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The Use of a Partially Simulated Exothermic Reactor to Test Nonlinear Algorithms

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Abstract−Two nonlinear control algorithms for controlling nonlinear systems include the receding horizon method and the nonlinear neural network inverse model methods. These methods have been found to be useful in dealing with difficult-to-control nonlinear systems, especially in simulated systems. However although much simulation work has been performed with these methods, simulation only is inadequate to guarantee that these algorithms could be successfully implemented in real plants. For this reason, a relatively low cost and simple online experimental configuration of a partially simulated continuous reactor has been devised which allows for the realistic testing of a wide range of nonlinear estimation and control techniques i.e. receding horizon control and neural network inverse model control methods. The results show that these methods are viable and attractive nonlinear methods for real-time application in chemical reactor systems.

Key words: Process Control, Nonlinear Methods, Receding Horizon, Neural Network, Simulated Reactor

INTRODUCTION

In practice, most systems encountered in the real world are to some extent nonlinear and in many of the control applications, nonlinear models are required to provide acceptable controls. In reality modelling and identification of nonlinear system is much more complex and difficult to obtain when compared to linear systems. This difficulty has limited the usage of nonlinear models to regions and systems where the model obtained is reliable. However in recent years many different techniques involving nonlinear control methodology have been proposed [Bequette, 1991]. Two such advanced control algorithms include the nonlinear receding horizon method, which is a model-based strategy and the other is the neural-network inverse-model based method, which is an input-output data based strategy. The receding horizon method is basically an extension of the open-loop optimal method. It incorporates plant nonlinearities, feedback and an end-point constraint while computing a control trajectory in time. While in the neural-network-based technique, the inverse neural network model acts as the controller in a one-step implementation action. The inverse model is obtained from using the input-output data of the plant or model of the system. Details of these two techniques will be given in later sections.

Both these techniques have been applied by other researchers in many simulation studies [Kershenbaum, 1993; Mayne, 1995; Hunt, 1992; Nahas, 1992] but since real plants do not behave in exactly the same manner as their models, the real performance and stability tests of any control strategy must include some plant-model mismatch. This can be introduced by subjecting these algorithms and methods to an actual plant. In fact plant/model mismatch and disturbances are inherently present in the real system. These control algorithms would only be useful for industrial applications if proven successful in these real plants. However before applying them in the industrial scale plants, they are normally tested in pilot plants, which is the common, safe and economical approach for testing new and advanced methods such as these. In fact up-to-date no other applications utilising any of these two techniques have been reported on a real reactor system, whether in a pilot-plant or an industrial plant [Hussain, 1999]. This paper presents an experimental investigation concerning the utilisation of these two techniques on a partially simulated pilot-plant reactor (PARSEX) system for controlling its temperature. Studies were made for set point tracking as well as for disturbance rejection cases under plant-model mismatches, as will be reported in the next few sections.

PILOT PLANT-PARTIALLY SIMULATED REACTOR SYSTEM

The PARSEX (Partially Simulated Exothermic Reactor) is a relatively low-cost, simple on-line experimental configuration, which approximates an exothermic reaction taking place in a batch or continuous reactor, as can be seen in Fig. 1 [Kershenbaum, 1994]. This plant has been devised for testing the performance of various nonlinear estimation and control algorithms. It basically consists of two main units: a continuous well-stirred reactor of approximate volume of 0.1 m^3 and a separate cooler section with approximately 0.7 m^2 of heat transfer area. The reactor is charged with water which represents the liquid reactants in this PARSEX system. Heat within these reactants is exchanged with the cooling medium by pumping the reactants through the external cooler via pump, M6 before being recycled into the reactor again. The cooler is provided with good circulation of cooling water by the pump, M10 and fresh

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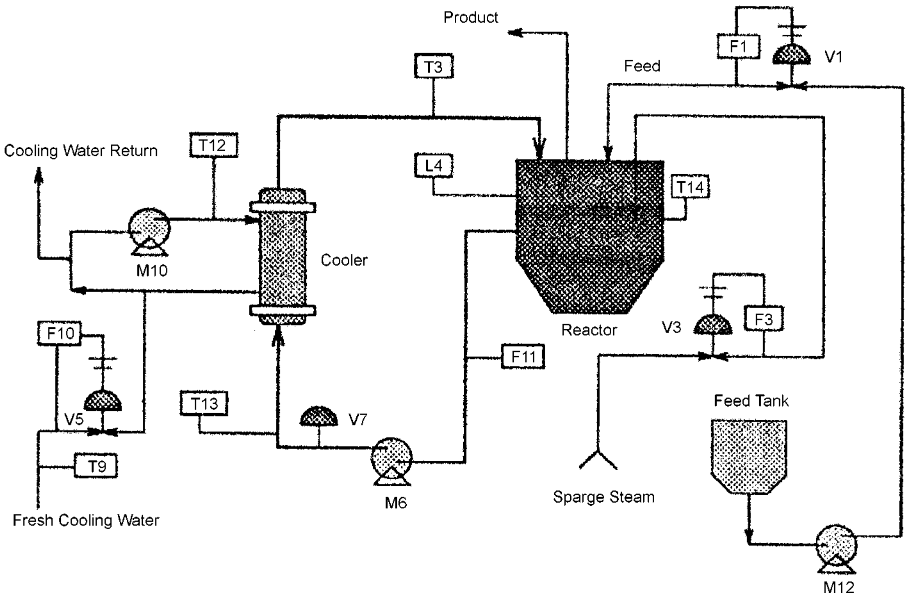

Fig. 1. Diagram of the PARSEX reactor.

make up water from the main water supply system. The feed to the reactor is pumped into the reactor from the feed tank through the pump M9. This feed flow is measured by the flowmeter F1 and controlled by the control valve V1. The temperature of the reactor, measured by detector T14 is regulated by the cooling water temperature, measured by detector T12. This cooling water temperature is manipulated by the fresh make-up cooling water flow, measured by flowmeter F10 and controlled by the control valve V5. The "reaction" is simulated by solving the relevant dynamic mass balance equations for the system. The concentration of reactant in the reactor denoted by C3 is a 'simulated' value obtained from solving these dynamic equations. The simulation also calculates the amount of heat liberated by the "reaction" as a function of time. An appropriate amount of steam is then sparged into the reactor, which is measured by flowmeter F3 and controlled by the control valve V3. Many exothermic reactions can be experimentally simulated quite realistically in this way and the effect of this operation is to achieve close resemblance in the pilot plant to the real reactor with true reactions. The controllers for all these control valves are "software-driven" by the Paragon data acqusition and

Table 1. Physical properties and process data for the reactor

U_r=68.0 kcal/(min·m^2 °C)	k_0=3.64∗10^6 min^{-1}
A_r=0.7 m^2	ΔH=8000.0 kcal/k·mol
V_r=0.24 m^3	E/R= 6000.0 °K^{-1}
C_{pr}=C_{pj} kcal/(kg^3 °C)	F=0.0036 m^3/min
C_{pj}=1.0 kcal/(kg·°C)	V_j=0.012 m^3
ρ_r=ρ_j kg/m^3	τ_j=1.1 min
ρ_j=1000.0 kg/m^3	T_{cw}=293.15 K (20 °C)
Initial Steady State Condition	
$C_a(0)$=5.364 kmol/m^3	$T_r(0)$=333.15 K (60 °C)
C_{ao}=25.0 kmol/m^3	T_{rsp}=333.15 K (60 °C)
T_{fo}=300.15 K (23 °C)	$T_j(0)$=324.15 K (51 °C)

control system. The process data for the reactor can be seen in Table 1. The model equations relating to the reactor can be seen in the Appendix.

The information flow for the reactor/computer interaction is shown in Fig. 2. The Paragon 550 Software (Intec Controls Corporation) manages the data acquisition and conventional PID control of slave loops. At a high frequency (typically every 2 seconds),

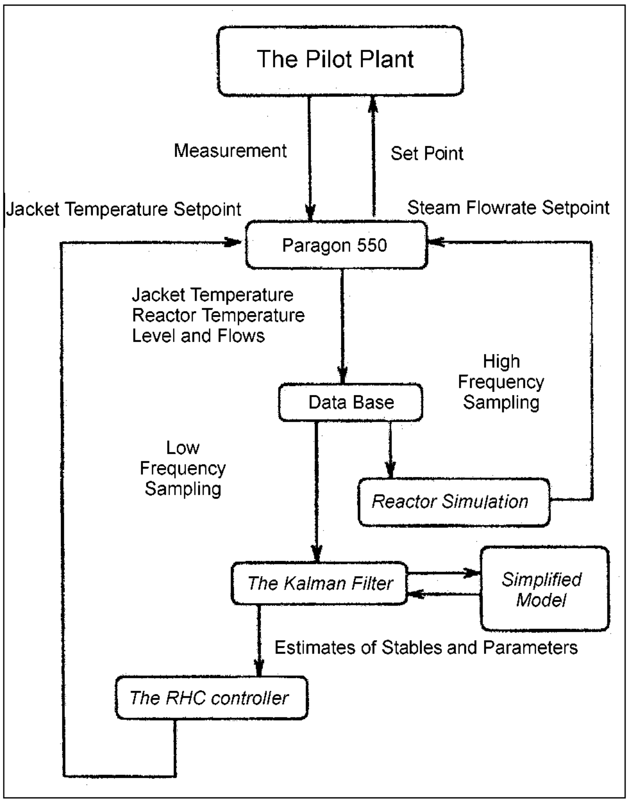

Fig. 2. Information flowchart of the experimental study.

measurements of the reactor temperature, level, and flowrates are sent to a reactor simulation programme. Although there are no real chemical reactions occurring in the reactor, any desired reaction processes with or without assumptions of perfect mixing, constant temperature, etc. can be simulated by solution of the dynamic material balance equations in real time, given the actual measurements of inlet and outlet flowrates, reactor level and temperatures and suitable rate expressions for the simulated reactions. Then, given knowledge of the heats of reaction for the simulated reactions, the amount of heat released by reaction can be calculated and converted to a desired flow rate of sparge steam which is controlled by the steam control valve (V3). Finally, at a lower frequency (typically every 6-12 seconds), the control and estimation algorithms being tested calculate the desired set point of the jacket temperature and/or the required cooling water flow rate and this information is passed back to the PARSEX reactor. Clearly, the PARSEX configuration can be used to test a wide range of control and estimation algorithms and the size of the equipment can be altered to suit individual requirements. In this work, we demonstrate the application of receding horizon control and neural-network-inverse-model based control on the reactor.

THEORETICAL DESCRIPTION

1. Receding Horizon Control

The idea of a Receding Horizon Control algorithm has been known for a long time. The basic concept of the RHC control design is to compute a control trajectory for a whole horizon time minimising a cost function of a plant subject to a dynamic plant model incorporating plant nonlinearities, and an end point constraint. The initial value of control is then applied to the plant. Some feedback is provided by measurements/estimates of state at the next interval and repeating the calculation [Mayne and Michalska, 1990; Kershenbaum et al., 1993].

As in several model-based controllers, RHC requires the measurement or estimation of the states of an appropriate process model. However, in most industrial processes, the state variables are not all measurable or not with sufficient accuracy for control purposes. Furthermore measurements that are available often contain significant amounts of random noise and systematic errors. In these situations, online estimation techniques have been applied to estimate the state variables. Sequential estimation techniques such as the extended kalman filter (EKF) produce estimates of true process values from noisy process measurement and suitable process models. They can also be easily incorporated into the RHC technique to cater for plant/model mismatches, as demonstrated in this work [Maybeck, 1982].

The basic concept of a receding horizon control algorithm is that the whole future control actions of the receding horizon control (RHC) algorithm are calculated from an optimal control problem including the current measurements, cost function, model parameters and constraints of states and controls. However, only the first element of control is applied to the system. Then, states are measured or estimated and used as initial conditions in order to recalculate the future controls by resolving the optimal control problem [Kwon, 1977; Biegler, 1993].

Typically, the optimal control problem can be given by a cost function (Performance Index):

$$\min \int_0^{\tau_f} W_1 (T_r - T_r^{sp})^2 d\tau \tag{1}$$

where W_1 is a weighting factor, subject to a final state constraint [$Tr(\tau_f)=Tr^{sp}$] and the system equations (state constraints), as taken from the Appendix i.e.

$$\frac{dT_{rm}}{dt} = \frac{Q_r}{\rho_r C_{pr} V_r} + \frac{F}{V_r}(T_f - T_{rm}) + \frac{U_r {*} Ar {*} (T_{jm} - T_{rm})}{\rho_r C_{pr} V_r} \tag{2}$$

$$\frac{dC_a}{dt} = -R_1 + \frac{F}{V_r}(C_{ao} - C_a) \tag{3}$$

The meanings of these symbols can be seen in the nomenclature. The model Eqs. (2) and (3) are obtained with standard assumptions such as perfect mixing and no heat lost, which are not neccessarily valid in an experimental system. Here, standard variational optimal control techniques are used to calculate U(t).

Since, in most processes, the state variables required for model-based controller implementation are not all measurable or, not with sufficient accuracy for control purposes, state estimation techniques have been utilised as well. In addition, it is possible to include uncertain model parameters such as the heat transfer coefficient and the rate constant within the state vector and estimate these along with the measured temperature, T_r and unmeasured concentration, C_a.

Fig. 3. illustrates the flowchart of the RHC with the EKF approach. As we see from the RHC algorithm, a set of control actions is determined on-line based on current states. Only the first element of control is applied to the system; the control action at time k+1 is the control $T_{jm}(1)$ of future controls calculated at time k. Some feedback is obtained by measurements of state at the next interval and repeating the calculation. The inclusion of the EKF is for estimating the unmeasured state, C_a, and unknown parameters,

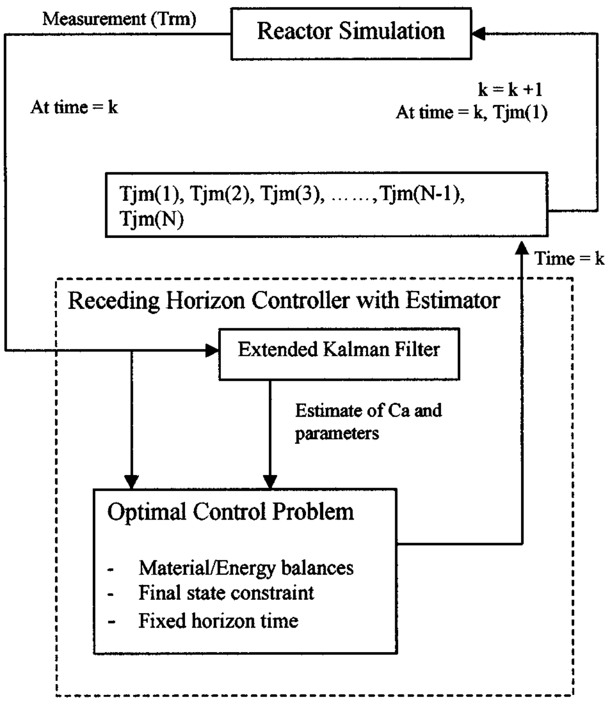

Fig. 3. Flowchart of the RHC with the EKF approach.

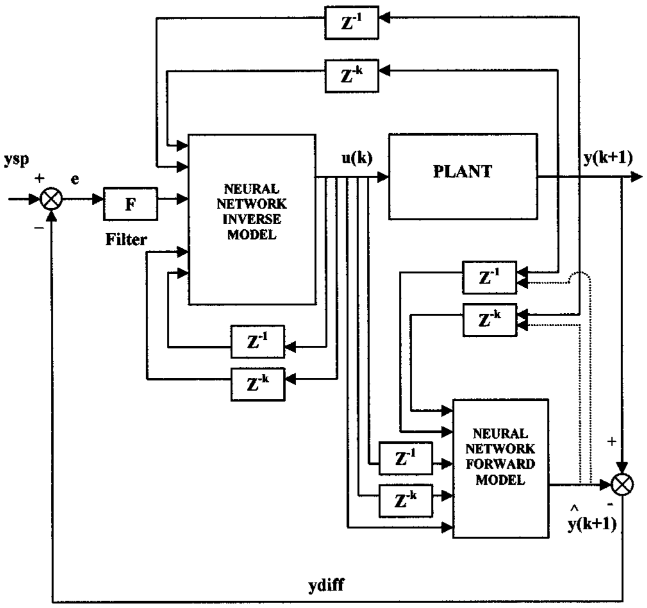

Fig. 4. Implementation diagram of neural-network based IMC strategy.

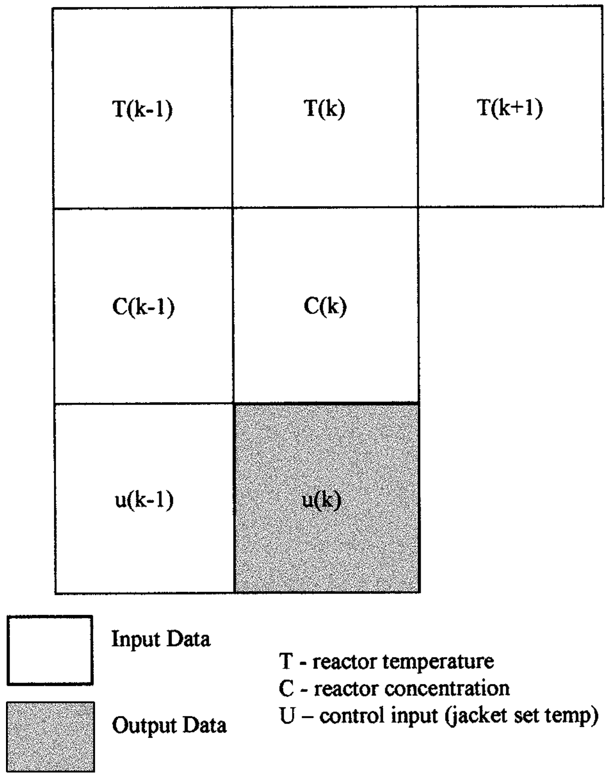

Fig. 5. Input-output pattern for the neural network inverse model.

the heat transfer coefficient and the rate constant, using the available measurement of T_r. Measurements and estimates are compared to a set point or predicted value. As a result, the error between the measurements and set point or predicted value caused by plant/model mismatch or disturbances can be utilised within the RHC algorithm. The RHC algorithm, then, produces the future controls which minimise this error based on the updated model parameters.

2. Neural-Network Inverse-Model Based Method

A robust and stable control strategy incorporating neural network is that of the nonlinear internal model control technique, which is basically an extension of the linear IMC method [Economou, 1986]. In this method both the forward and inverse models, as seen in Fig. 4 are used directly as elements within the feedback loop. In this case the neural network, acting as the controller, has to learn to supply at its output, the appropriate control parameters, u for the desired target, y_{sp} at its input. In this implementation u represents the jacket temperature, T_{jm} and the y is represented by the reactor temperature, T_m. The network inverse model is then utilised in the control strategy by simply cascading it with the controlled system or plant as seen in Fig. 4. In this control scheme the desired set point, ysp acts as the desired output temperature which is fed to the network together with the past values of inputs T_{jm} and outputs T_m and C_a respectively to predict the desired current plant input i.e current value of T_{jm}. The input output pattern for the inverse model in this implementation can be seen in Fig. 5. Further to this, the forward model placed in parallel with the plant, to cater for plant/model mismatches and in addition the error between the plant output and the neural net forward model is subtracted from the set point before being fed into the inverse model. In this case the forward model is fed with the current value of T_{jm} and the past values of T_{jm}, T_m and C_a respectively. The forward model can also be fed with its past outputs instead of the plant outputs, especially in cases of noisy plant output data (as seen from the dotted line of Fig. 4). A filter, F is introduced prior to the controller in this approach to incorporate robustness in the feedback system (especially where it is difficult to get exact inverse models) and also to project the error signal into the appropriate input space of the controller.

Other variations to this approach such as adding delay elements instead of the forward model (called dual neural net controller or direct network controller) and having a backup neural net in parallel with the neural net controller for online training and control refinement have also been discussed in the literature [Psichogios, 1991; Pao, 1992; Hunt, 1992]. In many of the cases, presented in the literature using this approach, the necessary control signals, u is computed by numerically inverting the neural network forward model at each interval by Newton's method or substitution methods based on the contraction mapping theorem. The first derivative with respect to the control input can be computed in these techniques by the usual bakpropagation method. These numerical techniques are however computationally intensive and time-consuming, they are very sensitive to the initial estimates and may not neccessarily give the global and unique solution. Hence they are not suitable for online implementation. For online implementation as in our study, we utilise the output of the offline trained inverse neural network model directly as the control signal, which has fast action and suitable for real life application such as described in this work.

EXPERIMENTAL STUDIES ON THE PARSEX REACTOR

1. Receding Horizon Control Implementation

The aim of this experimental work is to test the receding hori-

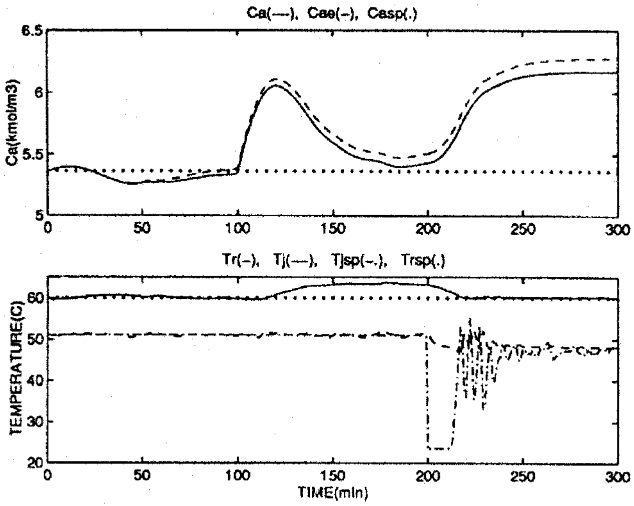

Fig. 6. Response of the RHC (nominal case).

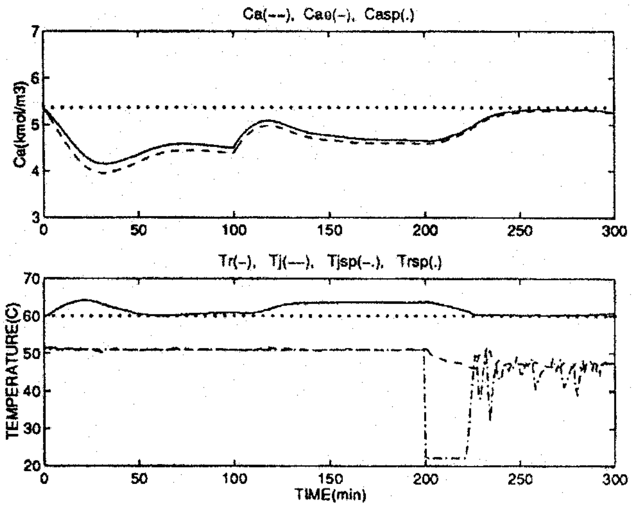

Fig. 8. Response of the RHC (mismatch in rate constant).

zon control algorithm performance on the PARSEX reactor. The experimental case study involves set point tracking under the disturbance of feed flow rate and parameter changes. In all the cases below, a 25% increase in feed flowrate was introduced at time 100 minutes and the control action initiated at time 200 minutes.

In reality, neither the parameters nor the true process model are known exactly. Therefore, the experimental results already include the effects of plant/model mismatch. The experimental results for a nominal case of the RHC controller with estimator and a corresponding PID controller are presented in Figs. 6 and 7 respectively. Fig. 6 shows that the RHC controller with estimator is able to provide good control response. This is because the EKF can give a good estimate of the reactant concentration. This estimated reactant concentration together with measured variables are used in the receding horizon control algorithm to determine the jacket temperature which can regulate the reactor temperature to the desired setpoint.

On the other hand, although the PID controller can control the reactor temperature at the desired setpoint, it provides control action which is rather noisy and the reactor temperature oscillates around the setpoint (Fig. 7). Without any special tuning, the receding horizon control gives the control action with less drastic control action than that of the PID controller.

Next, the RHC controller with the EKF is tested in a case where the true rate of reaction has been increased by 25%. It can be seen that the EKF can accommodate the mismatch and give good estimates of Ca as shown in Fig. 8. With these estimates, the RHC controller can control the reactor temperature to its set point and maintain it throughout the experiment.

Finally, the RHC controller with the EKF is tested in a case where the assumed value of the heat transfer coefficient has been decreased by 50%. It can be seen that the RHC controller with the EKF is still able to drive the reactor temperature to its set point. Then, it can control the reactor temperature at the set point throughout the experiment. In addition, this experimental result shows that the EKF can accommodate the mismatch and give good estimates of C_a as shown in Fig. 9.

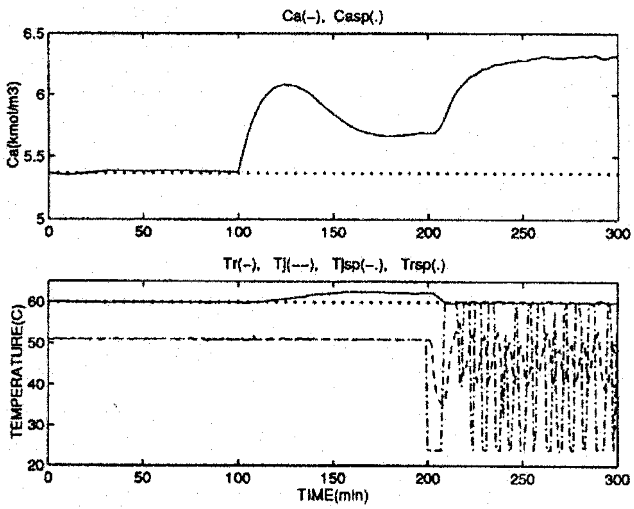

Fig. 7. Response of the PID (nominal case).

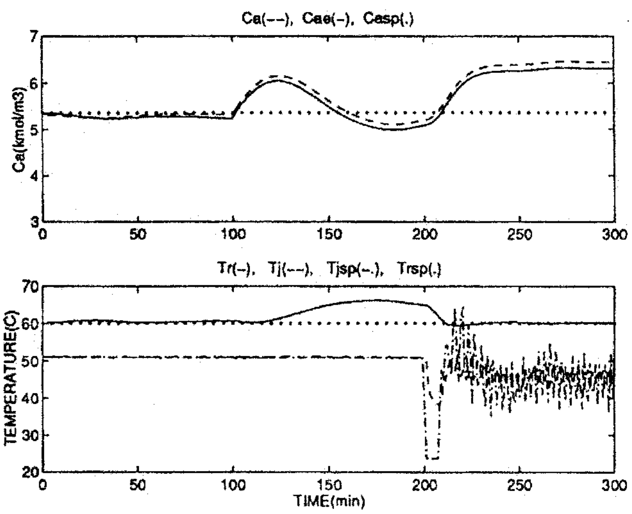

Fig. 9. Response of the RHC (mismatch in heat transfer coefficient).

2. Neural Network Inverse Model Based Implementation

In order to implement the neural-network method online, open loop testing was performed on the PARSEX reactor to generate the relevant data for training the forward and inverse model repectively. The open loop data was generated by varying the control input signal i.e. the cooling water jacket temperature set point, in various step sequences and then observing and recording the effect on the reactor temperature and concentration. The neural network models were trained by use of the backpropagation technique with adaptive learning rate. Various training and test data sets were used in validating the accuracy of the neural network utilised in the control strategy. The details of these methods and the neural network training can be found in Hussain [1996]. The forward and inverse models obtained from the training above were then implemented in the IMC strategy for performing set-point tracking and disturbance-rejection studies on the PARSEX reactor. These control implementations are discussed below: -

2-1. Set Point Tracking

The set point tracking experiment was done with step down in the required reactor temperature, to 42 °C, and step up, to 53 °C from the initial steady state temperature of 47 °C. A tuning filter value of 0.85 was used in this implementation. Each time step represents the concurrent data acquisition and control implementation sampling time of 6 secs. The experimental results obtained in this case can be seen in Fig. 10 The results overall showed that the reactor temperature could track the set point profile reasonably well even under the nonideal experimental conditions. However other observations seen from these results are as follows: -

(1) Offsets in the range 0.5-1.1 °C were observed at all set points and they were biggest at the highest and lowest set point values. These offsets were mainly due to the offset in the control prediction as given by the neural network controller, which depended on the accuracy of the trained inverse model offline.

(2) At the nominal set point value (of about 47 °C) in the beginning and middle of tracking, the jacket temperature could not reach its set point temperature due to the saturation of the valve, V5 and the fact that the jacket temperature cannot go higher than the reactor temperature in practice. However this high jacket temperature set point value of over 47 °C, set by the neural-network controller, enabled the jacket temperature to reach close to the value of 45 °C. This enabled the reactor temperature to keep close to the nominal set point, with small offsets.

(3) The set point tracking action was fast when stepping down but sluggish when stepping up. This is basically due to saturation of the control valve, V5 (controlling the temperature of the cooling water) at these lower set-point values, as seen in the valve % opening graph of Fig. 10. This speed of tracking in the response basically follows that of the jacket cooling water temperature in tracking the jacket set point temperature, as expected. This sluggishness however would not have happen if dual configuration for controlling the reactor temperature were available in the system: cooling water for cooling and hot water/steam for heating purposes.

2-2. Set Point Regulation under Plant/Model Mismatch Cases - Increase in ΔH

In this case study, the disturbance represents an internal disturbance in the form of plant/model mismatch introduced by an increase in the heat of reaction ΔH by 10% to 115558 kcal/min. This change was introduced by changing the relevant parameter within the reactor program, which re-calculates the amount of heat generated and hence the amount of steam injected into the system. At this instant also the controller action i.e jacket set point temperature, was frozen to its latest value (47.5 °C), which is the value prior to the introduction of the disturbance at the 300th time step. The system was then operated under open-loop control until the 900th time step. The increase in ΔH at the 300th time step, caused the reactor temperature to rise to another steady state temperature of about 50.7 °C. When the controller was initiated again at the 900th time step, the neural network controller immediately acted to reduce the jacket set point temperature and hence the reactor temperature to its initial nominal value. When the reactor temperature reached below its set point value at the 1040 time step the control action increased again to bring the reactor temperature back close to its steady state value at the 1300th time step. The result

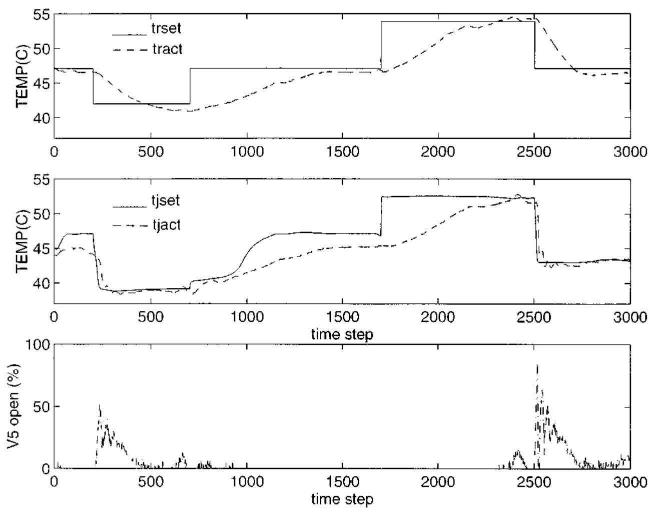

Fig. 10. Set point tracking - Neural Network inverse-model application.

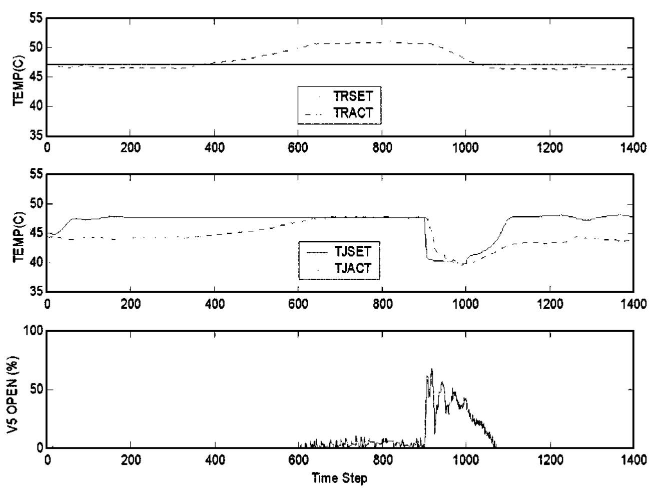

Fig. 11. Set point regulation with plant/model mismatch - Neural Network inverse-model application.

can be seen in Fig. 11.

CONCLUSION

The experimental results have clearly shown the effectiveness of these nonlinear control algorithms under the inherent presence of plant/model mismatches. The PARSEX reactor can be stabilised by the RHC controller with EKF in the presence of disturbances, plant/model mismatch and uncertainties. It gave better results than the conventional PID method which had nosiy responses. In the neural-network method, set point tracking and regulation under plant/model mismatch was achieved equally well with slight offsets in the responses. The PARSEX reactor can also complement simulation studies and lend credence to tests of proposed new and advanced control algorithms. However further tests on robustness will have to be carried out before such algorithms are implemented on the industrial scale.

Appendix: Model Equations for the Continuous Reactor

The reaction used by Limqueco et al. [1990] has been studied here. Some of the physical and model parameters in that work (specifically, the reactor volume, the heat transfer coefficient and the heat exchange area) have been modified to match those of the available experimental reactor. The system assumes a first order, irreversible reaction, A→B, occurring in the continuous reactor.

$$\frac{dC_a}{dt}=-R_1+\frac{F}{V_r}(C_{ao}-C_a) \tag{4}$$

$$\frac{dT_{jm}}{dt}=\frac{F_j}{V_j}(T_{cw}-T_{jm})-\frac{U_r*A_r*(T_{jm}-T_{rm})}{\rho_j C_{pj} V_j} \tag{5}$$

$$\frac{dT_{rm}}{dt}=\frac{Q_r}{\rho_r C_{pr} V_r}+\frac{F}{V_r}(T_f-T_{rm})+\frac{U_r*A_r*(T_{jm}-T_{rm})}{\rho_r C_{pr} V_r} \tag{6}$$

where

$$R_1=k_0\exp\left(\frac{-E}{RT_{rm}}\right)C_a$$

$$Q_r=(-\Delta H)R_1V_r$$

Note: The solution of these equations is required in order to calculate the amount of steam to be injected. Table 1 gives the physical properties and process data for the reactor.

NOMENCLATURE

A : component "A"
A_r : heat transfer area [m^2]
C_a : reactant concentration [mol/m^3]
C_{ao} : nominal feed concentration [mol/m^3]
C_p : specific heat capacity [Kcal/kg·K]
E : activation energy [J/mol]
F : volumetric flowrate [m^3/min]
F_j : jacket flowrate
ΔH : heat of reaction [Kcal/K·mol]
k_0 : Arrhenius pre-exponential constant [min^{-1}]
R : universal gas constant [J/mol·K]
t : time
T_{rm} : measured reactor temperature [K]
T_{jm} : measured jacket temperature [K]
T_{cw} : feed cooling water temperature [K]
T_f : feed temperature [K]
U_r : heat transfer coefficient [Kcal/min·m^2·K]
V_r : volume of reactor [m^3]

Greek Letters

ρ : reactant density [kg/m^3]
τ : time constant [min]

Subscripts

a : component "A"
c : cooling water
f : feed condition
o : initial condition or nominal condition
sp : set point
r : reactor
j : jacket

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