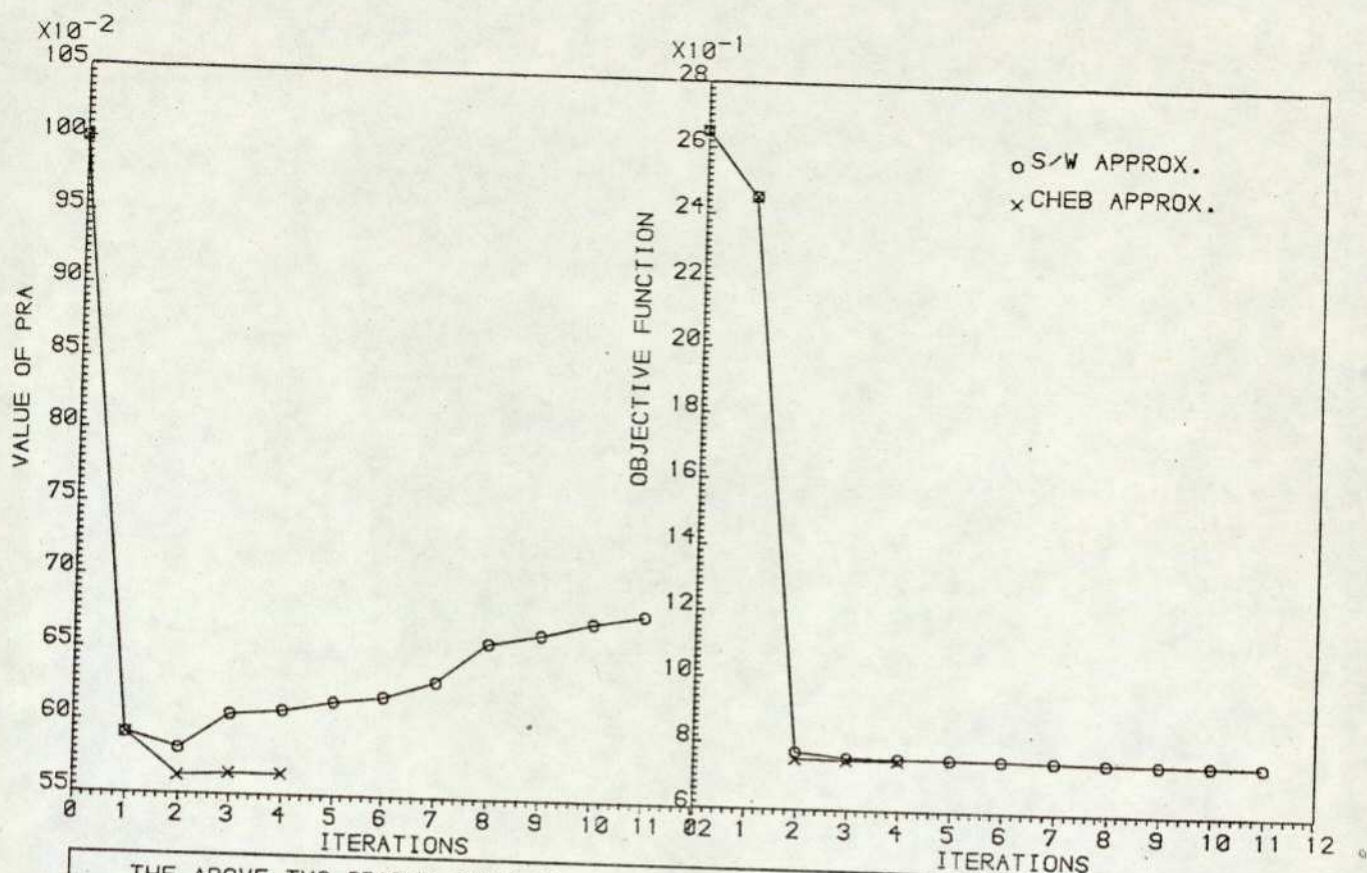


Fig.6.4.54. The Performances of the Classical Least Squares and the Smoothed Least Squares Techniques which Correspond to Cases 1 & 2 of Table 6.4.51.



THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF PRA AND OBJECTIVE FUNCTION VARY WITH THE NUMBER OF OVERALL ITERATIONS WHILST THE LOWER TWO GRAPHS COMPARE THE PERFORMANCE OF CLASSICAL LEAST SQUARES TECHNIQUE (AT ITERATION NO. 1) WITH THAT OF THE SMOOTHED LEAST SQUARES TECHNIQUE

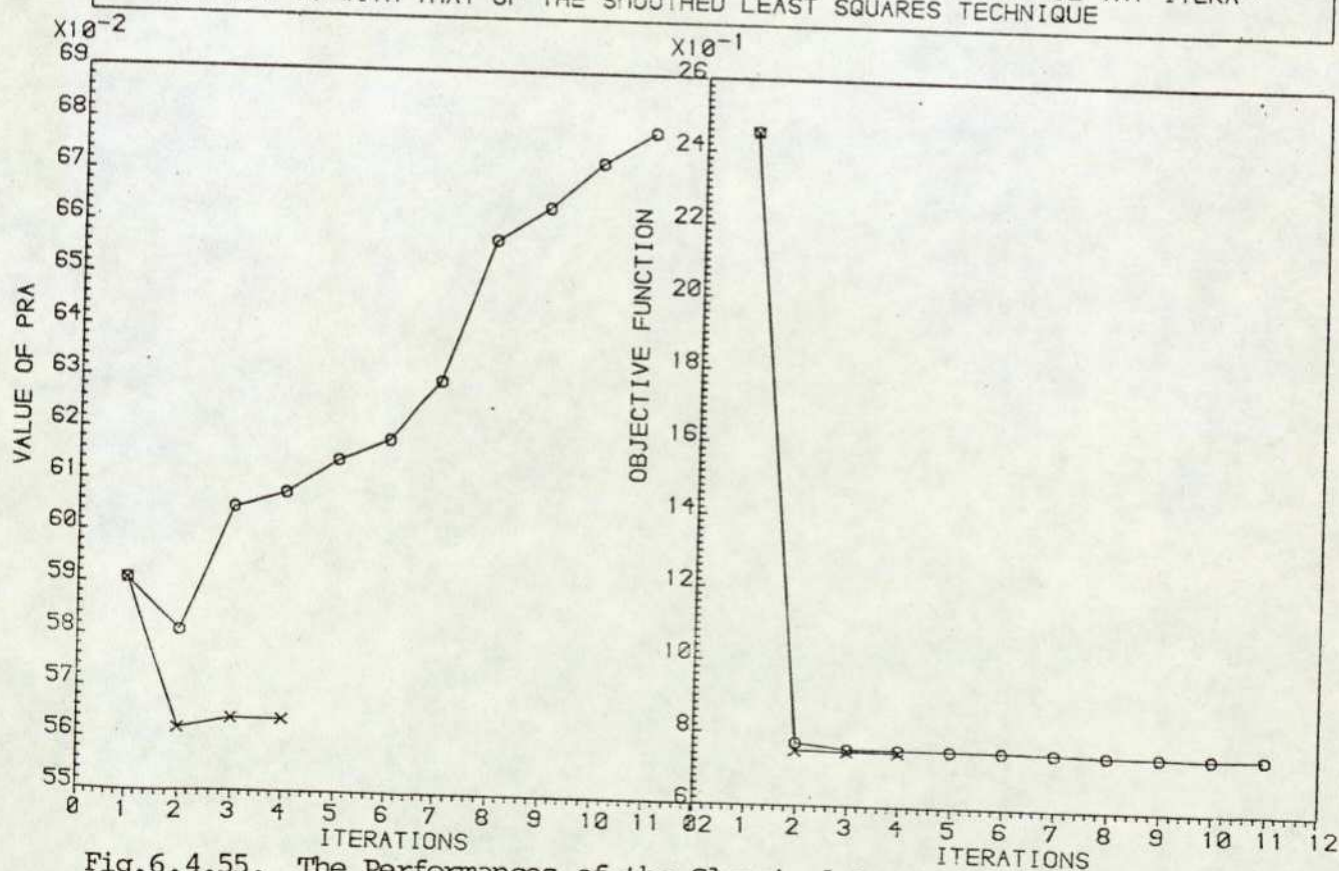


Fig.6.4.55. The Performances of the Classical Least Squares and the Smoothed Least Squares Technique which Correspond to Cases 3 & 4 of Table 6.4.51.

For the time-varying weighting matrices, the performances of the two techniques are shown in fig. 6.4.55. Again a major part has been played by the smoothed least squares technique though most of the improvement in the value of the objective function has been achieved after one solution of the smoothing problem.

The resulting time-varying uncertainties corresponding to fig. 6.3.55 are shown in Fig. 6.3.56. In this case, the departure of the uncertainties (of both forms) from their nominal trajectory is more than has been encountered in the previous cases. This has been done by the smoothing problem in order to reduce the gap between the system and model responses. Despite all this, the behaviour of the system has not been predicted by the model. This suggests that, in this case at least, other forms of time-varying uncertainties are necessary.

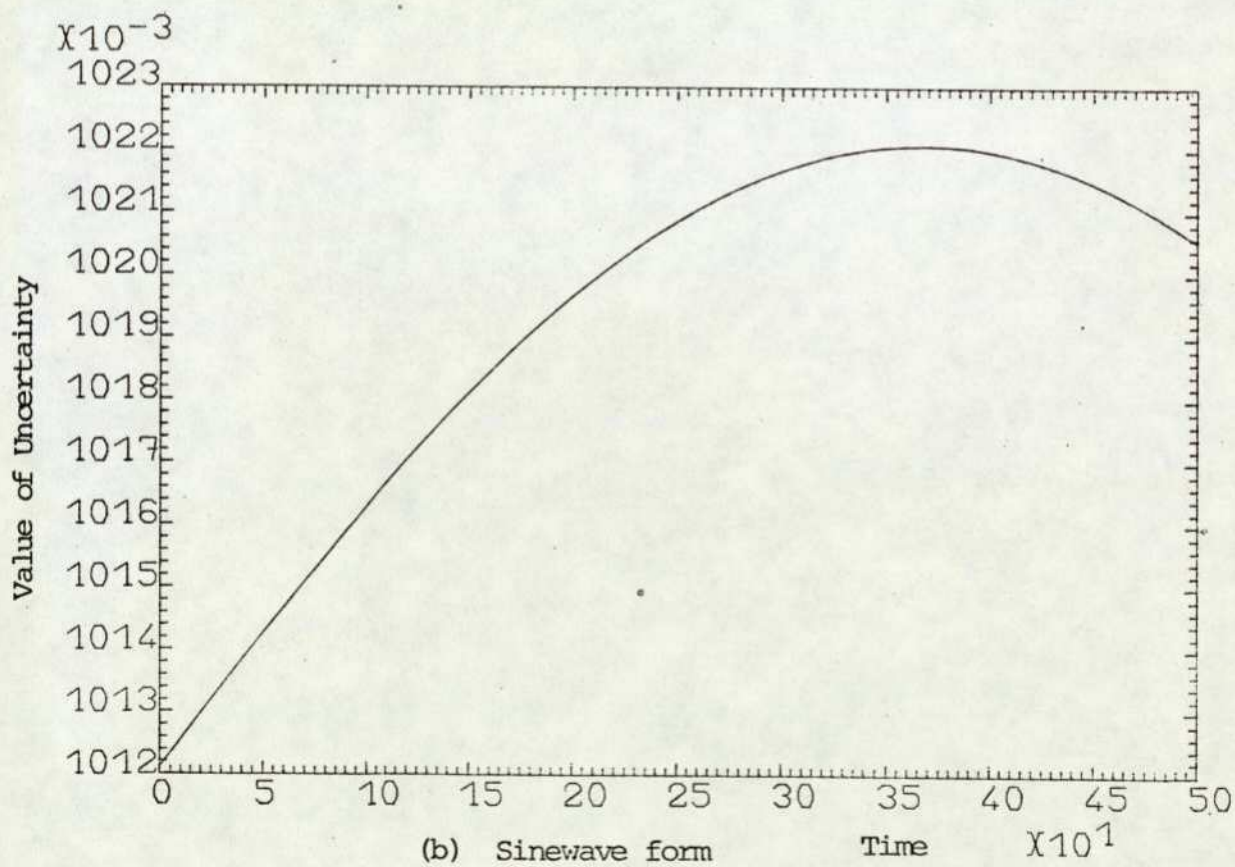
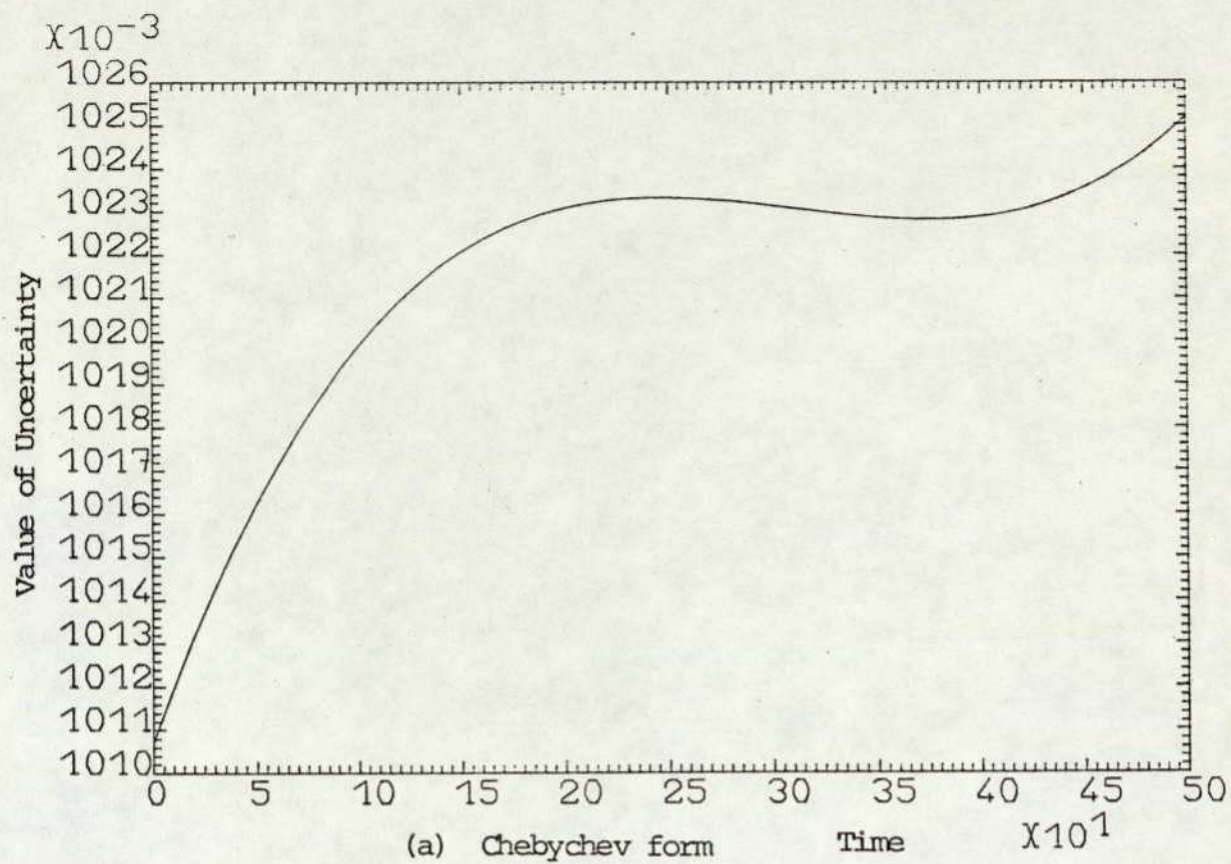


Fig.6.4.56. The Resulting Uncertainty Forms which Correspond to Fig. 6.4.55

Chapter 7

CONCLUSIONS

The research has been concerned with investigation into the performances of the classical least squares technique and the smoothed least squares technique which was proposed by Roberts and Leal (1977). The investigation has been carried out on a simulated mixing tank system based on an existing rig in the department and a pilot plant vaporiser system which has been developed in the department. In both systems the aim has been to predict accurate estimates of constant model parameters, but since both systems either have or are made to have responses unpredictable by the mathematical models i.e. uncertain dynamic systems, compensation for these model deficiencies has been made by the incorporation of time-varying "uncertainties" into the model, thus requiring the solution of a smoothing problem. Roberts and Leal's approach to the solution of this problem has been by the use of calculus of variations and a Riccati technique. The alternative approach to the solution of this problem which has been implemented in this research, is by the use of "parameterisation" concept which, it is thought, avoids the considerable computation complexity associated with the calculus of variations. However, the considerable computing time needed by the iterative process associated with the concept of parameterisation makes it necessary to review this idea.

Due to the seemingly periodical fluctuations on the output responses of the two systems, two forms of time-dependant periodical approximations; a sinewave and a Chebychev polynomial, have been used to approximate for the structural errors of the model.

Two models of the simulated mixing tank system have been considered; the first based on the assumption of a perfectly insulated system with no heat losses whilst the other takes the heat losses into consideration. Important results obtained from these two models are summarised below:

W(1)	W(2)	R	k_o True Value	Form of Uncert- ainties	k_o C.L.S. Estimate	k_o S.L.S.	No.of Overall Iters.	Computing time Seconds
0.1	0.5	20.0	1.00	CHEB.	0.9503	0.9555	6	. 60
				SINE	0.9503	0.9543	3	51
100.0	0.5	20.0	1.00	CHEB	1.0000	1.0000	12	120
				SINE	1.0000	1.0000	5	122
10	0.1	20.0	1.000		1.003	1.001	5	144
10	1.0	20.0	1.000		1.159	1.062	8	1000.0

Table 7.1 Typical results of the identification of the mixing tank system.

The first two cases relate to the model where no heat losses are accounted for whilst the second two cases relate to the model in which heat losses are taken into account.

These results represent the best and the worst results obtained by the identification process. When the weighting matrices are assigned the proper values, accurate estimates of the constant unknown model parameters have been obtained by the classical least squares technique and the need for smoothing has become less acute. On the other hand, for improper weighting values, the classical least squares technique has not been able to predict the accurate value of k_0 and the need for smoothing has become greater. In such cases, the smoothed least squares technique has resulted in improved estimate values, though in some cases the improvement is not significant. The weighting matrices have been found to be of prime importance in determining the behaviour of the two techniques and the computing time needed by the identification process.

The structural uncertainties have been approximated to by a time-varying uncertainty of two forms; a sinewave and a Chebychev polynomial. The identification process whose aim has been to predict accurate estimates of an unknown constant model parameter and to compensate for structural errors has managed to predict, in most cases, the accurate value of the unknown constant parameter. However, unlike the case where a sinewave approximation is employed for the uncertainty in which the exact behaviour of the system has been predicted including the variations on the

responses, the use of Chebychev polynomial has resulted in correct estimates of parameters, usually at lower computing time but variations on the responses have not been predicted.

When heat losses to the environment have been introduced into the system, the identification process which is assumed to lack knowledge of these losses, which had more difficulties in predicting the correct estimate, but at certain set of weightings these were near enough to the correct values.

As regards to the vaporiser system, where five different operating conditions have been considered, the parameter estimation problem has been concerned with the estimation of the value of the heat transfer coefficient (H_{tc}) between the wall of the heating glass tube and the freon liquid in the vaporiser tube. The inability of the model to predict the variations on the system responses have been thought to be due to periodical variations in the hot water temperature and has been approximated to by two forms; a sinewave and a Chebychev polynomial. The smoothing problem is concerned with estimating the coefficients of these time-dependent entities. The parameter estimates of H_{tc} obtained by the identification process (both by the classical least squares and the smoothed least squares techniques) are compared with the values obtained from steady state calculations and typical results are given in the following table where the values have been normalised relative to the values obtained by the steady state calculations:

Case No.	Form of Uncertainty	W(1)	W(2)	R	Steady State Calculation	Classical least squares	Smoothed least squares	No. of overall iterations	CP time
1	CHEB	10	0.5	20	1.0	0.596	0.598	7	1000
	SINE	10	0.5	20	1.0	0.596	0.572	12	1700
2	CHEB	10	0.5	20	1.0	0.4188	0.4183	3	614
	SINE	10	0.5	20	1.0	0.4188	0.4122	4	563
3	CHEB	10	0.5	20	1.0	0.4342	0.4348	2	382
	SINE	10	0.5	20	1.0	0.4342	0.4358	6	875
4	CHEB	10	0.5	20	1.0	0.386	0.391	3	745
	SINE	10	0.5	20	1.0	0.386	0.381	6	700
5	CHEB	10	0.5	20	1.0	0.591	1.157	5	3750
	SINE	10	0.5	20	1.0	0.591	1.070	16	3200

Fig. 7.2 Typical results of the identification of the vaporiser system.

In most of the cases, the parameter estimate has been significantly different from that obtained from steady state calculations with the classical least squares having to spend little effort to predict an estimate over which little improvement has been achieved by the smoothed least squares. Whereas the computing time needed by the classical least squares technique to converge to a solution is about 60 seconds (in the majority of cases), the little improvement achieved by the smoothed least squares technique has been achieved at a much higher cost of computing time. However, in dangerous situations where this improvement is critical, this cost may be justified.

Although the improvement in the parameter estimates achieved by the smoothed least squares technique over those obtained by the classical least squares technique is more significant in the cases of sinewave form uncertainty, the general behaviour of the smoothed least squares technique in terms of the number of overall iterations (an overall iteration comprises of consecutive solutions of parameter

estimation problem and smoothing) and computing time is almost the same for both forms of uncertainty.

Undoubtedly, the identified models of the vaporiser in all the five cases have yielded better responses than those in which the value of the H_{tc} obtained from steady state calculations were used though, the seemingly periodical variations on the height and vapour pressure responses have not been predicted even by the identified models. Furthermore, despite the fact that some identified models have yielded responses which fit into the average trend of the

- observational data, others have yielded models which followed the general trend of the observational data but did not pass through their average values.

7.1 Recommendations for Further Work

In the light of the work which has been done in this research, it is suggested that the following proposals be considered for further investigation.

- 1) the application of the calculus of variations and Riccati technique to the solution of the smoothing problem as related to the vaporiser system and comparing the results with those obtained using the parameterisation concept.
- 2) the application of the filtered least squares technique in conjunction with the classical least squares technique to the vaporiser system and the comparison of these results with the results obtained in this thesis.
- 3) the attachment of the time dependent uncertainty to a variable other than the hot water temperature such as the derivatives of height and vapour pressure.

APPENDIX 1

1.1 The Smoothing Problem

The incorporation of the smoothing problem into the identification process modifies the objective function to take the form

$$V_S = \int_0^T \left\{ [y(t) - \underline{z}(t)]^+ \cdot W \cdot [\underline{y}(t) - \underline{z}(t)] + [\beta(t) - \hat{\beta}(t)]^+ \cdot R \cdot [\beta(t) - \hat{\beta}(t)] \right\} dt$$

The aim is to minimise V_S w.r.t. $\beta(t)$ subject to

$$\dot{\underline{x}} = \underline{f}(\underline{x}, \underline{u}, \underline{\alpha}, \underline{\beta}(t), \quad \underline{x}(0) = \underline{x}_0$$

$\beta(t)$ may not represent physical quantities in the plant but may only be added for possible model inadequacies. If the degree of the uncertainty varies during the period of observation, R can be chosen as a function of time, and if the uncertain parameters $\underline{\beta}(t)$ are known to vary only slowly with time an additional term can be added to V to keep the derivatives of $\beta(t)$ small

$$\int_0^T \dot{\underline{\beta}}(t)' \cdot \underline{P} \cdot \dot{\underline{\beta}}(t) dt$$

where $\underline{P}$ is a positive semidefinite matrix.

To incorporate the uncertainty in the initial state of the plant caused by the uncertainty of the parameters $\underline{\alpha}$ and $\underline{\beta}(0)$ an additional term could be added to V_S of the form:

$$[\underline{x}(0) - \hat{\underline{x}}(0)]^T \underline{S} [\underline{x}(0) - \hat{\underline{x}}(0)]$$

where

$\underline{x}(0)$ = an estimate of the initial state

$\underline{S}$ = a symmetric positive definite weighting matrix

1.2 Optimum Control Solution to the Smoothing Problem (Calculus of Variations)

The constraint that the state variables satisfy the model equations, is adjoined by means of Lagrange Multipliers $\underline{\lambda}(t)$, to give the following augmented objective function:-

$$V = \int_0^T \left[\underline{y}(t) - \underline{z}(t) \right]^+ W \left[\underline{y}(t) - \underline{z}(t) \right] \\ + \left[\underline{\beta}(t) - \hat{\underline{\beta}}(t) \right]^+ R \left[\underline{\beta}(t) - \hat{\underline{\beta}}(t) \right] \\ + \underline{\lambda}'(t) \left[\dot{\underline{x}}(t) - \underline{f}(\underline{x}, \underline{u}, \underline{\alpha}, \underline{\beta}(t)) \right] dt$$

To solve this problem use is made of Calculus of Variations:

Theorem: If a set of continuously differentiable functions $\underline{x}$ minimises a functional V of the form:

$$V(\underline{x}) = \int_a^b L(\underline{x}, \dot{\underline{x}}, t) dt$$

where L has continuous first and second partial derivatives with respect to all its arguments, and if $\underline{x}$ satisfies the boundary conditions $\underline{x}(a) = \underline{k}_1$, and $\underline{x}(b) = \underline{k}_2$, then $\underline{x}$ satisfies the Euler Equations:

$$\frac{\partial L(\underline{x}, \dot{\underline{x}}, t)}{\partial \underline{x}_i} - \frac{d}{dt} \frac{\partial L(\underline{x}, \dot{\underline{x}}, t)}{\partial \dot{\underline{x}}_i} = 0 \\ i = 1, \dots, n$$

Applying this theorem to the above problem, we have

$$(a) \frac{\partial L}{\partial \beta(t)} - \frac{d}{dt} \frac{\partial L}{\partial \dot{\beta}(t)} = 0$$

$$\frac{\partial L}{\partial \beta(t)} = 2R (\beta(t) - \beta^0(t)) - f'_\beta \dot{\lambda}(t)$$

$$\frac{\partial L}{\partial \dot{\beta}(t)} = 0$$

$$\therefore 2R (\beta(t) - \beta^0(t)) - f'_\beta \dot{\lambda}(t) = 0$$

$$\beta(t) = \beta^0(t) + \frac{1}{2} R^{-1} f'_\beta \dot{\lambda}(t) \quad (3)$$

$$(b) \frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = 0$$

$$\therefore \underline{h}'_x W'(\underline{y}(\underline{x}) - \underline{z}(t)) + \underline{h}'_x W(\underline{y}(\underline{x}) - \underline{z}(t)) - f'_x \dot{\lambda}(t) - \dot{\lambda}(t) = 0$$

$$\left[\dot{\lambda}(t) = \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}} \right) \right]$$

$$\therefore \dot{\lambda}(t) = -f'_x \dot{\lambda}(t) + \underline{h}'_x W'(\underline{y}(\underline{x}) - \underline{z}(t)) + \underline{h}'_x W(\underline{y}(\underline{x}) - \underline{z}(t))$$

$$\dot{\lambda}(t) = -f'_x \dot{\lambda}(t) + 2 \underline{h}'_x W(\underline{y}(\underline{x}) - \underline{z}(t)) \quad (3)$$

$$\begin{aligned}
(c) \quad \frac{\partial L}{\partial \lambda} - \frac{d}{dt} \frac{\partial L}{\partial \dot{\lambda}} &= 0 \\
\dot{\underline{x}}(t) - \underline{f}(\underline{x}, \underline{u}, \underline{\alpha}, \underline{\beta}(t)) &= 0 \\
\dot{\underline{x}}(t) &= \underline{f}(\underline{x}, \underline{u}, \underline{\alpha}, \underline{\beta}(t)) \quad (3)
\end{aligned}$$

The usual method of obtaining optimum trajectories for $\underline{x}(t)$ and $\underline{\beta}(t)$ from Eqns. (3) is to use Riccati techniques. A solution of the form $\underline{x}(t) = \hat{\underline{x}}(t) + P(E) \underline{\lambda}(t)$ is attempted, where P is a symmetric matrix. Note that at $t = T$, $\underline{x} = \hat{\underline{x}}$. Assume initially that $\underline{\beta} - \underline{\beta}^0$ is small enough to allow linearisation W.R.T. $\underline{\beta}$, and that $P\lambda$ is small enough to allow linearisation W.R.T. $\underline{x}$,

$$\therefore \dot{\underline{x}} = \underline{f}(\underline{x}, \underline{u}, \underline{\alpha}, \underline{\beta}^0(t)) - 2Ph_x W (\underline{h}(\underline{x}) - \underline{y}(t))$$

$$\underline{x}(0) = \underline{x}_0$$

$$\dot{P} = Pf'_x + f'_x P + \frac{1}{2} f_{\beta\beta} R^{-1} f'_{\beta} - 2 Ph'_x W h'_x P$$

$$P(0) = 0$$

(The Riccati Equation)

1.3 Chebychev Approximation

Chebychev polynomials have the properties of both the Fourier series and orthogonal Polynomials.

These polynomials are defined by:

$$T_n(x) = \cos(n \arccos x) \quad (A)$$

Let $\theta = \arccos x$, we have

$$T_n(x) = \cos n \theta$$

By de Moivre's Theorem

$$(\cos n \theta + i \sin n \theta) = (\cos \theta + i \sin \theta)^n$$

Expanding the right member of the binomial theorem and then equating the real parts, we obtain:

$$\begin{aligned} \cos n \theta = & (\cos \theta)^n - \frac{n(n-1)}{2!} (\cos \theta)^{n-2} (\sin \theta)^2 \\ & + \frac{n(n-1)(n-2)(n-3)}{4!} (\cos \theta)^{n-4} (\sin \theta)^4 \\ & - \frac{n(n-1)(n-2)(n-3)(n-4)(n-5)}{6!} (\cos \theta)^{n-6} (\sin \theta)^6 + \dots \end{aligned}$$

But from $\theta = \arccos x$, we have $\cos \theta = x$ and $\sin^2 \theta = 1 - x^2$. Substituting in the above Equn.

$$\begin{aligned} T_n(x) = \cos n \theta = & x^n - \frac{n(n-1)}{2!} x^{n-2} (1-x^2) \\ & + \frac{n(n-1)(n-2)(n-3)}{4!} x^{n-4} (1-x^2)^2 \\ & - \frac{n(n-1)(n-2)(n-3)(n-4)(n-5)}{6!} x^{n-6} (1-x^2)^3 + \dots \end{aligned}$$

Hence $T_n(x)$ is a polynomial of degree n in x . The polynomials may be computed from above equation thus:

$$T_0(x) = 1$$

$$T_1(x) = x$$

$$T_2(x) = 2x^2 - 1$$

$$T_3(x) = 4x^3 - 3x$$

$$T_4(x) = 8x^4 - 8x^2 + 1$$

However, the easiest method of computing the polynomials is by use of the recursive formula:

$$T_{n+1}(x) = 2x T_n(x) - T_{n-1}(x)$$

The Fourier expressions for orthogonality may be written as:

$$\int_0^\pi \cos m\theta \cos n\theta d\theta = \begin{cases} 0 & m \neq n \\ \frac{\pi}{2} & m = n \\ \pi & m = n = 0 \end{cases}$$

From equation (A) this becomes

$$\int_{-1}^1 T_m(x) \cdot T_n(x) (dx / \sqrt{1-x^2}) = \begin{cases} 0 & m \neq n \\ \frac{\pi}{2} & m = n \\ \pi & m = n = 0 \end{cases}$$

Hence the Chebychev polynomials are orthogonal over the interval $(-1, 1)$ with respect to the weighting function:

$$W(x) = 1/\sqrt{1-x^2}$$

Correspondingly, in the discrete domain for N equally spaced data points, we have the relations :

$$\sum_{j=0}^{N-1} \cos m\theta_j \cos n\theta_j = \begin{cases} 0 & m \neq n \\ N/2 & m = n \\ N & m = n = 0 \end{cases} = \sum_{j=0}^{N-1} T_m(x_j) T_n(x_j) \quad (B)$$

Chebychev showed that of all polynomials of degree n , having a leading co-efficient equal to 1, the polynomial

$$\frac{T_n(x)}{2^{n-1}}$$

has the smallest upper bound for its absolute value in the interval

$$(-1 \leq x \leq 1)$$

since the upper bound of $|T_n(x)|$ is 1, then this upper bound is $1/2^{n-1}$.

This property is known as the Chebychev Criterion.

"Chebychev Approximation" is associated with those approximations which try to keep the maximum error to a minimum. This is known as the MINIMAX principle. Normal least squares approximation keeps the average square error down, but allows isolated extreme errors. Chebychev keeps extreme errors down but allows a larger average square error.

The n^{th} degree least squares polynomial approximation to $f(x)$ in $(-1,1)$ relative to the weighting function

$$w(x) = 1/\sqrt{1-x^2}$$

is defined by

$$y(x) = \sum_{k=0}^n a_k T_k(x) \quad -1 < x < 1 \quad (C)$$

where

$$a_0 = \frac{1}{\pi} \int_{-1}^1 \frac{f(x)}{1-x^2} dx$$

$$a_k = \frac{2}{\pi} \int_{-1}^1 \frac{f(x) T_k(x)}{\sqrt{1-x^2}} dx \quad k \neq 0$$

It has the property that, of all polynomials of degree n or less, the integrated weighted squared error

$$\int_{-1}^1 (1/\sqrt{1-x^2}) [f(x) - Y_n(x)]^2 dx$$

is least when $Y_n(x)$ is associated with the right hand member of (C).

In practice the above formulas are seldom used to evaluate a_k , but they do yield the following upper bounds:

$$|a_0| \leq 2M, \quad a_k \leq \frac{2M}{\pi} \int_0^\pi |\cos k \theta| d\theta = \frac{4M}{\pi} \quad k > 0$$

where M is the maximum value of $f(x)$ in $(-1,1)$.

A more useful method of evaluating the coefficients is based on relations of formular (B). The functions $T_0(x)$, $T_1(x)$ are orthogonal under integration over $(-1,1)$ relative to

$$w(x) = 1/\sqrt{1-x^2}$$

The functions $T_0(x)$, $T_1(x)$ $T_n(x)$ are orthogonal under Summation over the zeros of $T_{n+1}(x)$, relative to $w(x) = 1$. The n th degree Chebychev polynomial approximation to $f(x)$ is defined by:

$$f(x) = \sum_{k=0}^n ' a_k T_k(x)$$

where $\sum'$ indicates a finite sum whose first term is to be halved and

$$a_k = \frac{2}{n+1} \sum_{j=0}^n f(x_j) T_k(x_j),$$

$$x_j = -\cos \frac{(2j+1)\pi}{2n+2}, \quad j = 0, 1, \dots, n$$

APPENDIX 2

INTEGRATION PROCEDURE

The integration procedure used in the research is a dividend-difference formulation of Gear's method implemented by the NAG subroutine DO 2 AJF. This method is intended for "stiff" systems of ordinary differential equations of the form:

$$\frac{dy_i}{dx} = f_i(x, y_1, y_2, \dots, y_n) \quad i = 1, 2, \dots, N$$

from x to x_{end} .

Most stiff systems can be characterised as having complimentary functions (transients) which decay rapidly in comparison with the true solution, $y_1, y_2, \dots, y_N$. In most cases, the degree of stiffness of a system can be quantified by the size of the stiffness ratio (the larger the ratio the stiffer the system); if the eigenvalues of the Jacobian matrix $\frac{\partial f_i}{\partial y_j}$ are $\lambda_1, \lambda_2, \dots, \lambda_N$ with negative real parts, then the stiffness ratio is defined as the ratio of the largest real part to the smallest (in magnitude). In general, the values λ will depend on x and the solution $y_1, y_2, \dots, y_N$ and hence the degree of stiffness may vary across the range of integration. The routine chooses the step-size h and the order of the method to try to obtain specified accuracy with minimum computation. The maximum order used is six, giving a local error of h^6 . The differential equations are defined by a routine (MODEL), which evaluates the derivatives f_i in terms of x and $y_1, y_2, \dots, y_N$. The solution can be determined at intermediate points within the range of integration, if required.

APPENDIX 3

Programs of the Identification of the Mixing Tank System

3.1 Program Example

```

PROGRAM EXAMPLE(INPUT,OUTPUT,TAPE1=INPUT,TAPE2=OUTPUT)
C
C THIS PROGRAM CARRIES OUT IDENTIFICATION PROCESS ON A MIXING TANK SYSTEM
C
REAL KH,KC,KO
REAL MVH,MVT
DIMENSION DVH(100),DVT(100),MVH(100),MVT(100),TA(100)
DIMENSION ERS(200),W(3500),VB(4)
COMMON X(2),Y(2,100),KH,KC,KO,X1,X2,A,TH,TC,QH,QC,QO,H,PRA,
1 PRB(4),YY(2,100),XIC(2),IE(2,100),WT(2,100),YO(2),P(2,100),
2 PR(5),RR,F(2,4),DFDY(2,2),DIF(2,7,2),EB(2)
COMMON/DIF/DXX(2),DHT(100),DTEMP(100),RRS(100),BBM(100)
EXTERNAL SYSTEM,MODEL,OUT
C
C READ DESIGN VALUES AND SET INITIAL CONDITIONS
C
READ(1,20) NPA,NPB,NX,NY,IN3
READ(1,15) KH,KC,KO
READ(1,15) X1,X2,A,TH,TC
READ(1,15) PRA,(PRB(I),I=1,NPB)
15 FORMAT(5F15,10)
CALL CAM35MM
WRITE(2,5) KH,KC,KO,X1,X2,A,TH,TC
5 FORMAT(1H1,5H KH =,F12.7,5H KC =,F12.7,5H KO =,F12.7,/,
1 20H HW VALVE POSITION =,F12.7,/,
2 20H CW VALVE POSITION =,F12.7,/,
3 20H AREA OF THE TANK =,F12.7,/,
4 20H HOT WATER TEMP =,F12.7,/,
5 20H COLD WATER TEMP =,F12.7,/)
X(1)=0.1
X(2)=317.15
XIC(1)=X(1)
XIC(2)=X(2)
WRITE(2,7) X(1),X(2)
7 FORMAT(1H ,10H INITIAL CONDITIONS,/,
1 20H WATER HEIGHT =,F12.7,/,
2 20H MIXED WATER TEMP =,F12.7,/)
C
C SET PARAMETERS REQUIRED BY INTEGRATION PROCESS
C
NP=NPA+NPB
DO 13 I=1,NPB
VB(I)=9.11
13 CONTINUE
K=NP+3+NP/3

```



```

IERS=NY*NS
IW=2*IERS+4*NP+IERS*NP+(NP*NP+NP)/2+K*(2+IERS+2*NP)
DO 19 I=1,NX
  EB(I)=0.0001
19 CONTINUE
  DEL=0.03
  T=0.0
  TEND=2.0
  DLT=1.0
  IFAIL=0
  ITE=2
  TAB=0.0
  X2=0.75
  DO 24 I=1,NS
    DO 25 J=1,NX
      Y(J,I)=X(J)
25 CONTINUE
  BBS(I)=1.0+0.01*SIN(0.0314159*IT)
  TEND=TEND+DLT
  TA(I)=TEND
  CALL DB2AJF(T,TEND,X,NX,SYSTEM,DEL,EB,ITE,TAB,OUT,F,DFDY,DIF,
1      IFAIL)
29 CONTINUE
45 FORMAT(/,25H SYSTEM HEIGHT DERIVATIVE,/(6F15.6))
  WRITE(2,50)(DTEMP(N),N=1,NS)
59 FORMAT(/,39H SYSTEM TEMPERATURE DERIVATIVE,/(6F15.6))
  WRITE(2,30)(Y(1,I),I=1,NS)
39 FORMAT(1H1,24H DESIRED HEIGHT RESPONSE,/(6F15.6))
  DTEMP(1)=DXX(2)
  DHT(1)=DXX(1)
  WRITE(2,45)(DHT(N),N=1,NS)
  WRITE(2,40)(Y(2,I),I=1,NS)
49 FORMAT(/,1H,29H DESIRED TEMPERATURE RESPONSE,/(6F15.6))
C
C CALL THE IDENTIFICATION SUBROUTINE (OPTIM)
C
  CALL OPTIM(NY,NS,NX,NPA,NPB,INP,IERS,IERS,W,IW,VB,S,IER,IOPT)
C
C SET ARRAYS FOR PLOTTING
C
  DVH(I)=Y(1,I)
  DO 55 I=1,NS
    DVT(I)=Y(2,I)
    MVH(I)=P(1,I)
    MVT(I)=P(2,I)
55 CONTINUE
  CALL PLOT(TA,DVH,DVT,MVH,MVT)
  STOP
  END

```


3.2. Subroutine SYSTEM

```

C
SUBROUTINE SYSTEM(DX,X,T,INX)
C
C THIS SUBROUTINE SIMULATES A MIXING TANK SYSTEM WITH NO HEAT LOSSES TO
C THE SURROUNDINGS
C
REAL KH,KC,KO
DIMENSION DX(2),X(2)
COMMON G(2),Y(2,100),KH,KC,KO,X1,X2,A,TH,TC,QH,QC,QO,H,PRA,
1 PRB(4),YY(2,100)
COMMON/DIF/DXX(2),DHT(100),DTEMP(100),RBS(100),BBM(100)
TH=343.0
H=X(1)
T0=X(2)
QH=KH*X1
10 QC=KC*X2
12 QO=KO*SQRT(H)
TH=TH*(1.0+0.01*SIN(0.031+159*AT))
C LIQUID HEIGHT EQN
DX(1)=(QH+QC-QO)/A
DXX(1)=DX(1)
C TEMP EQN
DX(2)=(QH*(TH-T0)+QC*(T0-TC))/A/H
DXX(2)=DX(2)
RETURN
END
C

```

3.3. Subroutine MODEL

```

SUBROUTINE MODEL(DX,X,T,INX)
C
C THIS SUBROUTINE MODELS A MIXING TANK SYSTEM FOR THE CASE WHERE NO
C HEAT IS LOST TO THE SURROUNDINGS
C
REAL KH,KC,KO
DIMENSION DX(2),X(2)
COMMON G(2),Y(2,100),KH,KC,KO,X1,X2,A,TH,TC,QH,QC,QO,H,PRA,
1 PRB(4),YY(2,100)
COMMON/DIF/DXX(2),DHT(100),DTEMP(100),RBS(100),BBM(100)
TH=343.0
H=X(1)
T0=X(2)
IF(H.LE.0.0)GO TO 10
KO=1.58113E-5*PRA
QH=KH*X1
QC=KC*X2
QO=KO*SQRT(H)
TH=TH*(PRB(1)+PRB(2)*SIN(PRBS(3)*AT+PRB(4)))
DX(1)=(QH+QC-QO)/A
DXX(1)=DX(1)
DX(2)=(QH*(TH-T0)+QC*(T0-TC))/A/H
DXX(2)=DX(2)
RETURN
10 DX(1)=0.0
DX(2)=0.0
RETURN
END

```


3.4 Subroutine OPTIM

```

C
C SUBROUTINE OPTIM(NY,NX,NPA,NPB,NP,IERS,IERS,W,IW,VB,S,IER,IOPT)
C
C THIS SUBROUTINE COORDINATES THE JOINT SOLUTION OF THE PARAMETER
C ESTIMATION AND THE SMOOTHING PROBLEMSJ
C
REAL KH,KC,KO
DIMENSION ERS(IERS),W(IW),VB(NPB)
COMMON X(2),Y(2,100),KH,KC,KO,X1,X2,A,TH,TC,QH,QC,QO,H,PRA,
1 PRB(4),YY(2,100),XIC(2),JE(2,100),WT(2,100),YO(2),P(2,100),
2 PR(3),RR,F(2,4),JOFDY(2,2),JOF(2,7,2),EB(2)
COMMON/DIF/DXX(2),DHT(100),DTEMP(100),BBS(100),BBM(100)
COMMON/LOG/EST,SMD
EXTERNAL FUNCT,MONIT
EXTERNAL FUNCT1
WRITE(2,5)
5 FORMAT(17H0INITIAL RESPONSE)
CALL FUNCT(IERS,NPA,PRA,ERS)
WRITE(2,15)(DHT(N),N=1,100)
15 FORMAT(/,20H INITIAL HEIGHT DERIVATIVE,/(6F15.6))
WRITE(2,15)(DTEMP(N),N=1,100)
16 FORMAT(/,31H INITIAL TEMPERATURE DERIVATIVE,/(6F15.6))
S=0.0
DO 6 I=1,IERS
S=S+ERS(I)**2
6 CONTINUE
DO 7 J=1,NY
7 WRITE(2,8)J,(P(J,I),I=1,NX)
8 FORMAT(17H0MODEL OUTPUT NO.1,12/(1H,6F15.6))
WRITE(2,9)S
9 FORMAT(42H0INITIAL VALUE OF THE OBJECTIVE FUNCTION =,E15.6)
WRITE(2,10)
10 FORMAT(21H0OPTIMISATION MONITOR)
DO 100 KK=1,20
WRITE(2,11)
11 FORMAT(42H0 ***** ESTIMATION PROBLEM *****/)
C
C
SS=S
E1=0.1
E2=0.1
A1=0.1
B1=2.1
MAXCAL=30
IFAIL=1
CALL E04ABF(FUNCT1,E1,E2,A1,B1,MAXCAL,PRX,S,IFAIL)
PRA=PRX
CALL FUNCT1(PRA,S)
WRITE(2,21)IFAIL,MAXCAL
21 FORMAT(1H,/,10H IFAIL =,I5,5X,10H MAXCAL =,I5)
WRITE(2,12)S,EST,SMD,PRA
12 FORMAT(/,1H,7H SES =,F15.6,5X,6H EST =,F15.6,5X,6H SMD =,F15.6/)

```



```

1      14H PARAMETERS = ,F15.6)
  CALL SECOND(TT)
  WRITE(2,17)TT
17  FORMAT(1H ,24H CP TIME TO THIS POINT =,F8.3)
  WRITE(2,13)
C
13  FORMAT(1H0,42H ***** SMOOTHING PROBLEM ***** )
C
  EPSB=3.781
  ALFB=3.781
  IPRNTB=2
  MAXIT =400
  IFAIL=1
  CALL E24FAF(IERS,NPB,PRB,IERS,0,IEPSB,ALFB,VB,W,IW,FUNCT,MONIT,
1      IPRNTB,MAXIT,IFAIL)
  CALL SECOND(TT)
  WRITE(2,19)TT
19  FORMAT(1H ,24H CP TIME TO THIS POINT =,F8.3)
C
C CONVERGENCE CRITERIA
C
  IF(ABS(SS-SS) .LT. 10.000000) GO TO 99
C
100 CONTINUE
99  CALL FUNCT(IERS,NPB,PRB,ERS)
  S=0.0
  DO 50 I=1,IERS
  S=S+ERS(I)**2
50  CONTINUE
  WRITE(2,53)
55  FORMAT(/,30H FINAL RESPONSE AND PARAMETERS)
  DO 60 J=1,NY
60  WRITE(2,63)J,(P(I,I),I=1,NS)
65  FORMAT(/,17H MODEL OUTPUT NO1,12/(6F15.6))
  WRITE(2,66)(DHT(N),N=1,NS)
66  FORMAT(/,24H FINAL HEIGHT DERIVATIVE,/(6F15.6))
  WRITE(2,68)(DTEMP(N),N=1,NS)
68  FORMAT(/,29H FINAL TEMPERATURE DERIVATIVE,/(6F15.6))
  WRITE(2,70)S
70  FORMAT(/,1H,42H FINAL VALUE OF THE OBJECTIVE FUNCTION =,F15.6)
  WRITE(2,75)PRA
75  FORMAT(/,1H ,24H ESTIMATION PARAMETERS =,/(5F15.6))
  WRITE(2,80)(PRB(I),I=1,NPB)
80  FORMAT(/,1H ,23H SMOOTHING PARAMETERS =,/(5F15.6))
  RETURN
  END

```

3.5 Subroutine OUT

```

C
  SUBROUTINE OUT(I,X,HT,N,TAB)
C
C THIS SUBROUTINE IS A DUMMY ONE BUT MAY BE USED TO OUTPUT INTERMEDIATE
C RESULTS
C
  REAL X,Y,HT,TAB
  DIMENSIONX(2)
  RETURN
  END

```


3.6 Subroutine FUNCT1

```

C
C SUBROUTINE FUNCT1(PRA,S)
C
C THIS SUBROUTINE IS CALLED BY THE SUBROUTINE E24ABF AND CALCULATES THE
C MODEL RESPONSES AND THE OBJECTIVE FUNCTION
C
  REAL KH,KC,KO
  DIMENSION ES(200),SM(200)
  DIMENSION ERS(200)
  COMMON X(2),Y(2,100),KH,KC,KO,IX1,IX2,A,TH,TC,QH,QC,QO,H,PRAA,
1      PRB(4),YY(2,100),XIC(2),IE(2,100),WT(2,100),YO(2),P(2,100),
2      PR(5),RR,F(2,4),DFDY(2,2),DIF(2,7,2),EB(2)
  COMMON/DIF/DXX(2),DHT(100),DTEMP(100),BBS(100),BBM(100)
  COMMON/LOG/EST,SMO
  EXTERNAL MODEL,OUT
  NX=2
  NY=2
  NS=100
  IERS=200
  DO 2 I=1,NX
2  X(I)=XIC(I)
  PRAA=PRA
  ITE=2
  ITF=0
  T0=0.0
  TEND=0.0
  DEL=0.0
  DLT=1.0
  DO 3 I=1,NS
  T=T0
  BBM(I)=PRB(1)+PRB(2)*SIN(PRB(3)*T+PRB(4))
  CALL OUTP(T0,X,YO)
  S=0.0
  DO 10 J=1,NY
  P(J,I)=YO(J)
  E(J,I)=P(J,I)-Y(J,I)
  S=S+ABS(E(J,I))
  K=I+NS*(J-1)
  ES(K)=(WT(J,I)*E(J,I))**2
  SM(K)=(RR*(1-BBM(I)))**2
10 ERS(K)=SQRT((WT(J,I)*E(J,I))**2+(RR*(1-BBM(I)))**2)
  TAB=0.0
  IFAIL=2
  TEND=TEND+DLT
  CALL D02AJF(T0,TEND,X,NX,MODEL,DEL,IEB,ITE,TAB,OUT,F,DFDY,DIF,
1      IFAIL)
  DHT(I)=DXX(1)
  DTEMP(I)=DXX(2)
3  CONTINUE
  SMO=0.0
  EST=0.0
  S=0.0
  DO 4 I=1,IERS
  S=S+ERS(I)**2
  EST=EST+ES(I)
  SMO=SMO+SM(I)
4  CONTINUE
  RETURN
  END

```


3.7 Subroutine FUNCT

```

C
C SUBROUTINE FUNCT(IERS,NP,PRM,IERS)
C
C THIS SUBROUTINE IS CALLED BY THE SUBROUTINE E04FAF AND CALCULATES
C MODEL RESPONSES AND THE OBJECTIVE FUNCTION
C
REAL KH,KC,KO
DIMENSION PRM(NP),ERS(IERS)
DIMENSION ES(200),SM(200)
COMMON X(2),Y(2,100),KH,KC,KO,IX1,IX2,A,TH,TC,QH,QC,QO,H,PRA,
1 PRB(4),YY(2,100),XIC(2),IE(2,100),WT(2,100),YO(2),P(2,100)
2 PR(5),RR,F(2,4),DEFDY(2,2),DIF(2,7,2),EB(2)
COMMON/DIF/DXX(2),DHT(100),DTEMP(100),BBS(100),BBM(100)
COMMON/LOG/EST,SMO
EXTERNAL MODEL,OUT
NX=2
NY=2
NS=100
DO 2 I=1,NX
2 X(I)=XIC(I)
ITE=2
ITF=0
TB=0.0
TEND=0.0
DEL=0.0
DLT=1.0
DO 3 I=1,NS
T=TB
BBM(I)=PRB(1)+PRB(2)*SIN(PRB(3)*T+PRB(4))
CALL OUTP(T,X,YO)
S=0.0
DO 10 J=1,NY
P(J,I)=YO(J)
E(J,I)=P(J,I)-Y(I,I)
S=S+ABS(E(J,I))
K=I+NS*(J-1)
ES(K)=(WT(J,I)*E(J,I))**2
SM(K)=(RR*(1-BBM(I)))**2
10 ERS(K)=SQRT((WT(J,I)*E(J,I))**2+(RR*(1-BBM(I)))**2)
TAB=0.0
IFAIL=2
TEND=TEND+DLT
CALL D02AJF(T,TEND,X,NX,MODEL,DEL,EB,ITE,TAB,OUT,F,DEFDY,DIF,
1 IFAIL)
DHT(I)=DXX(1)
DTEMP(I)=DXX(2)
3 CONTINUE
EST=0.0
SMO=0.0
S=0.0
DO 4 I=1,IERS
S=S+ERS(I)**2
EST=EST+ES(I)
SMO=SMO+SM(I)
4 CONTINUE
RETURN
END

```


3.8 Subroutine MONIT

```

C
C SUBROUTINE MONIT(IERS,NP,P,S,ITERC,SING,LIM)
C
C THIS SUBROUTINE IS CALLED BY THE MINIMISATION SUBROUTINE TO WRITE THE
C REQUIRED RESULTS
C
COMMON/LOG/EST,SMD
LOGICAL SING,LIM
DIMENSION P(NP)
WRITE(2,200)ITERC,S,EST,SMD,(P(I),I=1,NP)
200 FORMAT(/,7H ITER =,15,3X,7H SES =,F15.6,5X,6H EST =,F15.6,5X,
1 6H SMD =,F15.6,/,14H PARAMETERS =,4E15.6)
RETURN
END

```

3.9 Subroutine PLOT

```

C
C SUBROUTINE PLOT(TA,DVH,DVT,MVH,MVT)
C
C THIS SUBROUTINE PLOTS THE RESULTS ON MICROFILM
C
REAL DVH,DVT,MVH,MVT
DIMENSION TA(100),DVH(100),DVT(100),MVH(100),MVT(100)
CALL SLIDE(00,801,0,1,00)
CALL MARGIN(0,0)
CALL XAXIS(00,1000)
CALL YAXIS(001,0015)
CALL LXTICK
CALL LXVAL
CALL LXLABEL(17H TIME IN SECONDS,17)
CALL LYTICK
CALL LYVAL
CALL LYLABEL(16H HEIGHT (METRES),16)
CALL EDGES(0011,2)
CALL PTPLOT(TA,DVH,100,15)
CALL INTRUPT(2,2)
CALL POLYS(TA,MVH,100)
CALL NEWFRAM
CALL SLIDE(00,100,0,1,00)
CALL MARGIN(0,0)
CALL XAXIS(00,1000)
CALL YAXIS(3101,317)
CALL LXTICK
CALL LXVAL
CALL LXLABEL(17H TIME IN SECONDS,17)
CALL LYTICK
CALL LYVAL
CALL LYLABEL(17H MIXED WATER TEMP,17)
CALL EDGES(0011,2)
CALL PTPLOT(TA,DVT,100,10)
CALL INTRUPT(2,7)
CALL POLYS(TA,MVT,100)
CALL NEWFRAM
CALL ENDFILM
RETURN

```


Programs of the Identification of the Vaporiser System

4.1 Program VAPOUR

```
PROGRAM VAPOUR(INPUT,OUTPUT,TAPE1=INPUT,TAPE2=OUTPUT)
```

C THIS PROGRAM CARRIES OUT IDENTIFICATION PROCESS ON A VPORISER SYSTEM.

```

REAL DVH,DVP,MVHT,MVPV
REAL MVPIC,MVHIC,MPBIC
REAL K1,K2,KG,LAMDA,MGIC,MC,MVH,MVP,LA
DIMENSION ERS(102),AJAC(102,51),JN(2260),VA(2),VB(4),A1(6,102),
      A2(6,6),A3(6,11),A4(6,51)
DIMENSION X(9),E(2,51),WT(2,51),YY(2),F(9,4),DFDY(9,9),DIF(9,7,2)
COMMON RL,SH,LAMDA,HTC,HV,JDV,JAV,VOLV,
      KG,K1,K2,SPH,SPP,LA,
      PH,PDS,TL,MVH,MVP,IOL,7,I08,ITB,PB,QV,
      FRA1(21),FVP1(21),FVP2(21),VPI,RA1,MG,
      VP2,RAD,SHW,RW,TO,FOW(21),QW,TW,PA,PI,
      ,VPIC1,VPIC2,SPICH,SPICP
COMMON/GDNTAB/PRA(2),PRB(4),XIC(9),JYA(2,51),Y(2,51),EBND,DT,NXX,
      NIS,TEIN,NSS,NYY,PR(6),ITRAJ,IRR,WT
COMMON/PLOT/TA(31),DVH(51),JDVP(51),MVHT(51),MVPV(51)

```

NAMELISTS

NAMELIST/DTA/RL,DV,AV,SH,LAMDA,JVOLV,KG,
HTC,K1,K2,HV,ISHW,IRW,IRAD,ILA

NAMLIST/FUNCS/FRA1,FVP1,FVP2,FDW

NAMLIST/CONT/OPH,SPICH,SPPP,SPICP

NAMLIST/BOUND/PH,PDS,TL,TD,PA

```
READ(1,DTA)
```

READ (1, FUNCS)

READ (1, BOUND)

```
READ(1,CONT)
```

```
READ(1,10)NY,NS,NX,NPA,NPB
```

```
10 FORMAT(5I10)
```

CALL CAM35MM

SET PARAMETERS REQUIRED BY THE IDENTIFICATION PROCESS.

$$NP = NPA + NPB$$

1ERS=NY*NS

$$K = NP + 3 + NP/3$$
$$I_N = 2 * I_{ERS} + 1 * NP + I_{ERS} * NP + (NP * NP + NP) / 2 + K * (2 + I_{ERS} + 2 * NP)$$

DO 1 I=1, NPA

$$Y_A(I) = 3.11$$

DO 11 I=1,NPB

19 VB(I) = 6.44

IOPT=1

PRA(1)=179

PRA(2) = 111a

$$HTC = 2.88 \times 10^4 \times PRA(1)$$

K2=7J14E14*PRA(2)

C
C CALCULATE INITIAL CONDITIONS
C

```

PVGIC=249.544*SPICP
PVIC=PVGIC+PA
RGIC=(PVIC/1.5E3+9.1079)/.1143
TBIC=(PVIC/53.17)**(1.09/8.1971)/RGIC
QVIC=KG*SQRT((PVIC+POS)*(PVIC-POS)/TBIC)/RGIC
QBIC=RGIC*QVIC/RL
MVPIC=SPICP
MVHIC=SPICH
MPBIC=MVPIC+(RL*MVHIC)/(RW*2.154*9.1071)
PBGIC=249.544*MPBIC
PBIC=PBGIC+PA
ZIC=(PBIC-PVIC)/(RL*9.1071)
MGIC=RGIC*(VOLV*AV*ZIC)
QLIC=QBIC
PI=PH+PA
RAIC1=QLIC*SQRT(K2/(PI-PBIC-K1*QLIC*QLIC))
CALL FUNC(RAIC1,FRA1,FVP1,121,VPIC1,JJ)
TWIC=(QBIC*RL*LAMDA*QLIC*RL*SH*(TL+TBIC)+LA)/(3.14159*DV*ZIC*HTC)
1  +TBIC
QWIC=2.0*HTC*(TWIC+TBIC)*ZIC*3.14159*RAD*RAD/(RAD*RW*SH*
1  (TO+TWIC))
CALL FUNC(QWIC,FQA,FVP2,21,VPIC2,JJ)

```

C
C CALL SUBROUTINE WHICH COORDINATES THE SOLUTION OF IDENTIFICATION PROCESS
C

```

CALL IDUNDYS(NY,NS,NX,NPA,NPB,INP,IER,SIERS,AJAC,W,IW,VA,VB,S,IER,
1  A1,A2,A3,A4,JOPTN
IF(IER.NE.0) WRITE(2,200)
200 FORMAT(23H0***IDUNDYS FAILURE***)

```

C
C CALL PLOTTING SUBROUTINE
C

```

CALL PLOT(TA,DVH,DVP,MVHT,MVPV)
STOP
END

```


4.2 Subroutine IDUNDYS

1 SUBROUTINE IDUNDYS (NY,NS,NX,NPA,NPB,NP,ERS,IERS,AJAC,W,IW,VA,VB,
S,IER,A1,A2,A3,A4,IOPT)

IDENTIFICATION OF NONLINEAR UNCERTAIN DYNAMIC SYSTEM
WITH SEVERAL OUTPUT SIGNALS

NY = NO OF SEPARATE OUTPUT SIGNALS (INPUT)
NS = NO OF SAMPLES PER OUTPUT SIGNAL (INPUT)
NX = NO OF STATE VARIABLES (INPUT)
NPA = NO OF PARAMETERS OF ESTIMATION PROBLEM (INPUT)
NPB = NO OF PARAMETERS OF SMOOTHING PROBLEM (INPUT)
NP = NPA+NPB
ERS = IERS ARRAY OF WEIGHTED RESIDUALS (OUTPUT)
IERS = DIMENSION OF ERS (INPUT) (IERS=NY*NS)
AJAC = IERS,NP JACOBIAN MATRIX (OUTPUT)
W = IW ARRAY OF WORKING STORE (OUTPUT)
IW = DIMENSION OF W (INPUT) (IW=2*IERS+4*NP+IERS*NP+
0.5*(NP*NP+NP)+K*(2+IERS+2*NP) WHERE K IS LARGEST
INTEGER LESS THAN NP+3+NP/3)
VA = NPA ARRAY OF SCALE FACTORS FOR ESTIMATION PROBLEM (INPUT)
VB = NPB ARRAY OF SCALE FACTORS FOR SMOOTHING PROBLEM (INPUT)
S = SUM OF SQUARE WEIGHTED RESIDUALS (OUTPUT)
IER = ERROR FLAG SET = 0 IF SUCCESSFUL (OUTPUT)
A1 = NP,IERS ARRAY OF WORKING STORE
A2 = NP,NP ARRAY OF WORKING STORE
A3 = NP,1 ARRAY OF WORKING STORE
A4 = NP,NP ARRAY OF WORKING STORE
IOPT = OPTION ON WEIGHTING SET = 1 IF SCALAR, = 0 IF TIME

USER TO SUPPLY TWO SUBROUTINES MODEL AND OUTP VIZ.

MODEL(DERX,X,T)
WHERE DERX = NX ARRAY OF DERIVATIVES, X = NX ARRAY OF STATES
AND T = CURRENT TIME. PURPOSE IS TO COMPUTE DERX GIVEN X

OUTP(T,X,Y)
WHERE Y = NY ARRAY OF CURRENT MODEL OUTPUTS. PURPOSE IS TO
COMPUTE Y GIVEN X

THE FOLLOWING NAMED COMMON BLOCK IS ALSO USED (ALSO SUPPLIED
BY USER

COMMON/GONTAB/PRA(),PRB(),X(),XIC(),YA(),Y(),E(),
C(9,),AA(9,),G(),IP(),R(),F(),EBND,DT,
EB(),NXX,NIS,WT(),TFIN,NSS,YY(),NYY,

PRAA(),PRBB(),PR()

PRA = NPA ARRAY OF PARAMETERS OF ESTIMATION PROBLEM
PRB = NPB ARRAY OF PARAMETERS OF SMOOTHING PROBLEM
X = NX ARRAY OF STATE VARIABLES
XIC = NX ARRAY OF INITIAL CONDITIONS ON X
YA = NY,NS ARRAY OF DESIRED OUTPUTS
Y = NY,NS ARRAY OF MODEL OUTPUTS
E = NY,NS ARRAY OF ERRORS
C = 9,NX ARRAY OF WORKING STORE
AA = 9,NX ARRAY OF WORKING STORE
G = NX,NX ARRAY OF WORKING STORE

76/76 OPT=1 MANTRAP

FTN 4.6+262

IP = NX INTEGER ARRAY OF WORKING STORE
R = NX ARRAY OF WORKING STORE
F = NX ARRAY OF WORKING STORE
EBND = INTEGRATION ERROR BOUND
DT = SAMPLING INTERVAL
EB = NX ARRAY OF ERROR BOUNDS
NXX = NUMBER OF STATE VARIABLES (NXX=NX)
NIS = NUMBER OF INTEGRATIONS PER SAMPLE
WT = NY,NS ARRAY OF WEIGHTING COEFFICIENTS
TFIN = FINAL CPU TIME
NSS = NUMBER OF SAMPLES (NSS=NS)
YY = NY ARRAY OF CURRENT MODEL OUTPUTS
NYY = NUMBER OF OUTPUTS (NYY=NY)
PRAA = NPA ARRAY USED IN CONVERGENCE CRITERION
PRBB = NPB ARRAY USED IN CONVERGENCE CRITERION
PR = NP ARRAY OF PARAMETERS
TRAJ = NOMINAL TRAJECTORY OF THE UNCERTAINTY
RR = WEIGHTING COEFFICIENT FOR THE UNCERTAINTY


```

1 DIMENSION ERS(IERS),AJAC(IERS,NP),W(IW),VA(NPA),VB(NPB),
  A1(NP,IERS),A2(NP,NP),A3(NP,1),A4(NP,NP)

```

C
C

```

  USER TO INSERT COMMON /GONTAB/ HERE
  REAL DVH,DVP,MVHT,MVPV
  DIMENSION X(9),E(2,51),WT(2,51),YY(2),F(9,4),DFDY(9,9),DIF(9,7,2)
  DIMENSION PRAA(2),PRBB(4)
  COMMON/GONTAB/PRA(2),PRB(4),XIC(9),YA(2,51),Y(2,51),EBND,DT,NXX,
  NIS,TFIN,NSS,NYY,PR(6),TRAJ,RR,WT
1 COMMON/PRINT/ EST,SNO
  COMMON/PLOT/TA(51),DVH(51),DVP(51),MVHT(51),MVPV(51)
  COMMON/CHECK/INN,IN
  COMMON/VALUE/D,ICOUNT
  EXTERNAL FUNCT1
  EXTERNAL FUNCT,MONIT

```

C

```

  READ DATA
  WRITE(2,199)
199 FORMAT(11H0DATA CHECK)
  DO 50 J=1,NY
  50 READ (1,100) (YA(J,I),I=1,NS)
  100 FORMAT (4E14.6)
  WRITE(2,200) NY,NS
200 FORMAT(28H0NUMBER OF OUTPUT SIGNALS = ,I2/20H0 NUMBER OF SAMPLES ,
  1 2H= ,I3)
  DO 1 J=1,NY
  1 WRITE(2,201) J,(YA(J,I),I=1,NS)
201 FORMAT(19H0DESIRED OUTPUT NO.,I2/(1H ,8E15.6))
  IF(IOPT.EQ.0) GOTO 3
  READ(1,100) (W(I),I=1,NY)
  WRITE(2,202) (W(I),I=1,NY)
202 FORMAT(30H0SCALAR WEIGHTING COEFFICIENTS/(1H ,8E15.6))
  DO 2 J=1,NY
  DO 2 I=1,NS
  2 WT(J,I)=W(J)
  GOTO 5
  3 DO 51 J=1,NY
  51 READ(1,100) (WT(J,I),I=1,NS)
  WRITE(2,203)

```

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1

```

203 FORMAT(26H0TIME DEPENDENT WEIGHTINGS)
  DO 4 J=1,NY
  4 WRITE(2,204) J,(WT(J,I),I=1,NS)
204 FORMAT(26H0WEIGHTINGS FOR OUTPUT NO.,I2/(1H ,8E15.6))
  5 READ (1,100) (PRA(I),I=1,NPA)
  READ(1,111) (PRB(I),I=1,NPB)
111 FORMAT(4F14.11)
  WRITE (2,205) NPA, (PRA(I),I=1,NPA)

```

```

205 FORMAT(41H0NO OF PARAMETERS OF ESTIMATION PROBLEM = ,
  1 I3/20H0INITIAL ESTIMATES =/(1H ,8E15.6))
  WRITE (2,2055) NPB, (PRB(I), I=1,NPB)
2055 FORMAT(41H0NO OF PARAMETERS OF SMOOTHING PROBLEM = ,
  1 I3/20H0INITIAL ESTIMATES =/(1H ,8E15.6))
  WRITE (2,206) (VA(I),I=1,NPA)
206 FORMAT(38H0SCALE FACTORS OF ESTIMATION PROBLEM =/ (1H , 8E15.6))
  WRITE (2,2066) (VB(I),I=1,NPB)
2066 FORMAT(38H0SCALE FACTORS OF SMOOTHING PROBLEM =/ (1H , 8E15.6))
  NXX=NX
  NSS=NS
  NYY=NY
  IF(NX.GT.1) GOTO 6
  WRITE(2,207)
207 FCRMAT(77H0*** THIS PROGRAM WILL NOT WORK WITH LESS THAN TWO DIFFE
  1RENTIAL EQUATIONS ***/29H0*** USE A DUMMY EQUATION ***)
  STOP
  6 READ(1,100) (XIC(I),I=1,NX)
  WRITE(2,208) NX,(XIC(I),I=1,NX)
208 FORMAT(16H0NO OF STATES = ,I3/22H0INITIAL CONDITIONS = /
  1 (1H ,8E15.6))
  READ(1,100) EBND,DT
  READ(1,100) EPS,DSTEP,ALF,TFIN
  READ(1,102) IPRNT,MAXIT,NIS
102 FORMAT(3I10)

```



```

WRITE(2,209) EBND,DT,EPS,DSTEP,ALF,TFIN,IPRNT,MAXIT,NIS
209 FORMAT(27H0INTEGRATION ERROR BOUND = ,E15.6/
1 27H SAMPLING INTERVAL = ,E15.6/
2 27H OPTIMISATION ACCURACY = ,E15.6/
3 27H DERIVATIVE STEP SIZE = ,E15.6/
4 27H RELATIVE ACCURACY = ,E15.6/
5 27H FINAL CPU TIME = ,E15.6/
6 27H PRINT CONTROL FLAG = ,I5/
7 27H MAX NO OF ITERATIONS = ,I5/
8 27H INTEGRATIONS PER SAMPLE = ,I5)
READ (1,100) ALFA,ALFB
WRITE (2,2098) ALFA,ALFB
2098 FORMAT (44H0RELATIVE ACCURACY FOR ESTIMATION PROBLEM = ,E15.6/
1 44H RELATIVE ACCURACY FOR SMOOTHING PROBLEM = ,E15.6)
READ (1,100) TRAJ,RR
WRITE(2,2099) TRAJ,RR
2099 FORMAT (44H0NOMINAL TRAJECTORY OF THE UNCERTAINTY = ,E15.6/
1 44H WEIGHTING COEFFICIENT FOR THE UNCERTAINTY = ,E15.6)
DO 53 I=1,NS
DVH(I)=YA(1,I)
DVP(I)=YA(2,I)
53 CONTINUE
INN=0
TA(1)=0.0
DO 54 I=2,51
54 TA(I)=TA(I-1)+DT
ICOUNT=0
WRITE(2,210)
210 FORMAT(17H0INITIAL RESPONSE)
CALL FUNCT (IERS,NPA,PRA,ERS)
S=0.0
DO 7 I=1,IERS
7 S=S+ERS(I)**2
DO 8 J=1,NY
8 WRITE(2,211) J,(Y(J,I),I=1,NS)
211 FORMAT(17H0MODEL OUTPUT NO.,I2/(1H ,8E15.6))
WRITE(2,212) S
212 FORMAT(42H0INITIAL VALUE OF THE OBJECTIVE FUNCTION = ,E15.6)
C OPTIMISATION
WRITE (2,213)
DO 444 KK=1,MAXIT
C PARAMETER ESTIMATION PROBLEM
IPRNTA=0
IFAIL=1
IF(IPRNTA.NE.0) WRITE (2,213)
213 FORMAT(21H0OPTIMISATION MONITOR)
DO 327 I=1,NPA
327 PRAA(I)=PRA(I)
WRITE(2,13)
13 FORMAT(/,1H ,41H ***** ESTIMATION PROBLEM ***** ,/)
E1=0.0
E2=0.0
B1=0.0
B2=2.0
MAXCAL=30
CALL ED4ABF(FUNCT1,E1,E2,B1,B2,MAXCAL,PRX,S,IFAIL)
PRA(1)=PRX
WRITE(2,16) IFAIL,MAXCAL
16 FORMAT(1H ,8H IFAIL = ,I5,5X,9H MAXCAL = ,I5)
CALL FUNCT1(PRX,S)
WRITE(2,17) PRA(1),S,EST,SMO
17 FORMAT(1H ,6H PRA = ,F15.6,5X,6H SES = ,F15.6,5X,6H EST = ,F15.6,5X,
1 6H SMO = ,F15.6)
IF(IFAIL.EQ.0) GOTO 99
C ERROR MESSAGE
WRITE (2,214) MAXIT, KK
214 FORMAT(13H0***MORE THAN,I5,5X,20HITERATIONS WHEN KK = ,I5,5X,
1 34HIN PARAMETER ESTIMATION PROBLEM***)
IER=1
GO TO 10
C SMOOTHING PROBLEM
99 IPRNTB=0
IPRNTB=2
ICOUNT=0
CALL SECOND(TT)
WRITE(2,220) TT
220 FORMAT(1H ,24H CP TIME TO THIS POINT = ,F10.3)
WRITE(2,14)
14 FORMAT(/,1H ,41H ***** SMOOTHING PROBLEM ***** ,/)
IFAIL=1
IF(IPRNTB.NE.0) WRITE (2,213)

```



```

DO 328 I=1,NPB
328 PRBB(I)=PRB(I)
EPSB=EPS
CALL E04FAF(IERS,NPB,PRB,ERS,S,EPSB,ALFB,VB,W,IW,FUNCT,MONIT,
1 IPRNTB,MAXIT,IFAIL)
CALL SECOND(TT)
WRITE(2,220)TT
IF(IFAIL.EQ.0) GO TO 3211
C ERROR MESSAGE
WRITE (2,2144) MAXIT,KK
2144 FORMAT(13H0***MORE THAN,I5,5X,20HITERATIONS WHEN KK =,I5,5X,
1 34HIN SMOOTHING PROBLEM ***)
IER=1
GO TO 10
C OPTIMISATION MONITOR
C CONVERGENCE CRITERION
3211 DO 321 I=1,NPA
IF(ABS(PRAA(I)-PRA(I)).GT.(ALF*VA(I))) GOTO 444
321 CONTINUE
DO 322 I=1,NPB
IF(ABS(PRBB(I)-PRB(I)).GT.(ALF*VB(I))) GOTO 444
322 CONTINUE
GO TO 9
444 CONTINUE
C ERROR MESSAGE
WRITE (2,323)
323 FORMAT (15H *** MORE THAN ,I5,15H ITERATIONS ***)
IER=1
GO TO 10
9 IER=0
C FINAL RESPONSE
10 CALL FUNCT (IERS,NPA,PRA,ERS)
WRITE(2,215)
215 FORMAT(30H0FINAL RESPONSE AND PARAMETERS)
ICOUNT=0
DO 36 I=1,51
MVHT(I)=Y(1,I)
MVPV(I)=Y(2,I)
36 CONTINUE
DO 11 J=1,NY
11 WRITE(2,211) J,(Y(J,I),I=1,NS)
WRITE (2,216) S,(PRA(I),I=1,NPA)
216 FORMAT(37H0FINAL VALUE OF OBJECTIVE FUNCTION =,E15.6/
1 46H0FINAL MODEL PARAMETERS IN ESTIMATION PROBLEM /(1H ,
2 8E15.6))
WRITE (2,2166) (PRB(I),I=1,NPB)
2166 FORMAT (46H0FINAL MODEL PARAMETERS IN SMOOTHING PROBLEM /
1 (1H ,8E15.6))
C SENSITIVITY ANALYSIS
WRITE (2,217)
217 FORMAT(55H0ACCURACY OF ESTIMATED PARAMETERS IN ESTIMATION PROBLEM)
DO 12 I=1,NPA
12 VA(I)=DSTEP*PRA(I)
CALL PERAS(IERS,NPA,PRA,ERS,S,VA,FUNCT,AJAC,A1,A2,A3,A4,W)
WRITE (2,218) (I,PRA(I),A3(I,1),I=1,NPA)
218 FORMAT(1H0,3X,9HPARAM.NO.,8X,5HVALUE,8X,9HTOLERANCE/(1H ,7X,I2,
1 6X,2E15.6))

WRITE (2,2177)
2177 FORMAT(55H0ACCURACY OF ESTIMATED PARAMETERS IN SMOOTHING PROBLEM)
DO 122 I=1,NPB
122 VB(I)=DSTEP*PRB(I)
CALL PERAS(IERS,NPB,PRB,ERS,S,VB,FUNCT,AJAC,A1,A2,A3,A4,W)
WRITE (2,218) (I,PRB(I),A3(I,1),I=1,NPB)
C
C RETURN
END

```


4.3 Subroutine MODEL

```

C
C
C      SUBROUTINE MODEL(DERX,X,T,INXX)
C
C THIS SUBROUTINE MODELS THE VAPORISER SYSTEM ON THE ASSUMPTION OF
C PERFECT MIXING CONDITIONS.
C
      REAL K1,K2,KG,LAMDA,MCIC,MC,MVH,MVP,LA,MPB
      DIMENSION DERX(9),X(9)
      DIMENSION X(9),Z(2,51),WT(2,51),YY(2),F(9,4),DFDY(9,9),DIF(9,7,2)
      COMMON RL,SH,LAMDA,HTC,HV,IV,AV,VOLV,
1      KG,K1,K2,SPH,SPP,LA,
2      PH,PDS,TL,MVH,MVP,IQL,Z,IQB,ITB,PB,QV,
3      FRA1(21),FVP1(21),FVP2(21),VPI,RA1,MC,
4      VP2,RAD,SHW,RH,TO,FOW(21),QW,ITW,PA,PI,
5      VPIC1,VPIC2,SPIC1,SPIC2
      COMMON/GDNTAB/PRA(2),PRB(4),XIC(9),YA(2,51),Y(2,51),EBND,DT,NX,
1      NIS,TFIN,NSS,NYY,PR(6),ITRAJ,RR,WT
      COMMON/CHECK/INN,IN
      COMMON/VAL/RC,PVW,PBW,V1,V2,V10,V11
      COMMON/VALUE75,ICOUNT
C
C CALCULATE CHEBYCHEV POLYNOMIALS
C
      T0=1.
      TOR=2./5000*T+1.
      T1=TOR
      T2=2.*(TOR**2)-1.
      T3=4.*(TOR**3)-3.*TOR
C
C ATTACH CHEBYCHEV POLYNOMIALS TO HOT WATER TEMPERATURE
C
      TIN=TO*(PRB(1)*T0+PRB(2)*T1+PRB(3)*T2+PRB(4)*T3)
      HTC=258000*PRA(1)
      K2=7.014E14*PRA(2)
      Z=X(1)
      IF(Z.GT.10.65)Z=10.65
      IF(Z.LT.10.1)Z=10.1
      MG=X(2)
      TW=X(3)
      MPB=X(4)
      VPI=X(5)
      MVP=X(6)
      VP2=X(7)
      IF(TIN.LT.TW)TIN=TW
      VPI=1.2*VPIC1
      VP2=VPIC2
      RG=MG/(VOLV*AV*Z)
      IF(RG.LT.7.44223)RG=7.44223
      PV=(-8.679+20.148*RG)*1.E5
      TB=(PV/53.7)*((1.30/0.1971)/RG)
      IF(TB.LT.TL)TB=TL
      PVG=PV-PA
      PVW=PVG/240.544
      QV=SIGN(KG*SQRT(ABS((PV+PDS)*(PV-PDS)/TB)))/RG,PV-PDS)
      IF(QV.LT.300)QV=300

```



```

CALL FUNC(VP1,FVP1,FRA1,Z1,RA1,IJY
CALL FUNC(VP2,FVP2,FQW,Z1,QW,IJY
PB=PV+RL*9.81*Z
PBG=PB-PA
PBW=PBG/249.544
IF(RA1.GT.0.00001)GO TO 2
QL=0.0
GO TO 3
2 QL=SIGN(SQRT(ABS(PI-PB)/(K1+K2*(RA1*RA1))),PI-PB)
3 V1=3.14159*HTC*DV*Z*(TW-TB)
V2=RL*QL*SH*(TB-TL)
IF(QL.LT.0.0)V2=0.0
IF(QL.LT.0.0)QL=0.0
IF(V1.LT.(V2+LA))V1=V2+LA
QB=(V1-V2+LA)/(RL*LAMDA)
V10=QW*(TIN-TN)/(Z*3.14159*RAD*RDY)
V11=2.0*HTC*(TW-TB)/(RAD*RW*SHW)
DERX(1)=(QL-QB)/AV
DERX(2)=RL*QB-RG*QV
DERX(3)=V10-V11
DERX(4)=2.0*(PBW-IX(4))
DERX(5)=0.0
DERX(6)=2.0*(PVW-IX(6))
DERX(7)=0.0
DERX(8)=0.0
DERX(9)=0.0
RETURN
END

```

4.4. Subroutine OUTP

```

SUBROUTINE OUTP(T,X,Y)
REAL K1,K2,KG,LAMDA,HCIC,MC,MVH,MVP,LA,MPB
DIMENSION X(9),Y(2)

```

C THIS SUBROUTINE CALCULATES THE HEIGHT AND VAPOUR PRESSURE USING THE
C CALCULATED VALUES OF STATE VARIABLES

```

COMMON RL,SH,LAMDA,HTC,HV,DV,AV,VOLV,
1 KG,K1,K2,SPH,SPP,LA,
2 PH,PDS,TL,MVH,MVP,QL,Z,QB,FB,PB,QV,
3 FRA1(Z1),FVP1(Z1),FVP2(Z1),VP1,RA1,MC,
4 VP2,RAD,SHW,RW,T0,FQW(Z1),QW,TW,PA,PI
5 ,VPIC1,VPIC2,SPICH,SPICP
Y(1)=2.54*2.0*0.01*RW*(X(4)-X(5))/RL
Y(2)=X(6)
MVH=Y(1)
RETURN
END

```


4.5 Subroutine MONIT

```

SUBROUTINE MONIT(IERS,NP,P,S,ITERC,SING,LIM)
LOGICAL SING,LIM
COMMON/PRINT/ EST,SMO
COMMON/VALUE/G,ICOUNT
DIMENSION P(NP)
WRITE(2,200) ITERC,S,EST,SMO,(P(I),I=1,NP)
200 FORMAT(1,7H ITER =,I5,3X,7H SES =,E15.6,3X,7H EST =,E15.6,3X,
1 7H SMO =,E15.6,/,14H PARAMETERS =,5E15.6,/)
WRITE(2,203) ICOUNT
203 FORMAT(1H,21H NO OF FUNCT CALLS =,I6,/)
IF(SING) WRITE(2,201)
201 FORMAT(26H *** LINEAR DEPENDENCE ***)
IF(LIM) WRITE(2,202)
202 FORMAT(33H *** PARAMETER CHANGE LIMITED ***)
RETURN
END

```

SUBROUTINE FUNCT(IERS,NP,P,ERS)

OPTIMISATION SUBROUTINE WHICH CALCULATES WEIGHTED RESIDUALS
E(I) AS FUNCTIONS OF MODEL PARAMETERS

DIMENSION P(NP),ERS(IERS)

USER TO INSERT COMMON /GONTAB/ HERE

DIMENSION ES(102),SM(102)

DIMENSION X(9),E(2,51),WT(2,51),YY(2),F(9,4),DFDY(9,9),DIF(9,7,2)

DIMENSION EB(9)

COMMON/GONTAB/PRA(2),PRB(4),XIC(9),YA(2,51),Y(2,51),EBND,DT,NXX,

1 NIS,TFIN,NSS,NYY,PR(6),TRAJ,RR,WT

COMMON/PRINT/ EST,SMO

COMMON/CHECK/INN,IN

COMMON/VALUE/S,ICOUNT

EXTERNAL OUT

EXTERNAL MODEL

STORE CURRENT MODEL PARAMETERS

DO 1 I=1,NP

1 PR(I)=P(I)

SET ERROR BOUNDS AND INITIAL CONDITIONS FOR INTEGRATION

PRX=PRA(1)

CALL INCON(PRX)

DO 2 I=1,NXX

EB(I)=EBND

2 X(I)=XIC(I)

ITE=2

ITF=0

T0=0.0

II=0

III=0

IIII=0

DLT=DT/FLOAT(NIS)

ICOUNT=ICOUNT+1

NPA=2

NPB=4

TEND=0.0

TAB=0.0

IFAIL=1

DEL=0.0

INTEGRATION LOOP

DO 3 I=1,NSS

T=T0

COMPUTE CURRENT OUTPUTS AND ERRORS

CALL OUTP(T0,X,YY)

S=0.0

DO 10 J=1,NYY

Y(J,I)=YY(J)

E(J,I)=Y(J,I)-YA(J,I)

S=S+ABS(E(J,I))

K=I+NSS*(J-1)

TOR=2./500.*T-1.

T00=1.

T1=TOR

T2=2.*(TOR**2)-1.


```

T3=4.*(TOR**3)-3.*TOR
BB22=PRB(1)*T00+PRB(2)*T1+PRB(3)*T2+PRB(4)*T3
RR=1.0/BB22
WT(J,I)=1.0/YA(J,I)
ES(K)=(WT(J,I)*E(J,I))**2
SM(K)=(RR*(BB22-TRAJ))**2
10 ERS(K)=SQRT((WT(J,I)*E(J,I))**2+(RR*(BB22-TRAJ))**2)
IF(S.GT.10.0E10) GOTO 5
C INTEGRATE OVER CURRENT SAMPLING INTERVAL
31 DO 3 N=1,NIS
TEND=TEND+DLT
CALL DO2AJF(T0,TEND,X,NXX,MODEL,DEL,EB,ITE,TAB,OUT,F,DFDY,DIF,
1 IF(INN.GE.1) GO TO 71
CALL SECOND(TT)
IF((TT.GT.TFIN).AND.(ITF.EQ.0)) WRITE(2,203) (PR(J),J=1,NP)
IF(TT.GT.TFIN) ITF=1
203 FORMAT(49H0*** TIME LIMIT EXCEEDED - CURRENT PARAMETERS ***/
1 (1H,8E15.6))
IF(IFAIL.NE.0) GOTO 4
30 CONTINUE
3 CONTINUE
C
71 EST=0.0
SMO=0.0
S=0.0
DO 7 I=1,IERS
EST=EST+ES(I)
SMO=SMO+SM(I)
7 S=S+ERS(I)**2
IF(INN.GE.1) GO TO 9
12 IF(ITF.EQ.0) RETURN
WRITE(2,204) S
204 FORMAT(47H0VALUE OF THE OBJECTIVE FUNCTION AT TIME LIMIT=,E15.6/)
STOP
C FAILURE INDICATORS
4 IF((IFAIL.EQ.1).AND.(IT.EQ.0)) WRITE(2,200) T,(PR(J),J=1,NP)
200 FORMAT(46H0*** INTEGRATION ACCURACY UNSATISFIED AT TIME ,E15.6,
1 4H ***/19H0CURRENT PARAMETERS//(1H,8E15.6))
IF(IFAIL.NE.1) GOTO 6
II=1
GOTO 30
5 IF(IIII.EQ.0) WRITE(2,201) T,(PR(J),J=1,NP)
201 FORMAT(29H0*** SYSTEM UNSTABLE AT TIME ,E15.6,4H ***/
1 19H0CURRENT PARAMETERS//(1H,8E15.6))
IIII=1
GOTO 31
6 IF(III.EQ.0) WRITE(2,202) T,(PR(J),J=1,NP)
202 FORMAT(43H0*** INTEGRATION CORRECTOR FAILURE AT TIME ,E15.6,
1 4H ***/19H0CURRENT PARAMETERS//(1H,8E15.6))
III=1
GOTO 30
9 IF(IN.GT.0) GO TO 14
WRITE(2,21) T0,(PR(I),I=1,NPA),(PRB(I),I=1,NPB),S,ICOUNT
21 FORMAT(1H,27HUNFEASIBLE REGION AT TIME =,F7.2,/,
1 25H ESTIMATION PARAMETERS =,2F15.6,/,
2 25H SMOOTHING PARAMETERS =,4F15.6,/,
3 25H OBJECTIVE FUNCTION =,F15.6,/,
4 25H NO OF FUNCT CALLS =,I6,/)
14 DO 13 I=1,IERS
13 ERS(I)=20.0
GO TO 12
C
END

```

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4.7 Subroutine FUNCTI

C
C THIS SUBROUTINE IS CALLED BY E24ABF AND CALCULATES THE MODEL RESPONSES
C AND OBJECTIVE FUNCTION]
C

```

DIMENSION ERS(102),ES(102),ISM(102)
DIMENSION EB(9)
DIMENSION X(9),E(2,51),WT(2,51),YY(2),F(9,4),DFDY(9,9),DIF(9,7,2)
COMMON/CONTAB/PRA(2),PRB(4),XIC(9),YA(2,51),Y(2,51),EBND,DT,NXX,
1 NIS,TFIN,NSS,NYY,PR(6),ITRAJ,RR,WT
COMMON/PRINT/EST,SMO
COMMON/CHECK/INN,IN
COMMON/VALUE/SS,ICOUNT
EXTERNAL OUT,MODEL
PRA(1)=PRX
TAB=2.0
25 CALL INCON(PRX)
DO 2 I=1,NXX
EB(I)=EBND
2 X(I)=XIC(I)
IERS=102
TB=0.0
DLT=DT/FLOAT(NIS)
ICOUNT=ICOUNT+1
TEND=2.0
DEL=2.0
IFAIL=1
ITE=2
DO 3 I=1,NSS
T=TB
CALL OUTP(TB,X,YY)
DO 10 J=1,NYY
Y(J,I)=YY(J)
E(J,I)=Y(J,I)+YA(J,I)
K=I+NSS*(J+1)

```

C
C CALCULATE THE TIME-VARYING UNCERTAINTY
C

```

TOR=2.0/500.0*T+1.0
T2=1.0
T1=TOR
T2=2.0*(TOR**2)+1.0
T3=4.0*(TOR**3)+3.0*TOR
BB22=PRB(1)*T2+PRB(2)*T1+PRB(3)*T2+PRB(4)*T3
ES(K)=(WT(J,I)*E(J,I))**2
SM(K)=(RR*(BB22+ITRAJ))**2
10 ERS(K)=SQRT((WT(J,I)*E(J,I))**2+(RR*(BB22+ITRAJ))**2)
DO 3 N=1,NIS
TEND=TEND+DLT
CALL D2AJF(TB,TEND,X,NXX,MODEL,DEL,EB,ITE,TAB,OUT,F,DFDY,DIF,
1 IFAIL)
3 CONTINUE
S=0.0
EST=0.0
SMO=0.0
DO 7 I=1,IERS
S=S+ERS(I)**2
EST=EST+ES(I)
SMO=SMO+SM(I)
7 CONTINUE
15 RETURN
END

```


4.8 Subroutine INCON

SUBROUTINE INCON(PRA)

C THIS SUBROUTINE CALCULATES THE INITIAL CONDITIONS WHICH ARE FUNCTION
C OF THE PARAMETER ESTIMATES.

```

C
REAL MVPIC,MVHIC,MPBIC
REAL K1,K2,KG,LAMDA,MGIC,MBG,MVH,MVP,LA
DIMENSION X(9),E(2,51),WT(2,51),YY(2),F(9,4),DEFDY(9,9),DIF(9,7),
COMMON RL,SH,LAMDA,HTC,HV,DV,AV,VOLV,
1 KG,K1,K2,SPH,SPP,LA,
2 PH,PDS,TL,MVH,MVP,QL,Z,QB,JB,PB,QV,
3 FRA1(21),FVP1(21),FVP2(21),JVP1,RA1,MBG,
4 VP2,RAD,SHW,RW,TD,FQW(21),QW,ITW,PA,PI
5 VPIC1,VPIC2,SPIC1,SPIC2
COMMON/CONTAB/PRF(2),PRB(4),XIC(9),YA(2,51),Y(2,51),ERND,DT,NXX
1 NIS,TFIN,NS3,YYY,PR(6),TRAJ,JRR,WT
HTC=2.8*PRA
TWIC=35.138
PVGIC=249.544*SPICP
PVIC=PVGIC+PA
RGIC=(PVIC/1.0E5+0.1079)/0.1143
TBIC=(PVIC/53.7)**(1.14/0.1971)/RGIC
QVIC=KG*SQRT((PVIC+PDS)*(PVIC-PDS)/TBIC)/RGIC
QBIC=RGIC*QVIC/RL
MVPIC=SPICP
MVHIC=SPICB
MPBIC=MVPIC+(RL*MVHIC)/(RW*2.154*0.1)
PBGIC=249.544*MPBIC
PBIC=PBIC+PA
ZIC=(PBIC+PVIC)/(RL*9.181)
MGIC=RGIC*(VOLV+AV*ZIC)
QLIC=QBIC
PI=PH+PA
RAIC1=QLIC*SQRT(K2/(PI+PBIC+K1*QLIC*QLIC))
CALL FUNC(RAIC1,FRA1,FVP1,21,JVPIC1,J)
LA=3.14159*DV*ZIC*HTC*(TWIC+TBIC)+QBIC*RL*LAMDA+QLIC*RL*SH*
1 (TL+TBIC)
QWIC=2.78*HTC*(TWIC+TBIC)*ZIC*3.14159*RAD*RAD/(RAD*RW*SHW*
1 (TO+TWIC))
CALL FUNC(QWIC,FQW,FVP2,21,JVPIC2,J)
XIC(1)=ZIC
XIC(2)=MGIC
XIC(3)=TWIC
XIC(4)=MPBIC
XIC(5)=VPIC1
XIC(6)=MVPIC
XIC(7)=VPIC2
XIC(8)=PI
XIC(9)=PI
RETURN
END

```


4.9 Subroutine FUNC

```

C
C
C SUBROUTINE FUNC(X,A,B,N,Y,IERR)
C THIS SUBROUTINE CALCULATES THE VALUE OF YCORRESPONDING TO X WHICH LIES
C IN THE RANGE A-B BY INTERPOLATION
C
  DIMENSION A(1),B(1)
  IF(X-A(1))3,1,1
1  I=2
2  IF(I-N)3,3,9
3  IF(X-A(I))4,4,6
4  Y=B(I-1)+(X-A(I-1))*(B(1)-B(I-1))/(A(1)-A(I-1))
  IERR=0
  GO TO 7
8  Y=B(1)
  GO TO 5
9  Y=B(N)
5  IERR=1
  GO TO 7
6  I=I+1
  GO TO 2
7  RETURN
  END

```

4.10 Subroutine OUT

SUBROUTINE OUT(T,X,HT,N,TAB)

```

C
C THIS SUBROUTINE IS CALLED BY THE IDENTIFICATION SUBROUTINES TO OUTPUT
C INTERMEDIATE RESULTS
C
  DIMENSION X(9)
  COMMON RL,SH,LAMDA,HTC,HV,IV,JAV,VOLV,
1  KG,K1,K2,SPH,SPP,LAJ
2  PH,PDS,TL,MVH,MVP,QL,I7,QB,ITB,PB,QV,
3  FRA1(21),FVP1(21),FVP2(21),VPI,RAI,MG,
4  VP2,RAD,SHW,RW,TD,FDWC(21),QW,TW,PA,PI,
5  VPIC1,VPIC2,SPICH,SPICP
  COMMON VAL,IRG,PVW,PRW,V1,IV2,V12,V11
  WRITE(2,15)T,X(1),MVH,X(2),IRG,IPVW,X(6),PRW,X(4),TB,TW,QV,QL,QB,V1,
1  V2,V12,V11
12 FORMAT(F7.1,4F3.1,4F8.1,2F5.1,13F10.1,7F6.1,F5.1,2F5.2)
  RETURN
  END

```


4.11 Subroutine PERAS

SUBROUTINE PERAS(NS, NP, P, E, S, DP, FUNCT, AJAC, A1, A2, A3, A4, W)

PARAMETER ERROR ANALYSIS - CALCULATES CONFIDENCE LIMITS ON
PARAMETERS ESTIMATED BY MINIMIZING SUM OF SQUARE RESIDUALS

NS = NO OF SAMPLES (INPUT)
NP = NO OF PARAMETERS (INPUT)
P = NP ARRAY OF OPTIMUM PARAMETERS (INPUT)
E = NS ARRAY OF MINIMIZED RESIDUALS (INPUT)
S = MINIMUM SUM OF SQUARE RESIDUALS (INPUT)
DP = NP ARRAY OF PARAMETER PERTURBATIONS (INPUT)
FUNCT = NAME OF EXTERNAL SUBROUTINE FUNCT(NS, NP, P, E) USED TO
COMPUTE RESIDUALS E FOR GIVEN PARAMETERS P
AJAC = NS, NP JACOBIAN MATRIX (OUTPUT)
A1 = NP, NS ARRAY OF AUXILIARY STORAGE - PERAS RETURNS WITH
A1 = PARAMETER SENSITIVITY MATRIX
A2 = NP, NP ARRAY OF AUXILIARY STORAGE - PERAS RETURNS WITH
A2 = AJAC TRANSPOSE AJAC
A3 = NP, 1 ARRAY OF AUXILIARY STORAGE - PERAS RETURNS WITH
A3 = PARAMETER 95 PER CENT CONFIDENCE TOLERANCES
A4 = NP, NP ARRAY OF WORKING STORAGE - PERAS RETURNS WITH
A4 = PARAMETER COVARIANCE MATRIX
W = NS ARRAY OF AUXILIARY STORAGE - PERAS RETURNS WITH
W = VARIANCE OF RESIDUALS

PERAS REQUIRES NAG SUBROUTINES F01AAF, F01CJF, F01CKF, G01BAF

DIMENSION P(NP), E(NS), DP(NP), AJAC(NS, NP), A1(NP, NS), A2(NP, NP),
A3(NP, 1), A4(NP, NP), W(NS), Z(1)

1 IF(NP.LT.2) WRITE(2, 200)
200 FORMAT(47H0*** PERAS REQUIRES AT LEAST TWO PARAMETERS ***)
IF(NS.LE.NP) WRITE(2, 201)
201 FORMAT(40H0*** INSUFFICIENT DEGREES OF FREEDOM ***)
IF((NP.LT.2).OR.(NS.LE.NP)) STOP

WRITE(2, 202)
202 FORMAT(57H0SENSITIVITY CALCULATIONS USED TO COMPUTE JACOBIAN MATRI
1X)
DO 4 J=1, NP
PT=P(J)
P(J)=PT-DP(J)
CALL FUNCT(NS, NP, P, W)
DO 1 I=1, NS
1 A1(1, I)=W(I)
P(J)=PT+DP(J)
CALL FUNCT(NS, NP, P, W)
DO 2 I=1, NS
2 A1(2, I)=W(I)
P(J)=PT
WRITE(2, 203) J, DP(J)
203 FORMAT(11H0PARAMETER , I3, 16H PERTURBATION = , E15.6)
WRITE(2, 204) (A1(2, I)-E(I), I=1, NS)
204 FORMAT(4H +VE/(1H , 8E15.6))
WRITE(2, 205) (A1(1, I)-E(I), I=1, NS)
205 FORMAT(4H -VE/(1H , 8E15.6))
DO 3 I=1, NS

3 AJAC(I, J)=0.5*(A1(2, I)-A1(1, I))/DP(J)
4 CONTINUE
WRITE(2, 206)
206 FORMAT(16H0JACOBIAN MATRIX/)
DO 5 J=1, NS
5 WRITE(2, 207) (AJAC(J, I), I=1, NP)
207 FORMAT(1H , 8E15.6)
MATRIX OPERATIONS TO COMPUTE APPROXIMATE ERRORS IN PARAMETERS
IFAIL=0
CALL F01CJF(A1, AJAC, NP, NS, 0, IFAIL)
CALL F01CKF(A2, A1, AJAC, NP, NP, NS, Z, 1, 1, IFAIL)
CALL F01CKF(A3, A1, E, NP, 1, NS, Z, 1, 1, IFAIL)
WRITE(2, 208) (2.0*A3(I, 1), I=1, NP)
208 FORMAT(28H0ESTIMATE OF GRADIENT VECTOR/(1H , 8E15.6))
CALL F01AAF(A2, NP, NP, A4, NP, A3, IFAIL)
CALL F01CKF(A1, A4, A1, NP, NS, NP, A3, NP, 3, IFAIL)
WRITE(2, 209)
209 FORMAT(19H0SENSITIVITY MATRIX/)
DO 6 J=1, NS
6 WRITE(2, 207) (A1(I, J), I=1, NP)
CALL F01CKF(A3, A1, E, NP, 1, NS, Z, 1, 1, IFAIL)


```

      WRITE(2,210) (-A3(I,1),I=1,NP)
210  FORMAT(33H0 APPROXIMATE ERRORS IN PARAMETERS// (1H ,8E15.6))
      B=0.5*S/FLOAT(NS-NP)
      WRITE(2,211)
211  FORMAT(32H0 COVARIANCE MATRIX OF PARAMETERS/)
      DO 7 J=1,NP
7    WRITE(2,207) (B*A4(I,J),I=1,NP)
C    95 PER CENT CONFIDENCE LIMITS COMPUTED USING STUDENT T DIST.
      IDF=NS-NP
      A=G01BAF(IDF,0.025,IFAIL)
      DO 8 I=1,NP
8    A3(I,1)=A*SQRT(B*A4(I,I))
      WRITE(2,212) (A3(I,1),I=1,NP)
212  FORMAT(48H0 95 PER CENT CONFIDENCE TOLERANCES ON PARAMETERS// (1H ,
1    8E15.6))
C    RESIDUAL VARIANCES AND 95 PER CENT TOLERANCES
      DO 11 K=1,NS
      W(K)=0.0
      DO 10 I=1,NP
      D=0.0
      DO 9 J=1,NP
9    D=D+AJAC(K,J)*A4(I,J)
10   W(K)=W(K)+D*AJAC(K,I)*B
11  CONTINUE
      WRITE(2,213) (W(I),A*SQRT(W(I)),I=1,NS)
213  FORMAT(1H0,5X,6HOUTPUT,6X,11H95 PER CENT/1H ,4X,8HVARIANCE,6X,
1    9HTOLERANCE// (1H ,2E15.6))
C
      DO 14 I=1,NP
      DO 13 J=1,NP
13   A4(I,J)=B*A4(I,J)
14  CONTINUE
C
      RETURN
C
      END

```

4.12 Subroutine PLOT

SUBROUTINE PLOT(TA,DVH,DVP,MVHT,MVPV)

C THIS SUBROUTINE PLOTS RESULTS ON MICROFILM
C

```

REAL DVH,DVP,MVHT,MVPV
DIMENSION TA(51),MVHT(51),MVPV(51),JDVH(51),DVP(51)
CALL SLIDE(00,100,00,80)
CALL MARGIN(0,0)
CALL XAXIS(00,500)
CALL YAXIS(0008,0,14)
CALL LXTICK
CALL LXVAL
CALL LXLABEL(17H TIME IN SECONDS,17)
CALL LYTICK
CALL LYVAL
CALL LYLABEL(16H HEIGHT (METRES),16)
CALL EDGES(0011,2)
CALL PTPLOT(TA,DVH,51,5)
CALL INTRUPT(2,2)
CALL POLY5(TA,MVHT,51)
CALL NEWFRAM
CALL SLIDE(00,100,00,80)
CALL MARGIN(0,0)
CALL XAXIS(00,500)
CALL YAXIS(00,14)
CALL LXTICK
CALL LXVAL
CALL LXLABEL(17H TIME IN SECONDS,17)
CALL LYTICK
CALL LYVAL
CALL LYLABEL(17H VAPOUR PRESSURE,17)
CALL EDGES(0011,2)
CALL PTPLOT(TA,DVP,51,10)
CALL INTRUPT(2,7)
CALL POLY5(TA,MVPV,51)
CALL NEWFRAM
CALL ENDFILM
C ***** C A S E 1 *****
RETURN
END

```


APPENDIX 5

Miscellaneous

5.1 Program Plotter

C THIS PROGRAM PLOTS THE PERFORMANCES OF THE CLASSICAL
C LEAST SQUARES AND THE SMOOTHED LEAST SQUARES TECHNIQUES
C AGAINST THE NUMBER OF OVERALL ITERATIONS WITH REGARDS
C TO THE PARAMETER ESTIMATE (PRA) AND THE OBJECTIVE
C FUNCTION.

```
C
      DIMENSION SPRA(20), CPRA(20), FIER(20), SESS(20), SESC(20)
      1  , SPRA1(20), CPRA1(20), FIER1(20), SESS1(20), SESC1(20)
      READ(5,5)NPLOTS
      5  FORMAT(I3)
      X1=15.
      X2=95.
      X3=175.
      Y1=15.
      Y2=110.
      Y3=140.
      Y4=235.
      CALL B1302
      DO 999 II=1,NPLOTS
      CALL DEVPAP(210.,297.,0)
      CALL WINDOW(2)
      CALL PENSEL(0,0.,0)
      CALL CHASIZ(2.,2.)
      CALL CHASWI(1)
      READ(5,10)ITERS
      ITERS=ITERS
      10  FORMAT(2I3)
      READ(5,15)(SPRA(I),I=1,ITERS)
      WRITE(6,88)(SPRA(I),I=1,ITERS)
      READ(5,15)(SESS(I),I=1,ITERS)
      WRITE(6,88)(SESS(I),I=1,ITERS)
      15  FORMAT(9E15.6)
      88  FORMAT(9E12.3)
      S=10.
      F=1.0E+4
      D=0.001
      U=0.001
      P=0.001
      R=0.001
      G=0.001
      H=0.001
      Q=10.
      A=0.001
      B=1.0E+4
      C=0.001
      FIER(1)=0.0
      DO 55 I=1,ITERS
      FIER(I+1)=FLOAT(I)
      55  CONTINUE
```



```

    ITERS1=ITERS-1
    DO 25 I=1,ITERS1
    SPRA1(I)=SPRA(I+1)
    SESS1(I)=SESS(I+1)
25  CONTINUE
    DO 37 I=1,ITERSS
    FIER1(I)=FIERS(I+1)
37  CONTINUE
    DO 20 I=1,ITERS
    IF(S.GT.SPRA(I)) S=SPRA(I)
    IF(F.GT.SESS(I)) F=SESS(I)
    IF(U.LT.SPRA(I)) U=SPRA(I)
    IF(A.LT.SESS(I)) A=SESS(I)
20  CONTINUE
    DO 45 I=1,ITERS1
    IF(P.LT.SPRA1(I)) P=SPRA1(I)
    IF(R.LT.SESS1(I)) R=SESS1(I)
45  CONTINUE
    IF(Q.LT.S) S=Q
    IF(A.GT.D) D=A
    IF(B.LT.F) F=B
    IF(C.GT.U) U=C
    IF(G.GT.P) P=G
    IF(H.GT.R) R=H
    SS=S-0.01*S
    DD=D+0.01*D
    UU=U+0.01*U
    FF=F-0.01*F
    PP=P+0.01*P
    RR=R+0.01*R
    WRITE(6,50)DD,FF
50  FORMAT(17HTHE VALUE OF DD= ,F12.6,17HTHE VALUE OF FF= ,F12.6)
    CALL AXIPDS(1,X1,Y3,80.,1)
    CALL AXIPDS(1,X1,Y3,95.,2)
    CALL AXISCA(1,ITERSS,0.0,FLOAT(ITERSS),1)
    CALL AXISCA(1,ITERSS,SS,UU,2)
    CALL AXIDRA(+2,+1,1)
    CALL MOVTO2(X1+30.,Y3-7.)
    CALL CHAHOL(15H*U ITERATIONS*. )
    CALL AXIDRA(+2,-1,2)
    CALL MOVTO2(X1-7.,Y3+40.)
    CALL ROTAT2(90.)
    CALL CHAHOL(17H*U VALUE OF PRA*. )
    CALL ROTAT2(-90.)
    CALL GRAPOL(FIERS,SPRA,ITERS)
    CALL GRASYM(FIERS,SPRA,ITERS,7,0)
    CALL AXIPDS(1,X2,Y3,80.,1)
    CALL AXIPDS(1,X2,Y3,95.,2)
    CALL AXISCA(1,ITERSS,0.0,FLOAT(ITERSS),1)
    CALL AXISCA(1,ITERSS,FF,DD,2)
    CALL AXIDRA(+2,+1,1)
    CALL MOVTO2(X2+30.,Y3-7.)
    CALL CHAHOL(15H*U ITERATIONS*. )
    CALL AXIDRA(+2,-1,2)
    CALL MOVTO2(X2-7.,Y3+40.)
    CALL ROTAT2(90.0)
    CALL CHAHOL(23H*U OBJECTIVE FUNCTION*. )
    CALL ROTAT2(-90.)
    CALL GRAPOL(FIERS,SESS,ITERS)
    CALL GRASYM(FIERS,SESS,ITERS,7,0)

```



```

CALL AXIPOS(1, X1, Y1, 80., 1)
CALL AXIPOS(1, X1, Y1, 95., 2)
CALL AXISCA(1, ITERSS, 0.0, FLOAT(ITERSS), 1)
CALL AXISCA(1, ITERSS, SS, PP, 2)
CALL AXIDRA(+2, +1, 1)
CALL MOVTO2(X1+30., Y1-7.)
CALL CHAHOL(15H*U ITERATIONS*. )
CALL AXIDRA(+2, -1, 2)
CALL MOVTO2(X1-7., Y1+40.)
CALL ROTAT2(90.)
CALL CHAHOL(17H*U VALUE OF PRA*. )
CALL ROTAT2(-90.)
CALL GRAPOL(FIERS1, SPRA1, ITESR1)
CALL GRASYM(FIERS1, SPRA1, ITESR1, 7, 0)
CALL AXIPOS(1, X2, Y1, 80., 1)
CALL AXIPOS(1, X2, Y1, 95., 2)
CALL AXISCA(1, ITERSS, 0.0, FLOAT(ITERSS), 1)
CALL AXISCA(1, ITERSS, FF, RR, 2)
CALL AXIDRA(+2, +1, 1)
CALL MOVTO2(X2+30., Y1-7.)
CALL CHAHOL(15H*U ITERATIONS*. )
CALL AXIDRA(+2, -1, 2)
CALL MOVTO2(X2-7., Y1+40.)
CALL ROTAT2(90.)
CALL CHAHOL(23H*U OBJECTIVE FUNCTION*. )
CALL ROTAT2(-90.)
CALL GRAPOL(FIERS1, SESS1, ITESR1)
CALL GRASYM(FIERS1, SESS1, ITESR1, 7, 0)
CALL MOVTO2(X3, Y1)
CALL LINTO2(X3, Y2)
CALL LINTO2(X1, Y2)
CALL MOVTO2(X3, Y3)
CALL LINTO2(X3, Y4)
CALL LINTO2(X1, Y4)
CALL MOVTO2(X1, Y3-8.)
CALL LINTO2(X1, Y2+7.)
CALL LINTO2(X3, Y2+7.)
CALL LINTO2(X3, Y3-8.)
CALL LINTO2(X1, Y3-8.)
CALL MOVTO2(X1+6., Y3-12.)
CALL CHAHOL('*U THE ABOVE TWO GRAPHS SHOW HOW THE VALUES OF*. ')
CALL CHAHOL('*U PRA AND OBJECTIVE FUNCTION*. ')
CALL MOVTO2(X1+6., Y3-15.)
CALL CHAHOL('*U VARY WITH THE NUMBER OF OVERALL ITERATIONS*. ')
CALL CHAHOL('*U WHILST THE LOWER TWO GRAPHS*. ')
CALL MOVTO2(X1+6., Y3-18.)
CALL CHAHOL('*U COMPARE THE PERFORMANCE OF CLASSICAL LEAST*. ')
CALL CHAHOL('*U SQUARES TECHNIQUE (AT ITERA-*. ')
CALL MOVTO2(X1+6., Y3-21.)
CALL CHAHOL('*U TION NO. 1) WITH THAT OF THE SMOOTHED LEAST*. ')
CALL CHAHOL('*U SQUARES TECHNIQUE*. ')
CALL MOVTO2(X3-40., Y4-10.)
CALL SYMBOL(7)
CALL CHAHOL('*U S/W APPROX. *. ')
CALL MOVTO2(X3-40., Y4-15.)
CALL SYMBOL(4)
CALL CHAHOL('*U CHEB APPROX. *. ')
CALL PICCLE
999 CONTINUE
CALL DEVEND
STOP
END

```


5.2 Program CHEB

C THIS PROGRAM PLOTS CHEBYCHEV-FORM UNCERTAINTY
C

```
      DIMENSION X(51),Y(51)
      CALL B1302
      CALL DEVPAP(170.0,120.0,0)
      CALL WINDOW(2)
      CALL PENSEL(0,0.,0)
      READ(5,25)N
25    FORMAT('READ NUMBER OF INPUT DATA',I3)
      DO 50 K=1,N
      READ(5,5)A,B,C,D,E,F
      5    FORMAT(6E15.6)
      WRITE(6,15)
15    FORMAT(4X,6H  TIME,8X,2HBB)
      T=0.0
      DO 20 I=1,51
      T00=1.0
      TOR=2.0/500.0*T-1.0
      T1=TOR
      T2=2.0*(TOR**2)-1.0
      T3=2.0*T2*TOR-T1
      T4=2.0*T3*TOR-T2
      T5=2.0*T4*TOR-T3
      BB=A*T00+B*T1+C*T2+D*T3+E*T4+F*T5
      X(I)=T
      Y(I)=BB
      WRITE(6,30)T,BB
30    FORMAT(F10.2,F15.8)
      T=T+10.
      20  CONTINUE
      CALL GRAF(X,Y,51,0)
      CALL PICCLE
      50  CONTINUE
      CALL DEVEND
      STOP
      END
```


5.3 Program SINE

C THIS PROGRAM PLOTS THE SINEWAVE-FORM UNCERTAINTY
C

```
      DIMENSION X(101),Y(101)
      CALL B1302
      READ(5,25)N
25    FORMAT(13)
      DO 50 K=1,N
      CALL DEVPAF(170.0,120.0,0)
      CALL WINDOW(2)
      CALL PENSEL(0,0.,0)
      READ(5,5)A,B,C,D
      5    FORMAT(4F15.8)
      WRITE(6,15)
15    FORMAT(4X,6H  TIME,8X,2HBB)
      T=0.0
      DO 20 I=1,101
      BB=A+B*SIN(C*T+D)
      X(I)=T
      Y(I)=BB
      WRITE(6,30)T,BB
      30    FORMAT(F10.2,F15.8)
      T=T+10.
      20    CONTINUE
      CALL GRAF(X,Y,101,0)
      CALL PICCLE
      50    CONTINUE
      CALL DEVEND
      STOP
      END
```

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