PRACTICAL MODELLING AND CONTROL IMPLEMENTATION STUDIES ON A pH NEUTRALIZATION PROCESS PILOT PLANT

A thesis submitted for the degree of Doctor of Philosophy

By

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March 2008

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To My Beloved Wife,

Nurlidia Mansor

And My Lovely Princesses

> Nur Azra Adli Nur Auni Adli Nur Ahna Adli

ABSTRACT

In recent years the industrial application of advanced control techniques for the process industries has become more demanding, mainly due to the increasing complexity of the processes themselves as well as to enhanced requirements in terms of product quality and environmental factors. Therefore the process industries require more reliable, accurate, robust, efficient and flexible control systems for the operation of process plant. In order to fulfil the above requirements there is a continuing need for research on improved forms of control. There is also a need, for a variety of purposes including control system design, for improved process models to represent the types of plant commonly used in industry.

Advanced technology has had a significant impact on industrial control engineering. The new trend in terms of advanced control technology is increasingly towards the use of a control approach known as an "intelligent" control strategy. Intelligent control can be described as a control approach or solution that tries to imitate important characteristics of the human way of thinking, especially in terms of decision making processes and uncertainty. It is also a term that is commonly used to describe most forms of control systems that are based on artificial neural networks or fuzzy logic.

The first aspect of the research described in the thesis concerns the development of a mathematical model of a specific chemical process, a pH neutralization process. It was intended that this model would then provide an opportunity for the development, implementation, testing and evaluation of an advanced form of controller. It was also intended that this controller should be consistent in form with the generally accepted definition of an "intelligent" controller. The research has been based entirely around a specific pH neutralization process pilot plant installed at the University Teknologi Petronas, in Malaysia. The main feature of interest in this pilot plant is that it was built using instrumentation and actuators that are currently used in the process industries. The dynamic model of the pilot plant has been compared in detail with the results of experiments on the plant itself and the model has been assessed in terms of its suitability for the intended control system design application.

The second stage of this research concerns the implementation and testing of advanced forms of controller on the pH neutralization pilot plant. The research was also concerned with the feasibility of using a feedback/feedforward control structure for the pH neutralization process application. Thus the study has utilised this control scheme as a backbone of the overall control structure. The main advantage of this structure is that it provides two important control actions, with the feedback control scheme reacting to unmeasured disturbances and the feedforward control scheme reacting immediately to any measured disturbance and set-point changes. A non-model-based form of controller algorithm involving fuzzy logic has been developed within the context of this combined feedforward and feedback control structure.

The fuzzy logic controller with the feedback/feedforward control approach was implemented and a wide range of tests and experiments were carried out successfully on the pilot plant with this type of controller installed. Results from this feedback/feedforward control structure are extremely encouraging and the controlled responses of the plant with the fuzzy logic controller show interesting characteristics. Results obtained from tests of these closed-loop system configurations involving the real pilot plant are broadly similar to results found using computer-based simulation. Due to limitations in terms of access to the pilot plant the investigation of the feedback/feedforward control scheme with other type of controllers such as Proportional plus Integral (PI) controller could not be implemented. However, extensive computer-based simulation work was carried out using the same control scheme with PI controller and the control performances are also encouraging.

The emphasis on implementation of advanced forms of control with a feedback/feedforward control scheme and the use of the pilot plant in these investigations are important aspects of the work and it is hoped that the favourable outcome of this research activity may contribute in some way to reducing the gap between theory and practice in the process control field.

ACKNOWLEDGEMENT

I would like to express my deepest appreciation to my supervisor, Professor David J. Murray-Smith for his admirable way of supervising the work, invaluable guidance, assistance and support throughout this research.

My special gratitude goes to my sponsor, Universiti Teknologi Petronas, Malaysia for giving me the opportunity and the scholarship for my studies. I would also wish to extend my thanks to Universiti Teknologi Petronas for allowing access to the pilot plant facilities for experimental investigations and the financial support in carrying out this research, especially the investment on the new system.

I would also want to acknowledge the funding provided by the Department of Electronics and Electrical Engineering, University of Glasgow, in support of conference attendance and aspects of the experimental work carried out at Universiti Teknologi Petronas.

An extended acknowledgment to Azhar Zainal Abidin for his assistance during my experimental work at the laboratory and also to PCA Automation for their technical support during installation of the new system.

My special thanks go to my beloved parents for their endless encouragement and prayers throughout the educational years of my life. To my wife and my lovely daughters, thank you very much for all their patience, understanding and priceless sacrifices.

Last but not least, 'Terima Kasih' to all my fellow friends and colleagues for their continuous encouragement especially to my badminton mates and Glasgow University's Badminton Club for providing a stress release session every week.

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ABBREVIATIONS

UTP	Universiti Teknologi Petronas
MPC	Model Predictive Control
FLC	Fuzzy Logic Control
PID	Proportional plus Integral plus Derivative
PI	Proportional plus Integral
LMPC	Linear Model Predictive Control
NMPC	Nonlinear Model Predictive Control
NGPC	Neural Generalised Predictive Control
DCS	Distributed Control System
XPC	Industrial Personal Computer
CSTR	Continuous Stirred Tank Reactor
H_2SO_4	Sulphuric Acid
NaOH	Sodium Hydrochloride
NN	Neural Network
TIC	Theil's Inequality Coefficient

CHAPTER ONE

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1.0 INTRODUCTION

The technology used within the process industries has changed rapidly in recent years as plant processes have become more and more complex. These changes are due to the increasing need for better product quality and requirements for minimisation of operating costs, including those associated with energy usage. As a result, significant new constraints have emerged which reflect directly on plant process technology. Another important factor that contributes to the development of process industry technology arises from environmental legislation which not only puts significant demands on the process industries but is also constantly being revised.

The capability and availability of new and modern hardware and software also plays an important role in this advancement of technology within the process industries. Previous researchers have had problems such as signal transmission delays, relatively low processing power for computational needs, and poor signal to noise ratios. However, with the new technology in instrumentation and measurement, for example, more accurate and precise data can be provided. Besides that, the introduction of modern computers with vastly increased processing power and improved networking capabilities also offers much better solutions in terms of speed and capacity. Thus researchers and process control developers in industry utilise these new hardware and software capabilities to improve the available technology and also introduce new and interesting developments in terms of control.

Generally, developments in classical control system technology have been based on linear theory, which is a well proven and generally successful approach when applied to process systems. Although all physical systems are nonlinear to some extent, some systems can be approximated in a very satisfactory fashion using linear relationships. However, certain types of chemical systems or processes have highly nonlinear characteristics due to the reaction kinetics involved and the associated thermodynamic relationships. In these circumstances, conventional linear controllers no longer provide adequate and achievable control performance over the whole operating range. Thus, designing a nonlinear controller which is robust in terms of its performance for different operating conditions is essential. There is also increasing interest in the potential of "intelligent" control methods for process applications. Intelligent control can be described as a control approach or solution that tries to imitate important characteristics of the human way of thinking, especially in terms of decision making processes and uncertainty. It is also a term that is commonly used to describe most forms of control systems that are based on artificial neural networks or fuzzy logic. The central theme of this research concerns problems of system modelling, control system development, implementation and testing for a specific application which involves a pH neutralization process. The control of a pH neutralization process presents a significant challenge due to the time-varying and highly nonlinear dynamic characteristics of the process.

In general terms this research study can be divided into two main activities. The first of these involves pH process model development, together with internal verification and external validation of the associated simulation model from test data obtained from open-loop and simple closed-loop tests carried out on the actual plant.

The second activity involves controller design and development, including preliminary controller evaluation using simulation and, finally, implementation and testing on a pH neutralization pilot plant. The key objective has been to develop an advanced control strategy that can provide accurate, efficient and flexible operation of the particular pilot process plant around which the project was based. Besides that, the work involves investigation of issues such as robustness, stability, implementation and overall performance optimisation.

1.1 Research Overview

This research project involves collaboration between the University of Glasgow, in the United Kingdom and the Universiti Teknologi Petronas (UTP) in Malaysia. This research is based upon a pH neutralization pilot plant which is installed at the Plant Process Control Laboratory, in UTP. Typically, pH neutralization plant can be found in a wide range of industries such as wastewater treatment, oil and gas and petrochemicals. It is a known fact that a pH process plant of this kind is very difficult to model and control. This is due to its highly nonlinear and time varying dynamic process characteristics. Research based on this pilot plant should provide new insight of value for other complex process applications involving highly nonlinear systems.

1.1.1 Problem Identification

Effective modelling of a pH neutralization plant is not a recent issue. However, due to the nonlinear characteristics and complexity of this type of system, research on how to provide a good dynamic model of a pH neutralization process, which was first started in the 1970s or earlier, still continues. Thus one of the first main issues faced in this research was the fact that currently available models for pH neutralization processes did not appear to be an adequate representation of the type of pH neutralization plant used in industry and could not be applied to the pilot plant at UTP without modification.

The second problem that has driven this research is the "*poor control performance*" which has been demonstrated by current control strategies. As described in the previous section, the major problems that contribute to unacceptable and inadequate control performance can be summarised as follows:-

- i. Increases in plant complexity and strict constraints in terms of environmental and other performance requirements present a significant challenge in applications such as pH neutralization.
- ii. The inherent and severe nonlinearity of a pH neutralization process is a major source of difficulty in terms of robust and stable control system design.

1.1.2 Research Objectives

There are two main objectives in this research. The first aim is to provide an adequate dynamic nonlinear pH neutralization model, based on physical and chemical principles that can represent the real pH neutralization plant available at UTP. The second goal for this research is to design, develop and implement an "intelligent" and advanced form of controller. The research work for the second objective mainly concerns the use of a combined feedback/feedforward system as an overall control structure and the implementation and testing of fuzzy logic controllers within that type of control scheme. The study focuses on the pH neutralization process but some aspects of the work have relevance for other process applications. Another aim is to investigate benefits and limitations of this type of control algorithm and the type of process model developed during this investigation.

1.1.3 Significance of the Research

As stated above, the research utilises the specific pH neutralization pilot plant at UTP. This pilot plant is based around the type of industrial instrumentation, measurement and actuation systems used within the process industries. Unlike some other laboratory test-bed neutralization reactor systems, measurement noise, time delays and control valve characteristics typical of full-scale industrial plant of this kind are well captured in the dynamic response of the pilot plant. Thus, the dynamic characteristics of the experimental system are believed to be representative of an actual pH neutralization plant used in industry.

Investigation and evaluation of the performance (e.g. accuracy, dynamic response etc.) of a developed simulation model of the pilot plant and detailed comparisons between the developed model and the plant behaviour has been an important feature of this research. Therefore, it is hoped that one outcome of this research should be the provision of a more reliable and more practical model for pH neutralization processes having a generic form that could be of some general value for industrial plant of this type.

It is hoped that the research work could also provide a significant impact in terms of the development of intelligent or advanced controllers for plant process control applications, especially in terms of the Fuzzy Logic Control approach. Indirectly, a further aim of this research is to try to provide additional insight regarding issues such as control performance, stability and robustness in an application of this specific kind, so that engineers in industry may feel more confident about the use of this flexible new industrial intelligent control technology. In this way it is hoped that the work may, in some small way, help to bridge the well known "gap" between theory and industrial practice.

1.2 Overview of the Thesis

Chapter 1: Introduction

This chapter introduces background information relevant to the research. It also highlights the main issues that drive this research study. The two main objectives of the research are presented and the chapter includes discussion of the practical significance of these aims.

Chapter 2: Literature Review

The chapter summarises the literature survey which has been conducted. It contains coverage of the main established concepts and techniques published in the literature concerning pH process modelling and control. A short summary of pH neutralization process characteristics is also presented in this chapter in order to help readers unfamiliar with this application develop a clearer understanding of the subject. A survey of the existing results for different controllers applied to pH neutralization processes is also highlighted. This chapter concludes by providing a basis or motivation for continuation of the research and also presents a discussion of the overall scope of the work.

Chapter 3: The pH Neutralization Pilot Plant

This chapter describes the configuration of the pH neutralization pilot plant used in this research. The chapter starts by describing the overall architecture of the pilot plant. It then continues with a short summary of the instrumentation and measurements involved and the associated hardware, including the pH meter, flowmeter, conductivity meter and control valves. It also highlights initial work required prior to experimentation, such as calibration work and configuring and testing of the data acquisition system. This section provides useful information relating to the capabilities and limitations of the pilot plant in general and the associated equipment. The chapter ends with some discussion of practical issues relating to the pilot plant.

Chapter 4: Modelling and simulation of pH neutralization process pilot plant

This chapter presents two aspects of the work concerning system modelling. The first part discusses the preliminary development of the first pH model used in this investigation. It is based on the mathematical modelling method used by McAvoy (McAvoy, Hsu, & Lowenthals 1972) for pH process modelling in an early paper that is still regarded as the key publication in this field. This chapter then goes on to describe the performance of the first pH model in comparison with the dynamic response obtained from preliminary experimentation on the pilot plant.

The second part of this chapter explains the investigation and modifications made to the first pH model in order to provide a transient response that better matches experimental findings. This section also describes the steps taken during internal verification and external validation, with a view to establish the validity and adequacy of the dynamic response from the modified pH model in comparison with the dynamic behaviour of the pilot plant.

Chapter 5: Conventional Proportional Integral (PI) controller

The chapter describes the performance of the system with a conventional controller (i.e. Proportional plus Integral (PI) controller) in controlling the pH neutralization process pilot plant. The control performance (i.e. experiment and simulation based) of the PI controller are also discussed in this section. The chapter ends with discussion of some objectives and the associated challenges for the design and implementation of more advanced forms of controller.

Chapter 6: Advanced controller design development, implementation and testing

This chapter starts with an overview of the formulation of the overall control structure which involves the combined feedback/feedforward principles. This chapter then describes in detail all measures taken during the development and implementation of the fuzzy inference system for the fuzzy controllers. The next section in this chapter presents results of the investigations on the use of the feedback/feedforward control scheme through the fuzzy logic approach to control the pH neutralization pilot plant. Results from the testing of the controller and associated investigations of the robustness and other potential benefits of the controller, involving investigations based on the actual pilot plant experiments, are presented. This section also presents results of computer-based simulation work on the fuzzy logic controller as well as PI controller with the same control structure (i.e. the feedback/feedforward control scheme).

Chapter 7: Conclusions and Recommendations

This chapter starts by summarising remarks relating to the first objective of the research concerning the performance of the modified pH neutralization model. It continues with conclusions relating to the second objective of the research in terms of the advanced controller. It highlights the main benefits of the fuzzy logic control scheme as an advanced controller for the pH neutralization process and discusses implementation issues. Finally, suggestions for further research are made towards the end of this chapter.

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2.0 BACKGROUND AND LITERATURE REVIEW

This chapter summarises the literature survey that was conducted as part of the research reported in this thesis. It covers pertinent established concepts and techniques published in the literature concerning pH process modelling and control. A short summary of the characteristics of the pH neutralization process is also presented in this section in order to present the subject more clearly in the context of the literature that is being reviewed. A survey of the existing published results for different controllers for the pH neutralization process is included. This chapter concludes with discussion which provides a basis or motivation for the research as well as outlining the scope of the work in more detail.

2.1 pH Process Characteristics

There are many excellent books and references in the field of equilibrium chemical processes involving reactions between acids and bases. This section describes, briefly, the general properties of acids and bases from a chemical perspective and continues with some explanations of the acid-base neutralization reaction process. It concludes with a description of methods for pH measurement. The main purpose of this section is to provide essential background information about the chemical process which is central this research. Sources of information used in this preliminary overview are mainly well established textbooks (e.g. (Bates 1973;Butler 1964;Christian 2004b;Harvey 2000),).

Concepts Relating to Acids and Bases

As described in the Arrhenius theory, an acid is a substance that ionises in water to give hydrogen ions (H^+) whereas a base is a substance that ionises in water to give hydroxyl ions (OH). The charge balance equations for acid and base reactions with water are given in Equation (2.1) and Equation (2.2) respectively. As shown in these equations, the hydrogen ion is actually a mere proton. Thus, based on the Bronsted-Lowry theory, an acid is described as a substance that can donate a proton and a base is a substance that can accept a proton.

$$\mathrm{HA} + \mathrm{H}_{2}\mathrm{O} \Leftrightarrow \mathrm{H}_{3}\mathrm{O}^{+} + \mathrm{A}^{-} \tag{2.1}$$

$$\mathbf{B} + \mathbf{H}_2 \mathbf{O} \Leftrightarrow \mathbf{H} \mathbf{B}^+ + \mathbf{O} \mathbf{H}^- \tag{2.2}$$

Acids and bases can be categorised as monoprotic or polyprotic (i.e. diprotic, triprotic, etc). This depends on the number of hydrogen ions or hydroxide ions that the substance has. To explain further, phosphoric acid (H_3PO_4) may used as a convenient example. This acid is considered as a triprotic acid. This substance ionises in three different stages since it has three hydrogen ions to donate, as shown in Equations (2.3), (2.4) and (2.5). Each stage has a different value of dissociation constant which describes the attributes or characteristic of the substance.

$$H_{3}PO_{4} \Leftrightarrow H^{+} + H_{2}PO_{4}^{-}$$
(2.3)

$$H_2 PO_4^- \Leftrightarrow H^+ + HPO_4^{2-}$$
(2.4)

$$HPO_4^{2-} \Leftrightarrow H^+ + PO_4^{3-}$$
(2.5)

The dissociation constant also describes the strength of the acids and bases. A large value of dissociation constant for an acid indicates that it is a strong acid that is able to donate or ionise all protons in water. On the other hand, a small value of dissociation constant for an acid shows that it is a weak acid and it dissociates partially.

$$K_{a1} = \frac{\left[H^{+}\right]\left[H_{2}PO_{4}^{-}\right]}{\left[H_{3}PO_{4}\right]}$$
(2.6)

$$K_{a2} = \frac{\left[H^{+}\right] \left[HPO_{4}^{2^{-}}\right]}{\left[H_{2}PO_{4}^{-}\right]}$$
(2.7)

$$K_{a3} = \frac{\left[H^{+}\right]\left[HPO_{4}^{3-}\right]}{\left[HPO_{4}^{-}\right]}$$
(2.8)

The acid-base neutralization reaction involves a chemical reaction in which hydrogen ions and hydroxide ions are neutralised or combined with each other to form water (H_2O) while the other ions involved remain unchanged.

As an example, Equation (2.9) shows the acid-base neutralization reaction between hydrochloric acid and sodium hydroxide.

$$H^{+} + Cl^{-} + Na^{+} + OH^{-} \rightarrow H_{2}O + Na^{+} + Cl^{-}$$
 (2.9)

In this example hydrogen and hydroxide ions combined together to form water and the mixed solution will also contain some salts.

A titration curve is normally used to describe the characteristic of the acid-base neutralization reaction. This curve is able to provide useful and important information about the reaction, such as the equilibrium point, the type of acid and base involved (strong or weak, and whether monoprotic or polyprotic) as well as the total volumes or amounts of the substances involved at the end point of the titration process. The titration curve can also show the level of complexity of the acid-base neutralization process, especially in terms of the nonlinearity and the time varying nature of the process.

As an example, Figure 2.1 shows the typical pattern of a titration curve for a monoprotic acid and a polyprotic acid (hydrochloric and phosphoric acids respectively). As shown clearly in the figure, the behaviour of the neutralization process is highly nonlinear. The figure shows an S-shaped curve in which the slope of the curve differs from one type of acid to another. The titration curve also depends on the concentration and composition of the acid and base involved in the reaction process. Thus it shows that the process gain can vary significantly and this creates an important challenge for pH control applications. The S-shaped curve also shows that the most sensitive point on the curve is in the region where the pH value is 7. At this point we should expect a significant change in output for a very small change of input. Thus this operating point involves difficult conditions for open-loop experimentation and for control.



Figure 2.1: Typical titration curves for monoprotic acid (left) and polyprotic acid (right)

The concentration of hydrogen and hydroxide ions determines whether the mixed solution is acidic or alkaline. The mixed solution becomes an acidic solution when the concentration of hydrogen ions is greater than the concentration of hydroxide ions. The opposite is true for the case of a mixed solution that is alkaline. However, if the concentration of both ions is the same then the mixed solution has reached a condition called a neutral solution. As described in (Christian 2004a), the concentration of H⁺ and OH⁻ in an aqueous solution can vary over an extremely wide range (normally between 10^{-14} M and 1M). Thus it is very convenient to measure the acidity of the solution by using the logarithm of the concentration of hydrogen ions,(log H⁺), rather than the concentration itself (H⁺). This concept of pH scaling for measuring the acidity of a substance was introduced by Sørenso in 1909 (Bates 1973;Christian 2004a;Mattock & Taylor 1961).

$$pH = -\log_{10}[H^+] \tag{2.10}$$

Based on this concept and Equation (2.10), the scale for measuring the acidity of a solution is between 1 and 14. At 25°C, if the pH value is below 7 the mixed solution has a higher concentration of hydrogen ions and thus the solution is acidic. If the pH value is 7 it shows that the mixed solution is neutral and if the pH value is more than 7, it indicates that the solution is alkaline.

2.2 pH Control Techniques

This section contains a short review of the significance of pH control in industry. It also summarises some of available control strategies and gives particular emphasis to the problems of control for the pH neutralization process. This section also includes discussion of the selected advanced control Fuzzy Logic Control (FLC) for an application of this kind. One objective of this section, through providing background information relating to the problems of pH control, is to establish appropriate boundaries for the research being undertaken.

2.2.1 Significance of pH control

The control of pH arises in a wide range of industries including wastewater treatment, biotechnology, pharmaceuticals and chemical processing. The general aim in this form of control is to maintain the pH value within a liquid at a specific level. This can be important in order to comply with and satisfy certain environmental requirements or quality standards.

Shinskey (Shinskey 1973) describes wastewater treatment applications as the one of the most challenging pH control problems encountered in industry. This is mainly due to disturbances in the feed composition which are difficult to handle as different compositions will require different sets of control parameters. There are many published papers that discuss pH control in the context of this type of application (e.g. (Mahuli, Russell Rhinehart, & Riggs 1993;Paraskevas & Lekkas 1997)). In general, in this case, the purpose of the chemical plant is to neutralise the waste product solution (which may arise as a result of some manufacturing process) before discharging it to the environment. In such cases the control of the pH value to a certain environmental and legislative standard is very important (Rudolfs 1953). The requirement in terms of the pH value for effluent from a wastewater treatment plant is usually in the range 6 to 8. This is mainly to protect life (both aquatic and human) and also to avoid or prevent damage due to corrosion.

A constant pH value is vital for some production processes in the biotechnology industry. As an example, efficient pH control is needed to maintain a pH value with a small tolerance in order to ensure the optimal performance (e.g. activity and growth) of certain cultures of microbial and animal cells (Roukas 1998;Roukas 1999;Roukas & Harvey 1988). Normally, in animal cell cultures, the optimal pH value for maximum cell growth is, approximately, a pH value of 7.4. In a bioreactor pH control is crucial in order to prevent the micro-organisms from dying as these microbial populations are very sensitive to the environment.

Pharmaceutical products (Lopes et al. 2002) are also produced under stringent and reliable controlled conditions in order to ensure the quality of the product. There are a few processes that require special attention such as sterilisation, fermentation, extraction and also neutralization. The instrumentation and control schemes used in such processes must be highly accurate and reliable.

2.2.2 Overview of pH control

In general pH control methods can be divided into three main categories. The first category is an open loop type of control scheme in which the control valve opening is kept at certain positions for specific time durations. A specific pH value in the reactor tank is not really the main concern. Normally this type of control approach is used for start-up and shutdown of a process or at an initial or pre-process stage within a multistage neutralization process in which at the later stages of the process involve a feedback controller to control the pH value to a specific value or within a range of values.

The second category is the most popular and commonly used approach and is based on feedback control principles. Unlike the open loop control approach, this type of control scheme involves a direct relationship between the control valve opening and the pH value in the process. The general idea is that when the pH value is higher than the desired value the control valve opening is decreased. Conversely, if it is lower than the set point then the control valve opening is increased. This control approach is also known as a corrective control approach. This is because the control action will take place once there is a discrepancy between the process variable and the required set point. There are many types of feedback control schemes that have been published and discussed by previous researchers. The most widely used type of controller for this feedback control approach is the Proportional, Integral and Derivative (PID) type of controller together with the closely associated variations on this control algorithm involving Proportional control (P) or Proportional plus Integral control (PI).

The third control method that is widely used in this type of application is feedforward control. In this control approach the controller will compensate for any measured disturbance before it affects the process (i.e. the pH value in the case of this application). In order to implement this control approach it will normally be necessary to make more measurements on the process. In the case of a pH process the disturbances could arise from unexpected changes in the concentrations of both solutions as well as changes in the flowrates for the two streams. Thus, with a properly designed feedforward scheme, if a disturbance occurs the controller will react before the pH value in the reactor tank is significantly affected. Based on this principle this feedforward control approach is also known as a form of preventive control. The preventive control approach is very much faster than the corrective control approach. Often, in an ideal case, a controller will involve a combination of corrective control and preventive control. It is unusual to have a controller which involves only feedforward control. This is because the feedback control scheme will handle or react to any unknown or unmeasured disturbances (which are unmanageable by means of feedforward control alone). At the same time the feedforward control scheme will react faster to any measured disturbance before it affects the process.

Review of selected papers describing previous research on pH control

In summary, pH control is an interesting and challenging research subject which has led to a large number of motivating and interesting published papers. As mentioned earlier this is mainly due to the nature of the reaction process, which is highly nonlinear, together with the challenge of disturbances caused primarily by variations in the influent composition and flowrate. In this section, several selected key papers were used as a basis for a review of previous work which includes some detailed explanations relating to a number of selected types of control schemes. This provides general information about previous research work done by other researchers working on problems of modelling and control in this field.

McAvoy and his fellow researchers (McAvoy, Hsu, & Lowenthals 1972) presented a paper on a rigorous and generally applicable method of deriving dynamic equations for pH neutralization in Continuous Stirred Tank Reactors (CSTRs). This paper and the associated model has been used as a platform for many subsequent investigations, such as those of Gustafsson & Waller, Henson & Seborg and Wright & Kravaris and formed the basis for their attempts to introduce new and improved forms of pH control, especially in the area of adaptive control.

T.K Gustafsson and K.V Waller have produced several interesting papers concerning modelling and control of the pH neutralization process and a number of these have been reviewed and cited by others as providing good reference material. In 1982 (Gustafsson 1982) introduced a new concept concerning the averaging pH value of a mixture of solutions. The idea was to utilise reaction invariant variables in calculating the pH value of mixtures of solutions instead of using a direct calculation involving a simple averaging of hydrogen ions. The paper introduced the concept of "invariants species" which represent the species that remain chemically unchanged by the governing of reactions in the neutralization process. Thus the paper suggested that the final pH value of a mixture of solutions needs to take into consideration the concentration of all variables involved in the reaction process.

In the following year this research group (Waller & Gustafsson 1983) published a systematic method for the modelling of the dynamics of the pH neutralization process. It was based on this concept of invariant species and the development of the dynamic nonlinear section involved mass balances of all the invariant species involved in the neutralization reaction process. This paper has been used as one of the key references by most researchers in this field. This is because the paper presents some simulation results which highlight the possible use of this pH model in implementing an adaptive pH control scheme. In the paper Gustafson and Waller also developed an adaptive controller where the developed model was incorporated in the controller in order to provide relevant information necessary for the controller. They used hypothetical species estimation to obtain the inverse titration curve so that overall linearization of the control loop can be utilised. Recursive least squares estimation was used in obtaining values of certain unknown parameters.

Gustafsson and Waller also produced another important paper on the investigation of the fundamental properties of continuous pH control (Waller & Gustafsson 1983). Some results on the investigation of standard and non-standard forms of PID controller are also presented in this paper and the paper includes simulation and experimental results for an adaptive reaction-invariant controller, the performance of which is compared with a conventional PID controller. Apart from these results relating to controller performance this paper is important in that it also provides a comparison of experimental results for two different capacities of the reactor tank (with PID control applied). These results suggest that taking into account the capacity of the reactor tank during plant design is important in order to have fast and efficient mixing in the tank. There are two further good papers on this subject entitled Nonlinear and Adaptive Control of pH (Gustafsson & Waller 1992) and Modelling of pH for Control (Gustafsson et al. 1995) which provide further reviews of the some of the above issues of dynamics and control that arise in this type of nonlinear control application. The research group of Henson & Seborg (Henson & Seborg 1994) is another group that has published work on adaptive nonlinear control applied to a pH neutralization process. That publication (Henson & Seborg 1994) is now recognised as an important paper and point of reference in the field of pH control. The group implemented the controller and evaluated its performance on a bench scale pH neutralization system in order to gain additional insight in terms of the practical application. The nonlinear controller was developed by applying an input-output linearization approach to a reaction invariant model of the process (Gustafsson & Waller 1983b; Waller & Makila 1981). The controller also utilised an open-loop nonlinear state observer and a recursive least squares parameter estimator. The paper highlights results for three different tests carried out to investigate the performance of the main types of controllers considered (i.e. a PI controller, and non-adaptive and adaptive forms of nonlinear controller). The first test involved set point changes; the second test involved buffer flowrate disturbances and finally the third test included acid flowrate disturbances. Based on the results from these tests the adaptive nonlinear pH control was found to provide the best results for the three controllers considered.

A research group from a control engineering laboratory at Helsinki University of Technology has also published a number of useful papers on modelling and control of pH neutralization processes In 1981 they published a paper on modelling of the pH neutralization process in a continuous stirred tank reactor which was based on a physico-chemical approach to process modelling (Jutila & Orava 1981). Their simulation focused on the changes of a dissociation process involving the use of the pH variable as a measure for the acidity. The pH model was able to calculate approximately the dissociation constant of the weak species by using a procedure of static fits to the titration curve of real liquid samples. The models developed by this Finnish group also allow estimation of the unknown concentration of the hypothetical species with the aid of a linear Kalman-filter algorithm.

In 1983 the research group produced another paper concerned with implementation of a form of adaptive pH control for a chemical waste water treatment plant (Jutila 1983). That paper is widely regarded as being important because the adaptive controller was actually being implemented at a chemical waste water treatment plant at Viinikanlahti, Tampere, Finland. The same approach presented in the earlier published work (Jutila & Orava 1981) was used in modelling and in controller design for the pH-reactor where the composition of the incoming waste-water is modelled with hypothetical chemical species. The paper reviewed and commented on previous work involving adaptive feedback algorithms. It was concluded that the main disadvantage of the approach adopted in earlier work was that the controllers were unable to implement a proper feedforward control loop. Thus the main idea presented in this paper (Jutila & Orava 1981) was to present a new approach for an adaptive combined feedback-feedforward control method for pH control which was based on a quantitative physico-chemical analysis of the pH neutralization process. As presented in the paper (Jutila 1983), the simulation and experimental results were very encouraging. Later this research group presented another paper on pilot plant testing of the adaptive pH control algorithm (Jutila & Visala 1984). The paper highlighted a few problems with the earlier adaptive control methodology and presented some improvements that had been made to the controller. The simulation results were presented to support the capability of the enhanced adaptive controller.

G.A. Pajunen (Pajunen 1987) published a paper in 1987 on comparisons of linear and nonlinear adaptive control of a pH process. She presented two different schemes of adaptive control involving linear and nonlinear adaptive controllers. The case involving the linear adaptive controller was based on flow and mixing models that were initially assumed to be known. The second scheme utilised piecewisepolynomial approximation to obtain an inverse of the titration curve for the pH process. It should be noted that the modelling approach for the pH model was different in this case from that of Gustafsson & Waller. It was more of an experimental method of modelling rather than involving derivation from a physical and chemical point of view. In summary the performance of the nonlinear adaptive controller was better than that of the linear controller. However in the case of frequent step disturbances the paper suggested use of the linear controller instead.

Wright and Kravaris, researchers from the Department of Chemical Engineering, at the University of Michigan, have also published several papers on pH control applications. In 1991 they introduced a new method of modelling and design of a nonlinear controller which was based on the concept of the strong acid equivalent. The first paper (Wright 1991) provides a comprehensive review of previous research work on pH modelling and control. The strong acid equivalent is one state variable of a reduced model which can be calculated online from the pH measurements given a nominal titration curve of the process stream. The formulation of the new approach transforms the control problem into an equivalent linear control problem which is expressed in terms of the strong acid equivalent. The paper presents some simulation results on the performance of the new control strategy, which is linear and nonadaptive. The second paper (Wright, Soroush, & Kravaris 1991) focuses on the implementation of the new approach (i.e. strong acid equivalent method) on a laboratory-scale pH neutralization process. The experimental results show that in addition to a nominal process stream titration curve the proposed control algorithm requires no chemical information, such as the dissociation constant and chemical species involved. These two main papers (Wright, Soroush, & Kravaris 1991) provided a foundation for further research to explore this subject in greater detail and this then led to some more interesting papers in later years from the same group.

Three papers were published on on-line identification and nonlinear control of pH processes (Wright & Kravaris 1995;Wright, Smith, & Kravaris 1998;Wright & Kravaris 2001b). These papers are based on a real industrial process for lime slurry neutralization. As described in these papers, the research work focuses on acidic flow of unknown contents and large acidic load changes. An online identification method for unknown chemical species was used, which is an approach that had been developed previously (Wright 1991;Wright, Soroush, & Kravaris 1991). As explained previously, the strong acid equivalent approach can be used once the identification is realised. In (Wright & Kravaris 1995) the results of the controller performance were briefly presented but the paper demonstrated the workability of the online identification concept for the unknown nonlinearity of an industrial pH process.

The next two papers (Wright, Smith, & Kravaris 1998;Wright & Kravaris 2001a) presented, in more detail, additional results relating to the investigation of the controller performance, such as tracking of the lime flowrate set point, investigation of different conditions of normal process operation (i.e. for pH values of 7, 4.5 and 2.5), and operation without agitation.

Another research group from Korea University, Seoul, has published several papers on adaptive nonlinear control for pH neutralization processes. In 1995 they presented a new approach to pH control that utilises an identification reactor to incorporate the nonlinearities of the pH neutralization process (Sung, Lee, & Yang 1995). As mentioned in their paper, they proposed a new method which uses an approach involving an identification reactor similar to that introduced previously by Gupta & Coughanowr (Gupta & Coughanowr 1978) and by Williams et al. (Williams, Rhinehart, & Riggs 1990). The titration curve was to be obtained from the identification reactor approach by using an interpolation method (cubic spline) and the titration curve was to be updated periodically. This proposed approach to control was based upon the Wright & Kravaris approach (Wright 1991; Wright, Soroush, & Kravaris 1991) especially in terms of the stability analysis and determination of controller parameters. In the year 2002, D.R. Yang and his group published another paper (Yoon et al. 2002) concerning indirect adaptive nonlinear control for the same process application (i.e. a pH neutralization process). However the proposed nonlinear control design strategy in this paper was different from their earlier paper (Sung, Lee, & Yang 1995) in which the backstepping technique was used instead. In addition to that, the general approach to pH model development described in the paper was also based on the work of Henson & Seborg (Henson & Seborg 1994), especially in terms of the dynamic model of the process. As described in the paper, the simulation results showed an adequate control performance using this approach.

In 2004, another paper was presented by the Korean researchers on nonlinear pH control (Yoo, Lee, & Yang 2004). Unlike the previous paper (Yoon, Yoon, Yang, & Kang 2002) this paper offers some insight into practical control design issues for a pH neutralization laboratory setup. The main concern of this study is to design an online identification method based on use of an extended Kalman filter.

The filter has been experimentally applied to the simultaneous estimation of states and process parameters of the pH neutralization process. The paper provides some comparison between simulation and experimental results.

Some groups of researchers have also investigated another type of advanced control strategy in the form of nonlinear model predictive control. As presented by Camacho & Bordons and Rossiter (Camacho & Bordons 1999;Rossiter J.A 2003), model predictive control can be described as an intelligent control algorithm that computes the future dynamic responses of a plant or system by using an explicit process model and determines the control input required on the basis of that predicted future response. Thus the main concern of this area of research is to develop a pH model that is able to demonstrate the nonlinearity of the pH process and will eventually be used to predict the future control signals for the controller. As an example, in 1994 Kelkar and Postlewaite presented a brief report on research work done on fuzzy-model based pH control (Kelkar & Postlethwaite 1994). The paper outlined the framework of the controller and the development of the fuzzy relational model which was based on a fuzzy bgic approach. The control scheme was implemented on a small-scale experimental rig and the performance of the controller was reported as satisfactory.. In the conclusions section of the paper experimental and instrumentation issues relating to reduction of electrical noise were emphasised, in order to provide better control performance.

A similar type of control strategy (i.e. nonlinear model predictive control) was also presented in a paper by Waller and Toivonen in 2002. Unlike Kelkar and Postlewaite (Kelkar & Postlethwaite 1994), this group of researchers has utilised a neuro-Fuzzy modelling technique which is also referred to as quasi-ARMAX to model the nonlinear characteristic of the pH neutralization process. As described in the paper, the developed neuro-fuzzy model is capable of representing the behaviour of a highly nonlinear pH neutralization process to a high level of accuracy. The simulation results for the nonlinear model predictive controller show that the controller works very well not only for set point changes but also with feed flow concentration disturbances.
Generally all of the papers that have been discussed in the previous sections were concerned with advanced control techniques that can be categorised as model-based control approaches. In summary, the primary issue of this type of control approach is to obtain an accurate pH model that can provide reliable state and parameter information for the controller. Based on this fact, most of the previous approaches mentioned above have focussed their efforts on the formulation of various methods for modelling the nonlinearity of the pH neutralization process. Their work shows that it is quite challenging to identify the process nonlinearity as well as to properly evaluate the response predictions of the model representing the actual pH neutralization process in a reliable and robust fashion. In addition, most of the abovementioned papers show that this model-based control technique involves quite complex numerical problems. Thus computational speed and assurance of a reliable solution in real time remains critically important and represents an interesting challenge for this type of control scheme.

As described previously in the first chapter of this thesis, this research study involves the development and implementation of advanced control approaches involving fuzzy logic control. The fuzzy logic approach has been chosen due to the fact that fuzzy logic control has made a breakthrough in some process industries involving highly nonlinear dynamic process behaviour. Besides that the fuzzy logic approach can be applied as a non-model-based technique. Instead, the fuzzy logic approach uses linguistic methods in control design and development. Thus it is believed that many of the problems outlined in the previous paragraphs dealing with model-based control methods can be avoided with this type of control approach. The following paragraphs will review several selected papers on pH control that utilise fuzzy logic techniques. Hopefully these papers will be able to provide some insight into the capabilities of fuzzy logic based methods and support the choice of this type of approach for this research.

In 1993, Karr & Genry presented a paper on the use of genetic algorithms in a fuzzy control approach for a pH process (Karr & Gentry 1993). The paper basically describes work done by researchers at the U.S. Bureau of Mines as an extension of previous investigations on adaptive fuzzy logic controllers (Karr 1991).

As described in these papers (Karr 1991;Karr & Gentry 1993), the researchers at the Bureau had developed a technique in which the genetic algorithm approach is employed to alter membership functions in response to changes in the process. The idea presented in the later paper (Karr & Gentry 1993), is to utilise the ability of genetic algorithm in terms of optimizing the membership functions for different requirements in terms of set point or concentration disturbances. The developed controller was implemented on a small scale laboratory setup in which the volume of the beaker that represents the reactor tank is 1000mL. The paper presented some experimental results showing that the performance of this form of controller is very encouraging.

A short paper on enhanced fuzzy control of a pH neutralization process was presented in 1993 by Kwok and Wang (Kwok & Wang 1993). The paper proposes a new control strategy consisting of three different parts: a fuzzy controller which represents the Proportional and Derivate control action, an integrator and a Smith predictor. As described in that paper the simulation results demonstrate the effectiveness of the proposed controller in comparison with the classical control approach involving the conventional PID controller.

In 1994 Parekh and his colleagues published a paper on a new form of advanced control system for pH neutralization processes (Nie, Loh, & Hang 1994;Parekh et al. 1994;Proll & Karim 1994) involving a technique based on the fuzzy logic approach. As described in the paper, the main advantages of the new proposed controller included a wider operation range, robustness of the controller in hand ling random disturbances as well as a relatively simple implementation. The paper highlighted the fact that, during the formulation of the fuzzy logic controller, experimental data and practical experience of the real process play an important role. It also shows at this design stage that the complexity of the mathematical formulation has been reduced through the use of linguistic terms. The paper included quite comprehensive experimental results which allowed the conclusion to be drawn that the proposed form of fuzzy logic controller works very well and provides good control performance.

2.2.3 The Conventional Approach

The most widely used simple feedback control strategy applied to pH control involves the PID algorithm. Equation 2.10 describes the most basic form of continuous PID algorithm in the time domain. As shown in the equation, the PID algorithm is actually a simple single equation with three control terms; proportional gain, (K_P) , integral gain, (K_I) and derivative gain, (K_D) . The variable mv(t) represents the controller output while the variable e(t) is the error, which is the difference between the system output (the measured pH in this case) and the set point.

$$mv(t) = K_{P}e(t) + K_{I} \int_{0}^{t} e(t)dt + K_{D} \frac{de(t)}{dt}$$
(2.10)

This simple feedback control approach will be discussed further in Chapter 4. The dynamic performance of a PI controller on the pH neutralization pilot plant is used as a benchmark against which more advanced schemes can be compared. As discussed in Chapter 4, the conventional controller was not able to provide a good overall performance and this is consistent with previously published findings in the literature (e.g. (Alvarez et al. 2001)).

2.2.4 Fuzzy Logic Control

Historical Background of Fuzzy Logic

In 1965, Lofti A. Zadeh published an interesting and ground-breaking paper on "Fuzzy Sets" (Zadeh 1965b). This paper describes the mathematics of fuzzy set theory which then led to the development of the fundamental ideas of fuzzy logic. As described in the paper, a fuzzy set is a class of objects with a continuum of grades of membership. Such a set is characterised by a membership function which assigns to each object a grade of membership ranging between zero and one. Zadeh then elaborated on this idea in a subsequent paper in, 1975, which introduced the concept of linguistic variables (Zadeh 1975a;Zadeh 1975b;Zadeh 1975c).

Since the 1960s many papers on fuzzy logic have been published by Zadeh and by other researchers who have followed his lead. As described by Zadeh (Zadeh 1976c), the primary aim of fuzzy logic is to provide a formal, computationally-oriented system of concepts and techniques for dealing with modes of reasoning which are approximate rather than exact.

In 1987, Yager, Ovhinnikov, Tong and Nguyen published an edited volume entitled "Fuzzy Set and Applications" (Yager et al. 1987). This book is a compilation of selected papers by Zadeh on fuzzy logic. The editors have divided the papers into three main categories as follows: formal foundations, approximate reasoning, and meaning representation. The first category involves seven papers (Zadeh 1965a;Zadeh 1968;Zadeh 1971;Zadeh 1973;Zadeh 1976a;Zadeh 1978a;Zadeh & Bellman 1970) that introduce fuzzy sets and possibility theory. The second category includes six papers (Zadeh 1975a;Zadeh 1975b;Zadeh 1976b;Zadeh 1976c;Zadeh 1976d;Zadeh 1983b;Zadeh 1985) that define the concept of linguistic variables. The last category involves papers that describe directly the problem of meaning representation in natural language (Zadeh 1972;Zadeh 1978b;Zadeh 1983a;Zadeh 1984;Zadeh 1986).

In 1975, Mamdani and Assilian published a paper entitled "An Experiment in Linguistic Synthesis with a Fuzzy Logic Controller" (Mamdani & Assilian 1975). This paper described the first application of fuzzy set theory in a practical control systems context. The paper presented the steps taken to control a steam engine and boiler combination by synthesizing a set of linguistic control rules obtained from experienced human operators. The inputs for the fuzzy logic control in this case were "error" and "change of error" and this was in many ways similar to the inputs used in conventional PI controllers. Other papers presented subsequently by Mamdani and his co-authors described the application of this concept of linguistic synthesis to a number of control applications (Mamdani 1976;Mamdani 1977;Mamdani & Assilian 1999;Mamdani & Baaklini 1975). This approach remains one of the most popular and commonly used methods in the development of fuzzy logic controllers. In this research the Mamdani type of approach has been used to develop a fuzzy logic controller for the pH neutralization pilot plant.

Apart from the work of Mamdani and his colleagues there are other interesting approaches that have proved useful for fuzzy logic control system development and the work of Sugeno is particularly important in this respect (Ishii & Sugeno 1985;Takagi & Sugeno 1985). In this approach the fuzzy logic controller utilises experimental data to develop the control strategy. Another important difference between Mamdani's method and Sugeno's method is in terms of the output membership function. For Sugeno's method the output membership functions are either linear or constant (The Math Works 2000).

Although the first literature on fuzzy logic (Zadeh 1965c) was presented and introduced in the U.S.A., researchers and manufacturers in North America were not keen to adopt this technology in the initial stages. The Europeans and Japanese were the first to aggressively apply the fuzzy approach to real engineering problems and to build real products around it. It has been reported that the first industrial application that implemented fuzzy logic as a control scheme was a cement kiln built in Denmark in 1975 (Jamshidi, Ross, & Vadiee 1993). A decade later, Seiji Yasunobu and Soji Miyamoto constructed a simulation that demonstrated the superiority of a form of fuzzy control system for the Sendai railway. Two years after that the idea was adopted and fuzzy systems were used to control the acceleration, braking and stopping of the trains (Schwartz & Klir 1992). In 1987 the first fuzzy chips were announced in Japan (Jamshidi, Ross, & Vadiee 1993;Ross, Booker, & Parkinson 2002) and since then there have been many Japanese-designed electrical appliances such as washing machines, dishwashers, air conditioning units, televisions and photocopying machines which use fuzzy logic concepts in some form of control scheme.

The Basic Concepts of Fuzzy Logic

This main purpose of this section is to present the general ideas of the fuzzy logic approach. Firstly it is necessary to have a basic understanding of fuzzy and classical sets, as introduced by Zadeh (George & Yuan B 1995;Jamshidi, Ross, & Vadiee 1993;Ross, Booker, & Parkinson 2002;Zadeh 1965d).

Using the definition provided by Ross (Ross 1993) a fuzzy set is a collection of elements in a universe of information where the boundary of the set contained in the universe is ambiguous, vague, and thus "fuzzy" in some respects. In a classical set, the boundary is certain and rigid so that the boundary can be used to establish, in an unambiguous fashion, the set to which the element belongs.

Let X denote the ground set or universe of discourse and let an element of that universe be denoted as 'x'. Set A is a group of real numbers between 0 and 1 which is a subset of the universe, X. Figure 2.2 shows the graphical representation of the membership function of the classical set for this case and Figure 2.3 shows a corresponding graphical membership function of the fuzzy set



Figure 2.2: Membership function of a classical set



Figure 2.3: Membership function of a fuzzy set

As shown in the Figure 2.2, there are only two elements for set A which is 0 and 1. For the fuzzy set, besides the value of 0 and 1, set A has other values between these extremes, as shown in the figure. These values will depend on the membership function of set A. Figure 2.4 shows some other examples of membership functions that are available and commonly used in fuzzy logic systems.



Figure 2.4: Typical membership function for fuzzy logic systems

The simplest membership function which is applicable to most process system is the triangular membership function, as shown in Figure 2.3. At the moment there are no proper rules or laws that can determine which membership function is most suitable for a given system or application.

Table 2.1 shows the basic notations involved in fuzzy sets and provides a basis for a comparison between classical and fuzzy set operation. Table 2.2 shows the graphical representation of the membership function for each fuzzy set operation given in Table 2.1.

Descriptions	Classical Set	Fuzzy Set
Union	$A \cup B = \{x \mid x \in A \text{ or } x \in B\}$	$\mathbf{m}_{A\cup B}(x) = \mathbf{m}_{A}(x) \lor \mathbf{m}_{B}(x)$ $= Max[\mathbf{m}_{A}(x), \mathbf{m}_{B}(x)]$
Intersection	$A \cap B = \left\{ x \mid x \in A \text{ and } x \in B \right\}$	$\boldsymbol{m}_{A \cap B}(x) = \boldsymbol{m}_{A}(x) \wedge \boldsymbol{m}_{B}(x)$ $= Min[\boldsymbol{m}_{A}(x), \boldsymbol{m}_{B}(x)]$
Complement	$\overline{A} = \left\{ x \mid x \notin A, \ x \in X \right\}$	$\boldsymbol{m}_{\overline{A}}(x) = 1 - \boldsymbol{m}_{A}(x)$

 Table 2.1: Comparison between classical and fuzzy set operations

Set Operation	Set A and Set B	Set C
Union	m_x A B $1 \rightarrow x$	m_x C C C C C C C C C C C C C C C C C C C
Intersection	m_x A B 1 0 x	m_x 1 C 0 x
Complement		m_x C C C C C C C C C C C C C C C C C C C

Table 2.2: The graphical representation of fuzzy set operations

These two tables provide some basic ideas of fuzzy set operation. Zadeh explained these fuzzy set operations and provided some relevant theorems (e.g. De Morgan's Theorem and the Distributive Theorem) in his first paper on Fuzzy Sets (Zadeh 1965e).

Generally the development of the fuzzy logic systems or control schemes involves three steps or processes, as shown in Figure 2.5. The first step that is shown is the fuzzification process. This process involves a domain transformation in which the system inputs or *crisp inputs* are converted into fuzzy set inputs. In the pH neutralization process the system inputs are actually the measured process variables such as the pH value in the reactor tank, the flowrates of the streams and the conductivity values of the solutions. In this process each input will be transformed into its own group of membership functions or fuzzy sets. Thus the development of the controller must include identifying the crucial system inputs, determining the type of membership function, as well as establishing the degree of the membership function for the input set.



Figure 2.5: General procedures of designing a fuzzy system

The second step is the Fuzzy Inference process which is described as a process that forms the mapping of the fuzzy input and output sets. The main process involves establishing the relevant Fuzzy Set and Fuzzy Operator, as well as developing a set of "if-then rule statements". As described in most of the literature such as (George & Yuan B 1995;Jamshidi, Ross, & Vadiee 1993;Ross, Booker, & Parkinson 2002) fuzzy sets and fuzzy operators are the subjects and verbs of fuzzy logic. Thus the "ifthen" rule statements are used to formulate conditional statements. Each rule statement will provide the result of implication. The last process prior to the next step is the aggregation process in which all the results of implication of each rule are combined into a single fuzzy set. The third step is an inverse process of the first step and is called "defuzzification". The process involves transforming the fuzzy set output into the system output so that the output signal can be used to drive some actuators or can be further processed by the controller. As described in the previous paragraph, the input for this process is actually a fuzzy set. This set comprises all the results of implication of each rule and thus contains a range of output values. The final output from the defuzzification process is a single value.

There are a variety of methods to transpose the range of output values into a single value. These include methods such as the "centroid", the "bisector" and the "middle of maximum" techniques. However the most commonly used method is the centroid method in which the centroid of the fuzzy set is calculated.

Advantages of Fuzzy Logic

From the literature, it appears that the main advantages of fuzzy logic control are as follows:

- i. Fuzzy logic is capable of controlling nonlinear processes by formalising the expertise of an operator who has vast experience in handling and tuning the process or a designer who has engineering knowledge in that particular area of process control engineering.
- ii. Fuzzy logic is able to provide a simple solution for model development in areas where it is difficult to derive a precise model using mathematical approaches based on the application of fundamental physical laws and principles. A complex and highly nonlinear process is usually difficult to describe quantitatively using such fundamental knowledge.
- Fuzzy logic is also capable of resembling human decision making processes, with an ability to produce accurate and reliable solutions from vague or imperfect information.

iv. Formulation of a fuzzy logic system is relatively easy and the resulting controllers are usually straightforward to implement, as compared with other advanced forms of control system. This is mainly due to the fact that fuzzy logic uses a linguistic approach that is easy to understand rather than a more complex mathematical form of description.

2.3 Summary and Research Motivation

This chapter has given an overview of the pH neutralization process as well as the significance of pH control in industry. The review of the literature on pH neutralization processes shows that there is still a considerable challenge in the development of good dynamic models for pH neutralization processes and that pH control still remains an interesting research activity. This is mainly due to inherent nonlinearities in the process.

The availability of a pH neutralization pilot plant (to be described in the next chapter -Chapter 3) that uses industrial standard instrumentation, measurement systems and control valves has also provided an important stimulus for this research. Although numerous papers and research activities have been published and presented on pH neutralization processes, the scope of this research is different since it focuses particularly on the problems of plant modelling, model validation from experimental data and the implementation of advanced forms of control. The process equipment on this pilot plant also differs, in a number of important respects, from the equipment used in other published experimental investigations. These are important features of this research.

This research involves investigation of an advanced form of control strategy which is based on fuzzy logic techniques within an overall control structure that involves both feedback and feedforward control. Interest in so-called "intelligent control" approaches, such as fuzzy logic, has been gradually increasing over the last few years. Although there are various other approaches available, such as adaptive control and model predictive control, there are a number of issues associated with the performance of these methods in practical industrial applications that are still being actively pursued. These include problems of optimisation, constraints and disturbance handling, process model nonlinearities and uncertainties and also issues of stability and robustness. Due to these issues associated with model-based approaches to control, this research has been directed towards investigation of a nonmodel-based type of control strategy that involves a fuzzy logic approach.

In general terms, fuzzy logic is now recognised as one of the most successful technologies for developing and implementing control systems for a wide range of industrial applications. This is due to the fact that fuzzy logic is capable of managing complex applications efficiently, even with uncertainties or vague information about the system to be controlled. The fuzzy logic concept has also been shown to be capable of mimicking human decision making processes for applications where manual control is known to produce acceptable control performance. Thus the successful application of fuzzy control concepts in other fields has encouraged this research activity to investigate the benefits and limitations of fuzzy control in the pH neutralization process. These research activities also reflect interest in improving the operation and control of systems involving highly nonlinear process plant.

CHAPTER THREE

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3.0 THE pH NEUTRALIZATION PILOT PLANT

This section describes the pH neutralization pilot plant in detail. The main advantage of this plant for research of the type described in this thesis is that it has the characteristics that are comparable with a pH neutralization plant used in industry and its design uses industrial instrumentation and measurement technology throughout.



Figure 3.1: Piping and Instrumentation Diagram (P&ID) of the pilot plant

Figure 3.1 depicts the main section of the Piping and Instrumentation Diagram (P&ID) of the pilot plant. Such a diagram provides useful information relating to the overall process configuration and piping layout as well as details of instrumentation and control related features. As shown in the figure, the pilot plant consists of three main tanks, an acid tank (VE100), an alkaline tank (VE110) as well as a mixing or reactor tank (VE120). The acid stream and the alkaline stream are pumped into the reactor tank by pump P100 and pump P110 respectively. As shown in the diagram, there are two flow transmitters FT120 and FT121 that indicate the flowrate for the acid and alkaline streams respectively.

The flowrate for both streams can be controlled individually by using the control valve CV121 for the acid stream and control valve CV122 for the alkaline stream. There is a motorised agitator (AG120) in the reactor that is used to mix the solution. A pH sensor (AT 122) measures the pH value of the solution in the reactor tank. The conductivity meters in the acid (CT100) and alkaline (CT110) tanks are used to monitor the concentrations of the solutions. There is another section which is not included in this P&I diagram. This is the discharging section which starts from the outlet of the reactor tank (i.e. the product of the neutralization process) and ends at the discharged tank. The solution in the discharged tank will be treated before being released into the environment.



Figure 3.2: Photograph of the pH neutralization pilot plant

Figure 3.2 shows a photograph of the pH neutralization pilot plant. It gives additional information about the pilot plant configuration. In general the design of this pilot plant involves control of the pH value of the solution in the reactor to a desired level by controlling the feed flow of the alkaline stream. This desired level is, in practice, usually between pH value 6 and pH value10.

3.1 Overall System Architecture

The overall system architecture of the pilot plant is shown the Figure 3.3. As shown in the figure there are three different functional levels for this pilot plant. The first level is known as the Plant and Field Instrument Layer, the second level is the Data Acquisition System Layer and the third level (shown at the top) is the Supervisory Computer System Layer.



Figure 3.3: Overall system architecture of the pilot plant showing the three functional levels

The first level (the Plant and Field Instrument Layer) involves the physical plant itself and consists of the primary elements such as the pH meters, conductivity meters and flow transmitters that provide information about the relevant process variables to the system. This level also has some final elements such as the control valve, pumps and agitator. In addition, this level will also provide some status input information to the upper levels (e.g. ON/OFF switch status input).

The main function of the second level is to establish communication between the first layer and the third layer as well as data retrieval and processing functions. The second and the third levels are normally very closely interconnected and can be considered as one system although they involve more than one processor. Such a system may be termed a Distributed Control System (DCS). The computer system in the third layer should be compatible and comply with all protocols used in the data acquisition system. The third layer provides a platform for monitoring and controlling the whole operation of the pilot plant.

The pilot plant was originally equipped with a DCS system which consisted of second and third level systems from Honeywell. The PlantScape Honeywell System however has some constraints and limited capabilities for experimental work and research, as it is a proprietary system. Thus, at an early stage in the current project, the Honeywell DCS system was replaced by a new system that has the capability to operate as an open system and allows the investigator considerable freedom in terms of open-loop testing and controller implementation. This new DCS system uses MATLAB/SIMULINK as a platform which provides more flexibility in monitoring and controlling of the pilot plant. Thus the author was involved directly with testing and configuration work as well as development of the MATLAB/SIMULINK model and controllers for the new system. This new system will be described further in the next section.

3.2 The Reactor Tank

The reactor tank is very crucial in this research as this is where the neutralization reaction process takes place and where the output measurements are taken. Figure 3.4 shows the simplified diagram of the physical arrangement of the reactor tank and Figure 3.5 shows a photograph of the actual reactor tank on the pH neutralization pilot plant.



Figure 3.4: The reactor tank

The outlet point is positioned to provide a maximum storage volume for this tank of 80L. The minimum operating volume is 30L, as the agitator will not be able to mix the solution properly if the volume is smaller than this value. Thus most of the simulation and experimental results are based on a volume of mixing solution of approximately 80L. As shown in the figure, the pH meter (AT 122) and the agitator (AG 120) are installed near the acid feed stream inlet. The main purpose of this agitator is to mix both solutions completely and homogeneously. In addition to that, it will also accelerate the neutralization reaction process. The agitator produces some turbulence in the tank in order to mix the solution satisfactorily. The pH value from the online pH meter is also relatively consistent, indicating that the agitator works adequately and its turbulence does not adversely affect the measured signals.

The outlets for the acid and alkaline streams as they flow into the tank are separated by 44cm. In practice, both solutions will take some time to travel and merge before the neutralization reaction takes place. Theoretically, if both inlet streams are close to each other some of the delays will be eliminated but there will inevitably be further lags or time delays before the concentration in the whole tank reaches a steady uniform level following a change of an input. Thus this arrangement introduces additional dynamic behaviour in the neutralization reaction, especially in terms of reaction lags and transport time delays. Most models described in the literature (e.g (Gustafsson & Waller 1983a;Henson & Seborg 1994;McAvoy, Hsu, & Lowenthals 1972;Mwembeshi, Kent, & Salhi 2001)) do not include pure time delays as the models are based on laboratory scale equipment where delays are much smaller, possibly due to more efficient mixing. As a result, the development of the pH neutralization plant model was found to be more challenging than originally expected.



Figure 3.5: Photograph of the reactor tank at the pilot plant

3.3 Instrumentation and Measurements Involved

There are five main process variables that will determine the behaviour of the pH neutralization process for this pilot plant. As given in the table below (i.e. Table 3.1), the instrumentation that provides the main required process variables from the pilot plant involves one pH meter, two flowmeters and two conductivity meters These three main measuring instruments are crucial for the control strategy.

No	Process Variable	Instrument
1	pH value from the reactor tank	pH Meter
2	Concentration in acid tank	Conductivity Meter
3	Concentration in alkaline tank	Conductivity Meter
4	Flowrate for acid stream	Flowmeter
5	Flowrate for alkaline stream	Flowmeter

Table 3.1: List of process variables

The pH meter provides the main feedback of the process variable to the controller whereas the flowmeters and conductivity meters can be used to provide inputs that indicate whether or not the system can be controlled. Therefore the accuracy and reliability of these instruments are also important in order to ensure that the performance of the controller is satisfactory and consistent.

The pH neutralization pilot plant was installed in the process control laboratory at Universiti Teknologi Petronas in the year 2000. Since that time no instrument recalibration work had been done until the current project began. Thus the main activity at the pilot plant before performing any experiments involved a major recalibration of all the instruments. Results (see Appendix I) show that the performance of the instruments before recalibration was poor. However, after the recalibration work was carried out the performance of the instruments was found to be satisfactory. Full details are included in Appendix I.

3.3.1 pH Meters

The pH meter used in the pilot plant is the alpha-pH1000 model from EUTECH Instruments. The detailed specification for this product is given in Appendix II. The pH meter can be divided into two parts. The first part is the process electrode, which acts as a sensor. This electrode will measure the electrical potential (i.e. in mV), which is developed across the surface of a sensing membrane. The second part is the controller, the main function of which is to convert the measured electrical potential signal into a pH value according to the Nernstian Slope.

The meter is normally installed in waste and water treatment plants, and in chemical and food processing industries as well as neutralization process plants. As mentioned earlier, the primary objective of this pH neutralization process is to control or maintain the pH value in the reactor tank to a desired value. Thus this pH meter will provide an important feedback signal for the controller.

The measurement range for the pH meter is set to pH values in the range 0 to 14 and the corresponding output range for the meter is 4 to 20mA. The pH meter has been calibrated with three standard buffer solutions (of pH values 4, 7 and 9). The readings from this meter have been compared and verified with readings from a laboratory pH meter that acts as a primary standard and the results are satisfactory and acceptable. A few experiments involving a simple laboratory bench-top pH neutralization process have been carried out to ensure the consistency of the pH meter. The results are encouraging and details can be found in Appendix I. The pH meter needs to be re-calibrated from time to time and the measuring probe cleaned in order to ensure its reliability and accuracy. Occasionally, samples are taken from the reactor tank and the pH value of the mixing solution is measured using the laboratory pH meter as a comparison to certify the reliability of the meter used on the pilot plant.

3.3.2 Conductivity Meters

The conductivity meters used for the pilot plant are also from EUTECH Instruments. The model is alpha-CON1000 ¹/₄ DIN and the detailed specification is given in Appendix III. The meter also has two parts: the process electrode and the controller. The main function in each case is similar to the functions within the pH meter. The process electrode measures the density of ions in the aqueous solution in the form of an electrical current. Normally the range of the generated electrical current is very small. The controller displays the measured current using suitable basic units of measurement, which are milliSiemens/cm (mS/cm) and microSiemens/cm (μ S/cm).

The conductivity value relates to the concentration value of an aqueous solution and a different solution will involve a different relationship. A few sets of laboratory experiments had been carried in order to find a suitable or appropriate range for concentrations for the pilot plant. The main factor was to be able to achieve a linear relationship between the conductivity and the concentration of the solution. In addition to that, other factors also had to be considered such as the safety of the pilot plant and the cost of the experiments. After considering all factors the best concentration values for sulphuric acid and sodium hydroxide range from 0.01M to 0.1M.

Based on the results from the tests carried out on the meter the relationship between conductivity and concentration for the two solutions are as follows:-

i. Sulphuric acid

Concentrat ion value $=\frac{\text{Conductivi ty Value}}{487.88}$

ii. Sodium Hydroxide

Concentrat ion value $=\frac{\text{Conductivi ty Value}}{210.43}$

As mentioned above, there are two conductivity meters. One meter is installed at the acid tank and the other at the alkaline tank. The maximum volume of these tanks is 280L. Both these tanks were cleaned during the refurbishment and recalibration work on the pilot plant. This was to ensure that the tanks were free from any contamination and thus would not lead to the occurrence of any unwanted reactions. Concentrated sulphuric acid and sodium hydroxide are used to prepare the solutions at the required concentrations. During the preparation process each solution is stirred manually with a special rod in order to ensure that the solution is uniformly mixed.

The measurement range for the conductivity meter is between 0mS and 200mS, which correspond to an output range for the meter from 4 to 20mA. The meter has also been calibrated with standard buffer solutions that have conductivity 1413μ S and 12.88mS. The reading from this meter has also been compared and verified with the reading from a laboratory pH meter. After cleaning of the process probe and recalibration work the performance of the meters was judged to be satisfactory and acceptable. The results of the recalibration process are shown in Appendix I. Occasionally, samples are also taken from both the acid and alkaline tanks and are measured using the laboratory conductivity meter as a comparison to certify reliability of the meters used on the pilot plant.

3.3.3 Flowmeters

There are two magnetic flowmeters installed on the pilot plant. These flowmeters or flow transmitters will provide flowrate indications for the acid stream (FT120) and for the alkaline stream (FT121). A magnetic flowmeter is suitable for wastewater or other dirty fluid applications as there is no direct contact between the fluids being measured and the measuring parts or elements. The operating principle of a magnetic flowmeter is based on Faraday's law of electromagnetic induction. The fluid acts as a conductor and the induced potential is proportional to the average flow velocity which is perpendicular to the flux lines. The magnetic flowmeter can also be considered as divided in two parts. The first part is a sensor in which the magnetic field is normally mounted along the pipeline. The second part is the transducer. This is where all the conversions of the measured variable into a desired form in terms of the electrical signal take place. Figure 3.6 involves two photographs **h**at show the actual physical form of the sensor and transducer parts of the type of flowmeter installed on the pilot plant. The operating range for FT 120 is 0.300L/h and as for FT121 is between 0.350L/h. Again the output range for these meters is 4-20mA. There was no need for adjustment or recalibration of these meters as they were found, from initial tests, to serve the intended purpose perfectly.



Figure 3.6: Photographs of the magnetic flowmeters

3.3.4 Control Valves

In a process control application control valves represent an important form of final element that will determine the performance of a controller. In general there are three types of control valve characteristics, which determine the relationship between the control valve opening and the actual stream flowrate as shown in Figure 3.7 (Spirax-Sarco Limited 2007). The first type of control valve characteristic is termed linear opening, the second type is called quick opening and the third type is called an equal percentage type of valve. In general terms the physical shape of the plug and the seat arrangement of the control valve characteristics. Thus the actual setting of the trim (i.e. the shape of the plug and seat arrangement) of each control valve is unique as it also depends on the process involved.



Figure 3.7: Typical characteristic of a control valve

However any given control valve is likely to have a form and characteristics broadly similar to one of these three types shown in the figure. As for the linear opening type, this form of control valve is generally required for applications in which the differential pressure drop across the control valve is relatively constant over the valve travel range. This type of situation commonly arises for control of liquid level and flow.

As shown in the figure, the quick opening characteristic valve exhibits a rapid increase in flowrate as the valve opens even with a small change of opening. The movement of this type of valve can be extremely small relative to small changes in the controller output thus the valve has an inherently high range of operability. The typical application for this type of control valve is a frequent on-off service and this type of characteristic is also useful for processes where immediate large flowrate is required.

As mentioned above, the third type of control valve is the equal percentage characteristic valve. The trim for this type of control valve has been designed so that each increment in the control valve opening will lead to an increase of the flowrate by a certain percentage of the previous flow. In general, the response for the equal percentage type of control valve is much slower or less sensitive compared to the fast opening type. This type of control valve is normally being used in processes where large changes in the pressure drop are expected. The type of control valve is also common in temperature and pressure control applications.

As mentioned previously, there are two main control valves installed on this pilot plant. Figure 3.8 shows a photograph of the actual control valves installed. The first control valve (i.e. CV121) will control the flowrate of the acid stream and the other control valve (i.e. CV122) controls the flowrate of the alkaline stream.



Figure 3.8: Photograph of the control valves

The author was not involved in designing and commissioning of the pilot plant and relatively little plant documentation was available at the start of the project. Thus the author was required to perform experiments to investigate the characteristics of each control valve. Each experiment was performed by manually controlling the opening of the control valve. As shown in the figure the "up scale" curve was obtained when the percentage of opening was initially at 0% opening and the valve opening was continuously increased upwards until the valve was fully open (i.e. 100% opening).

The "down scale" curve was obtained when the initial control valve opening was at 100% and the percentage of control valve opening was steadily decreased until the control valve was fully closed. This exercise also allowed investigation of the hysteresis error. The results of the experiment are shown in Figure 3.9. Based on the graphical evaluation, the results from the experiments show that the installed characteristic of the control valve that is controlling the acid stream is of the equal percentage type. The control valve that is controlling the alkaline stream is of the quick opening type. The results also indicate that the control valves do not have very significant hysteresis error.



Figure 3.9: Control valve characteristics

As shown in Figure 3.9, there is clear evidence of leakage at the control valve CV121 since there should be zero flow when the control valve has a 0% opening and the results indicate that there is still a measured flow of approximately 20L/h under these conditions.

This situation might be due to problems with the diaphragm or some other mechanical part of the control valve. Normally, recalibration work for a control valve involves a few specific tests such as the leak test and also a pressure test which requires special equipment and expertise. For the intended application in the work reported in this thesis the leakage does not adversely affect closed-loop experiments on the pH neutralization process as a selected and suitable range of control valve opening can be identified for normal operating conditions.

The characteristic of the control valve CV121 can be divided into three different responses as described in the Table 3.2. The responses for the first part of the range can be termed as "Low Gain Factor". This is when the control valve opening is in the range from 0% to 60% and provides a flowrate for the acid stream of approximately 20L/h to 40L/h. The second response is called a "Moderate Gain Factor" response and the corresponding range of the control valve opening is between 60% and 80%. This range will give a much greater variation of flowrate (from 40L/h to 120L/h). Within this part of the range the relationship between the control valve movement and the flowrate is more predictable and linear compared with the first range of control valve response. The last column in Table 3.2 shows the effective gain factor obtained by linearising the response over the specific range. As an example for the case of the moderate gain factor (referring to second-last column), the effective gain factor is calculated as follows:-

Effective Gain Factor =
$$\frac{\left[\text{Maximum Range - Minimum Range}\right]_{Flowrate}}{\left[\text{Maximum Range - Minimum Range}\right]_{\% \text{ controlvalveopening}}}$$
$$= \frac{\left[120 - 40\right]L/h}{\left[80 - 60\right]}$$
$$= 4L/h$$

Range		Control Valve	Effective Gain		
Control valve Opening (%)	Flowrate(L/h)	Gain factor	Factor (L/h)		
	CV121				
0-60	20-40	Low	0.33		
60-80	40-120	Moderate	4		
80-100	120-240	High	6		
CV122					
5-10	0-100	High	20		
10-60	100-300	Moderate	4		
60-80	300-320	Low	1		

Table 3.2:	Categories	of control	valve	responses
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As shown in the table a 1% change of the control valve movement will provide a 4L/h change in the flowrate in this part of the operating range. The third range is from an 80% to 100% opening and is termed a "High Gain Factor" response range. It should be noted that this third part of the range involves the same amount of control valve movement or variation as the second part (i.e. 20%). However, the fast response range will provide an even wider range of acid stream flow, from 120L/h to the maximum flowrate which is approximately 240L/h. As shown the slope of the fast response part of the range is much steeper. Thus it shows that a small movement of control valve opening will result in a large change of flowrate. Therefore the suitable range for the experiment ranges from 60% to 80% opening that is in the moderate response range.

For the control valve CV122 the response is an inverse form of the response of control valve CV121. The first 5% of the control opening provides 0L/h of alkaline flow. In order to provide 0-100L/h of flowrate the control valve opening needs to be controlled between 5% and 10%. This suggests that it is very difficult to manage the control valve movement since a 1% change of opening can produce a change of flowrate of the order of 20L/h.

As shown in Figure 3.9 for control valve CV122 the flowrate of the alkaline stream will reach 300L/h when the control valve opening is at 60%. This gives a 50% variation of control valve movement which can produce a flowrate in the range 100L/h to 300L/h. As given in Table 3.2, for this part of the range, there is a change of approximately 4L/h for every 1% opening of the control valve movement. Therefore, this is a sensible operating range for experimental work on pH neutralization process.

3.4 Data Acquisition System

As briefly explained in the previous section describing the overall system architecture the first data acquisition system installed for monitoring and controlling the pilot plant was the PlantScape Honeywell system. The system was designed for use in demonstration of the pilot plant in normal operation and was not intended for research and development. As a proprietary system it does not allow any modification of the control scheme or implementation of new control strategies. The system can only allow modification or parameter changes of its controller of specific kinds.

These limitations within the existing control system led to a need for modification and upgrading of the pilot plant to make it more suitable for research. The plant modification involved installation of a new data acquisition and supervisory computer system. Much rewiring work and testing was required and specific tests carried out included a loop test and a continuity test in order to ensure the integrity of the signals to and from the pilot plant. The new system offers much more flexibility in terms of implementation of new control schemes and dynamic testing of the system under open-loop conditions. Figure 3.10 shows a photograph of the cabinet in which the new data acquisition system was installed.



Figure 3.10: Photograph of the new data acquisition system

Some preliminary experiments were performed using the original Honeywell system. These experimental results were used to verify the pH neutralization process model which had been derived from the physics and chemistry of the system. However all work concerning the implementation of intelligent controllers and the development of a modified pH neutralization model was based on the new system.

The new supervisory computer system uses MATLAB/SIMULINK software as a tool to handle all activities of the pilot plant such as process monitoring, data manipulation and processing, process control development as well as the human-machine interface system. In addition, the system requires additional software which includes a Microsoft Visual C/C++ compiler (Version 5.0, 6.0, or 7.0) to translate the source code from programs developed in MATLAB/SIMULINK environment into a low-level machine language for real-time implementation.

The new data acquisition system is also MATLAB based and operates within the same Industrial PC (XPC) platform. The main function of this system is to allow real time communication between the engineering workstation in the control room and the field instruments on the pilot plant. While being based upon a normal PC, this system also includes analogue and a digital I/O cards and a communication card.

There are five I/O cards in total. There are two Digital Input cards and one Digital Output card to provide a gateway for digital signals. Analogue Input and Output cards cater for analogue signals in the pilot plant. A detailed list of input and output signals for the pilot plant may be found in Appendix IV. There are selector switches on the I/O cards to provide options in configuring the function of the cards. Appendix IV also provides some information about pin layout of the I/O cards and the settings selected for the switches.

The data acquisition system does not require operating system software such as DOS, Windows or Linux. It uses a boot disk that includes the XPC Target kernel to start up. There are a few settings and tests that need to be performed in order to create the boot disk and establish communication between the supervisory computer system and the data acquisition system (i.e. XPC). The communication between these two systems is based on the TCP/IP protocol. All communication settings or configurations can be made at a special user interface menu called *xpc explorer*. This user interface can be retrieved by typing a callout function called *xpcexplr* at the MATLAB command window.

The main advantage of the new system is that the users have the flexibility to develop their own Graphical User Interfaces (GUIs). The GUI is used to control and monitor the status of the pilot plant or system. Appendix V shows the layout of the developed GUI used for the experimental work on the pilot plant.

In between the XPC and field instruments there are signal conditioners. This is because all the signals to and from the field instruments are normally in current form (i.e. 4-20mA) whereas the XPC can only receive or send signals in voltage form (i.e. 1-5V).

3.5 Practical Issues Associated with the Pilot Plant

It is worth pointing out that there are some practical issues associated with the pilot plant that impact upon the overall performance and implementation of the pH neutralization process.

i. Process for Preparation of the solutions

As explained earlier, the concentration of both solutions is very important. Concentration values can have a major influence on the pH process even though the difference between the actual concentration value and the desired concentration value may be very small. Thus it is important to prepare the concentration value as close as possible to the desired value. However, due to practical issues, this is not a straightforward task.

In order to prepare each solution the conductivity value must first be recorded. The next step is to fill the appropriate tank with water until it reaches the maximum operating level, which is 250L. There is no accurate measurement available to provide an exact indication of the level of the solution but an attached sight glass provides some guidance. The highly concentrated solution (i.e. 18M for acid and 17.5M for alkaline) must then be added. The required amount of the concentrated solution, AV, is based on the formula given below in Equation 3.1.

$$AV = \frac{(DC \times MV) - (CC \times MV)}{HC - DC}$$
3.1

In this equation the desired concentration value is DC, the current concentration value is CC and the concentration value for the concentrated solution is HC, while MV represents the maximum volume of solution.

The solution must be stirred by means of a rod to ensure that it mixes perfectly. Usually the process will not end at this point and an additional adjustment involving further amounts of the concentrated solution is required and sometimes additional water in order to obtain the required concentration.

ii. Limitations of the new DCS system

The new DCS system, which is based on the MATLAB/SIMULINK environment, is not an established distributed control system intended specifically for process control applications. Thus initial setting up of the system required a considerable amount of work and proved very time consuming. The communication between the data acquisition system and the supervisory computer system was found to be somewhat unreliable and it is suspected that this problem may be associated with hardware issues.

There are also some limitations in terms the software. The graphic user interface for the system is too simple and is not sufficiently user friendly. Thus process monitoring, trending and achieving the process variable can be less straightforward that it ideally should be and can be somewhat limited in scope. Some of the toolboxes are not capable of being used in this real-time application. Although the software allows development of new functions there are however too many functions that need to be developed. In addition, the development of new functions requires time and an in-depth knowledge of the MATLAB software system.

CHAPTER FOUR

<i>4.0</i>	MODELLING AND SIMULATION OF THE pH	
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4.0 MODELLING AND SIMULATION OF THE pH NEUTRALIZATION PROCESS PILOT PLANT

In broad terms, this research study can be divided into two main activities. The first of these involves process model development, together with internal verification of the associated simulation model and subsequent external validation of the model from test data obtained from open-loop and simple closed-loop tests carried out on the actual plant. The second, activity is controller design and development, involving preliminary controller evaluation using simulation and, finally, implementation and testing on the pH neutralization pilot plant itself.

The dynamic model of the process has been derived from the application of fundamental physical and chemical principles to the system, using a conventional mathematical modelling approach. This chapter describes in detail the development of this pH neutralization plant model. The model of the pH neutralization plant is based on the system configuration described in Chapter 3. Figure 4:1 is a flowchart which summarises, in a simplified fashion, the modelling approach adopted and this flowchart provides a useful guideline which was followed throughout the process of developing the model of the plant.

The first stage of the process involves defining the goal, or the required specification, for the developed model at the end of the modelling process. This goal is to develop a pH process model that is adequate in terms of the intended application which is the development of an improved form of controller. It was decided that the simulation model should be able to represent the behaviour of the pH neutralization pilot plant with sufficient accuracy in terms of the type of steady state and transient performance measures that commonly provide a basis for control system design.


Figure 4:1: The flowchart of the modelling process

As shown in Figure 4:1, the modelling process is not a straightforward task involving simple linear progression from one stage to the next. There are two decision points that may make the modelling process return to earlier stages until a model that is acceptable for the intended application is produced. The first decision point is at the Simulation Model Analysis block and the other is at the Model Validation block. At the simulation model analysis stage, the main concern is internal verification of the simulation model to determine whether or not the computer representation is consistent with the underlying mathematical representation and also whether or not the solution of the model using simulation tools is correct.

Internal verification (Gong & Murray-Smith 1998;Murray-Smith 1998;Murray-Smith 2000;Rudolfs 1953) of the simulation model involves ensuring that the equations of the simulation are the equations of the model so that it fully represents the underlying mathematical description and also ensuring that there are no issues of numerical inaccuracy or numerical instability in the implementation of the simulation model. Some more fundamental validation can also be carried out at this stage to check, for example that the simulation behaves in a fashion that is generally appropriate for the given sets of test conditions. Theoretical knowledge and physical understanding of the plant itself, together with results from previous work done by other researchers, can provide a useful basis for comparison at this stage.

At the formal model validation stage, the emphasis is on external validation processes, with the dynamic response from the developed simulation model being critically evaluated through comparison with experimental results. The main idea of this exercise is to determine whether the developed simulation model is able accurately to represent the pilot plant in terms of the given specification.

As shown in the figure, at both these stages in the flow graph, the developed model is being evaluated. If the model is satisfactory it will be possible to move to the next stage of the process of model development but, if it is not acceptable, the procedure must then involve returning to an earlier stage. The evaluations and decisions must be based on the goal set at the beginning of the modelling process.

4.1 Overview of the pH Neutralization Process Modelling

A rigorous and generally applicable method of deriving dynamic equations for pH neutralization in Continuous Stirred Tank Reactors (CSTRs) was presented by McAvoy in the year 1972 (McAvoy, Hsu, & Lowenthals 1972). The research work done by McAvoy was essential to the development of the fundamental modelling approach of the pH neutralization process in CSTRs.

As cited and described in other literature, the use of the CSTR in developing the pH neutralization model was started over 50 years ago by Kramer (1956) and by Geerlings (1957). However those early studies concentrated largely on the dynamic behaviour of the pH electrode system. Subsequently, two crucial points in developing a pH neutralization process model which describes the nonlinearity of the neutralization process have emerged from published research. The two points are as follows:-

- i. Material balances in terms of hydrogen ion or hydroxyl ion concentrations would be extremely difficult to write down. This is due to the fact that the dissociation of water and resultant slight change in water concentration would have to be accounted for.
- ii. Instead, material balances are performed on all other atomic species and all additional equilibrium relationships are used. The electroneutrality principle is used to simplify the equations.

The basic equations describing the chemistry underlying the pH neutralization process in the early work by McAvoy was tested and validated through experimental work involving small-scale bench-top processes. In those investigations the stirred tank typically had a volume of 1L and the total flowrate for acid and alkaline was held constant at 600cc/min. The translation of such models to represent the processes involved in a full-scale process or pilot plant presents a further challenge. The challenges might be due to mixing efficiency, transport delays, unwanted signal noise, accuracy of the measurements and some other unexpected causes.

In 1983 Gustafsson and Waller (Gustafsson 1982;Gustafsson & Waller 1983a) reinforced McAvoy's modelling principles for pH neutralization processes and emphasised the fact that mass balances on the invariant species are inherently independent of reaction rates. As described in this paper, the "invariant species" is actually the species that remain chemically unchanged by the governing of reactions in the neutralization process whereas the "variant species" are the species that change in the neutralization process, such as the hydrogen ions.

The main contribution of this work by Gustafsson and Waller was a matrix formulation that generalised the approach. Their model and all the associated research were also based on the CSTR configuration.

Another interesting and widely used account of work involving the modelling of a pH neutralization process is by Wright and Kravaris (Wright & Kravaris 1991). Their work provided a new approach to the design of nonlinear controllers for pH processes by defining an alternative equivalent control objective. That new approach results in a control problem that is linear. A minimal order model was produced by assuming that the flowrate of the titrant required to operate the reactor was negligible in comparison with the flow rate of the process streams.

There are many useful papers that have presented and discussed issues concerned with the design of an appropriate controller for the pH neutralization process using the fundamental pH model. Some of the references such as (Shinskey 1973, Kelkar & Postlethwaite 1994, Henson & Serborg 1994, Wright & Kravais 1991, (Gustafsson 1982;Gustafsson & Waller 1983a)) have been discussed in Chapter 2. These papers have been used as a guideline in this work concerned with developing an adequate mathematical model of the pilot plant.

All the procedures outlined in the publications mentioned above have involved the making of assumptions to reduce model complexity. Without such assumptions models can present computational difficulties and can involve major problems in terms of validation and tuning. As suggested in previous studies, the assumptions underlying the modelling of the pH neutralization process are as follows:-

- i. The acid and alkaline solutions in the reactor tank are perfectly mixed at all times and a lumped parameter compartmental form of model can be used.
- ii. The acid-base reaction process in the reactor tank is instantaneous and isothermal.

- iii. The dissociation of acid and base reaction is complete and the attainment of equilibrium is fast.
- iv. No other reactions occur in the reactor tank.
- v. The time constants for the control valves and measuring instruments are negligible compared to those of the process.
- vi. The volume of the solution in the tank is constant.

Generally, most of the assumptions mentioned above are suitable for a bench-top laboratory-scale reactor setup. Results from the previous studies show that the assumptions are appropriate and that the responses from the developed models are similar to the results obtained from the laboratory test-bed configuration. Thus these assumptions will be used and applied as an initial step in the modelling approach.

The primary advantage of this research is the availability and configuration of the pH neutralization pilot plant. The pilot plant configuration represents a practical industrial system, albeit on a relatively small scale. As described earlier, the volume of the reactor tank is 100 times bigger than the one used in the McAvoy experimental setup. Theoretically, a small volume of a stirred reactor tank should provide a more efficient and a more perfectly mixed process. With a larger volume in the stirred reactor tank it is more difficult to remove the influence of uncertainties on the dynamic response of the process especially in terms of the mixing process. Therefore, it was recognised, from the outset of the work, that at the model validation stage the experimental results should provide some important insight concerning the model structure, especially in terms of the mixing process. This could well result in some additional function blocks being added to form a modified pH process model to represent the pilot plant. Thus the combination of the fundamental approach based on physical principles used by previous researchers and suitable practical measured data should, hopefully, provide a more realistic pH neutralization model having a level of accuracy that is at least sufficient for the intended control application.

4.2 Preliminary Development of the Mathematical Model

The second block in the flowchart of Figure 4:1 involves identifying and specifying the pH process in detail. The common approach that facilitates this exercise involves sketching the process diagram of the system. In the case of the pH neutralization process model for this stage, the configuration of the plant has been simplified into the form of a Continuous Stirred Tank Reactor (CSTR) model as shown in Figure 4:2. A detailed description of the pH process neutralization pilot plant can be found in Chapter 3. However this diagram and the current section provide a useful summary of some of the most important information relating to the reactor tank, including the key variables involved and boundaries of the model.

In this schematic diagram the volume of the reactor tank is 80L. The flowrate for the acid and alkaline streams are F_1 and F_2 respectively. The flowmeters provide a flowrate of between 0-300L/h and 0-350L/h for the acid stream and alkaline stream respectively. The concentration for acid in tank VE100 is C_1 and the concentration of alkaline in tank VE110 is C_2 . The selected range for both conductivity meters is from 0 to 200mS.



Figure 4:2: A schematic diagram for the pH neutralization process

As mentioned earlier, the formulation of the process dynamic model is based on fundamental principles. The first principle that is applied is known as the conservation balance principle. The conservation balance equations that are commonly used in process control are the equations for conservation of material, energy and momentum. As far as this research is concerned the variables involved relate to the total liquid mass in the reactor tank and the principle of conservation of material is used in the derivation of the basic equations of the process. The general equation for the conservation of material for the pH process may be written as follows:



Based on this general equation, two equations have been derived to express the pH process in the CSTR system. The derivation of these equations follows the general approach adopted by previous researchers in this field (e.g. (McAvoy, Hsu, & Lowenthals 1972;Mwembeshi, Kent, & Salhi 2001;Nie, Loh, & Hang 1996)).

$$V\frac{d\boldsymbol{a}}{dt} = F_1 C_1 - (F_1 + F_2)\boldsymbol{a}$$

$$\tag{4.1}$$

$$V\frac{d\boldsymbol{b}}{dt} = F_2 C_2 - (F_1 + F_2)\boldsymbol{b}$$
(4.2)

As described earlier, the volume V represents a constant volume of 80L of the reactor tank. The flowrates for the acid and alkaline streams are F_1 and F_2 respectively. The concentration for acid in tank is C_1 and the concentration of alkaline in tank is C_2 .

The non-reactant components in the system are a for acid and b for alkaline. These variables are defined in Equation (4.3) and Equation (4.4) as:

$$\boldsymbol{a} = [H_2 S O_4] + [H S O_4^-] + [S O_4^{-2}]$$

$$\tag{4.3}$$

$$\boldsymbol{b} = [Na^+] \tag{4.4}$$

The next step is to identify and derive the electroneutrality condition of the nonreactant components. Based on the principle of electroneutrality all solutions are electrically neutral. There is no solution containing a detectable excess of positive or negative charge because the sum of positive charges equals the sum of negative charges.

The total electroneutrality condition is,

$$[Na^{+}] + [H^{+}] = [OH^{-}] + [HSO_{4}^{-}] + 2[SO_{4}^{-2}]$$
(4.5)

The equilibrium constant expressions that apply to the acid-base system are,

i. Water (H_2O)

$$K_{w} = [H^{+}][OH^{-}] \tag{4.6}$$

ii. Sulphuric Acid (H_2SO_4)

$$K_1 = \frac{[H^+][HSO_4^-]}{H_2SO_4}$$
(4.7)

$$K_{2} = \frac{[H^{+}][SO_{4}^{-2}]}{HSO_{4}^{-}}$$
(4.8)

The quantity K_w (the constant value for the ionic product of water), is equal to 1.0 x 10^{14} . There are two acid dissociation constants for sulphuric acid $K_I = 1.0 \times 10^3$ and $K_2 = 1.2 \times 10^{-2}$ since sulphuric acid falls under category of a diprotic acid, having two equilibrium points or dissociation points. However for this case, the first point is negligible as the first dissociation constant, K_I is too large. Theoretically the titration curve for this acid-base reaction process will only show one break point or equilibrium point.

The pH scale is a measure of the hydrogen ion concentration, thus the pH value can be calculated by using the equation below.

$$pH = -\log_{10}[H^+] \tag{4.9}$$

Equation (4.5) needs to be solved in order to find the value of the hydrogen ion, $[H^+]$. Eventually, after substitution of Equations (4.3), (4.4), (4.6), (4.7) and (4.8) into Equation (4.5) the final equation can be written as a polynomial equation (4.10).

This is commonly referred to in the literature as the *pH equation*.

$$[H^{+}]^{4} + a_{1}[H^{+}]^{3} + a_{2}[H^{+}]^{2} + a_{3}[H^{+}]^{1} + a_{4}$$
(4.10)

Where the coefficients a_1 to a_4 are defined as follows;

$$a_1 = K_1 + \boldsymbol{b} \tag{4.11}$$

$$a_{2} = \boldsymbol{b}K_{1} + K_{1}K_{2} - K_{w} - K_{1}\boldsymbol{a}$$
(4.12)

$$a_{3} = \boldsymbol{b}K_{1}K_{2} - K_{1}K_{w} - 2K_{1}K_{2}\boldsymbol{a}$$
(4.13)

$$a_4 = -K_1 K_2 K_w \tag{4.14}$$

Figure 4:3 shows the MATLAB/Simulink blocks that represent the pH neutralization process model resulting from the above physico-chemical modelling procedure. Generally, there are three main parts that influence the behaviour of this physically based model of a pH neutralization process and these relate to the above equations. The first block is the dynamic part, which involves the differential Equation (4.1) and Equation (4.2). Apart from these equations, the nonlinearity of the model will be influenced by Equation (4.10) which forms the second main block. The final block involves calculation of the pH value, and this is based on Equation (4.9).



Figure 4:3: MATLAB/Simulink blocks of the pH neutralization on process model

The next stage of the process modelling process is Model Analysis. At this stage the main objective is to analyse and evaluate the dynamic response of the developed model to determine whether the response is acceptable, at least to the extent that it satisfies the formulation. If the developed model does not produce the expected dynamic response then the previous stage of process modelling will have to be repeated. The selected simulation results and analysis are described in the next section. Following completion of Model Analysis it is then necessary to compare simulation results with the experimental results in greater detail within the Model Validation stage.

4.3 Experimental Results from the Enhanced Data Acquisition System

As explained in the previous chapter, the software environment for the enhanced data acquisition system is based on MATLAB/Simulink software. At this stage in the research (i.e. external model validation) it was appropriate to use the capability of the software available in the new combined data acquisition and simulation system to further analyse and investigate the dynamic response of the pilot plant and the corresponding behaviour of the simulation model. Further investigations involving the developed pH model and comparisons with experimental results were all based on data obtained using the enhanced data acquisition system.

For these tests, which involve a continuous process, the reactor tank is filled with solution up to the maximum level (i.e. 80L) and the level will be constant as there is flow going out from the tank at this point. The initial pH value of the solution in the reactor tank may be set to a desired value by controlling the two valves for the acid and alkaline streams manually. In order to represent this experiment in terms of a computer simulation it is appropriate to use the pH model for the continuous process of Figure 4.3.

Two experiments were carried out to provide more information about the dynamic behaviour of the pH neutralization process. The results from these experiments were used to validate, in a more quantitative way, the developed pH model described in the previous section and led to important refinements of the model. The first of these experiments involves a step change of flow in the alkaline stream. During the experiment the control valve for the acid stream was set to the fully closed position.

Figure 4:4 shows the dynamic response of the pH neutralization process for the pilot plant for the first experiment. In principle, in this experiment the initial pH should be set to the lowest possible value. However the process to achieve the lowest pH value is quite time consuming as the reaction process in this region is very slow. In addition it requires quite a lot of acid solution to bring down the pH value to the

lowest value possible. Thus it is a rather impractical and expensive procedure. Based on several trials, a pH value of 3 was chosen as a reasonable initial pH value for this experiment.



Figure 4:4: Experimental results obtained using the enhanced data acquisition system during a test involving a step change of the flow rate for the alkaline stream.

As shown in Figure 4:4, before the experiment started the pH value had been brought down, approximately, to the specified initial pH value of 3. At t = 150 sec. the process continues with the average flowrate for alkaline stream in the reactor tank being suddenly increased from zero to a steady value of 135.92L/h. The conductivity meters provided average readings for the acid and alkaline solutions of 23.68mS and 10.29mS respectively. Based on these values for the conductivities of the solutions in the two tanks, the results indicate that the concentrations of both of the solutions were slightly below the expected concentration value of 0.05M, with a concentration value for the acid solution of 0.0485M and a value of 0.0489M for the alkaline solution. Figure 4:4 shows clearly the nonlinearity of the process with various different reaction rates as the response moves through the operating range in terms of pH values. The dynamic response can be divided into five different regions with three different reaction rates as given in Table 4.1.

Range of pH Value	Reaction rate
3-4	Low
4-6	High
6-8	Moderate
8-10	High
10-12	Low

 Table 4.1: Process reaction rate of the dynamic response

The dynamic behaviour shows two different equilibrium points. The first equilibrium point, pK_1 is approximately at a pH value of 3.2 and the second point, pK_2 is at a pH value of 6.8. As explained previously, the equilibrium (or break point) depends on the value of the dissociation constants. Theoretically, sulphuric acid will have two break points as it is categorised as a diprotic acid. However, due to the first dissociation constant being fairly large, the first break point cannot be seen on the titration curve.

As shown in Figure 4:4, it is believed that the dissociation constant for the acid solution has been decreased due to some other reaction in the acid tank. In this experiment the sulphuric acid was added to water and it is believed that an additional and unknown source of hydrogen and hydroxyl ions existed. Such a situation will make the ionic strength of the solution decrease and as a result the dissociation constant will also decrease.

The results from the second experiment are presented in Figure 4:5. It shows another interesting dynamic response of the pH neutralization pilot plant. The idea of this experiment is not exactly the same as the previous experiment where the main aim was to obtain the process reaction curve of the neutralization process.



Figure 4:5: The dynamic response from the neutralization pilot plant for square-wave variation of alkaline flowrate with constant flowrate of acid solution.

The objective for this second experiment was to obtain further insight about how to control the alkaline stream and the pH value in the reactor tank with a constant flow in the acid stream. The initial pH value was set to a pH value of 7. The valve that is controlling the acid stream was set to an opening which provided an average flow value of the acid stream of 61.5L/h. The alkaline stream was set to behave as a square wave signal with a period of 50s. The average flowrate value of the alkaline stream at the peak was 273.68L/h.

The average concentration value for the acid was slightly higher (0.0475M) than for the alkaline solution (0.0465M). As shown in the figure, the initial pH value is at a pH value of 7 and the dynamic response of the pH value increases towards the upper range of the pH scale as the experiment continues. This is an expected dynamic response as the flowrate of the alkaline stream is three times larger than the flowrate of the acid stream. Thus there will be more sodium hydroxide than sulphuric acid at the end of the experiment.

Computational work was carried out to simulate the two experiments outlined above. The simulated experiments were based on the actual settings and configuration as given in Table 4.2 and described in the previous paragraph. The simulation results in terms of the dynamic responses obtained from the developed model for both experiments are shown in Figure 4:6 and Figure 4:7.

Simulation	Concentration		Flowrate	
Simulation	Acid	Alkaline	Acid	Alkaline
Experiment 1 (Process reaction curve)	0.0485M	0.0489M	Step change from 60L/h to 0L/h at 500 th second	Step change from 0L/h to 135.92L/h at 1150 th second
Experiment 2 (Square wave signal for alkaline stream)	0.0475M	0.0465M	Constant flowrate at 61.5L/h	Square wave signal with period of 50s and peak flowrate of 273.68L/h

 Table 4.2: Parameter settings for the simulation work

Figure 4:6 shows the dynamic response for the first experiment. This simulated dynamic response should be similar to the actual response obtained experimentally from the pilot plant during the step response test, as shown in Figure 4:4. The simulated dynamic response that represents the second experiment (i.e. using a square-wave signal to vary the flowrate of the alkaline stream) is shown in Figure 4:7. The dynamic response obtained from this simulation experiment should be similar to the corresponding experimental result obtained from the test carried out on the pilot plant and shown in Figure 4:5. The simulation results shown in Figure 4:6 and Figure 4:7 show clearly that the dynamic responses from the actual pilot plant in a number of ways. These results suggest that there are further investigations and modifications of the pH process model that need to be carried out.



Figure 4:6: Dynamic response – simulation of Experiment 1



Figure 4:7: Dynamic response – Simulation of Experiment 2

As mentioned earlier the pH process model was developed following some assumptions introduced to make the model simpler in structure and computationally more convenient to translate into a simulation. The experimental results and the findings from the simulation model suggest that some of the assumptions should be reconsidered. The next section describes some modifications to the pH process model introduced in order to make the pH dynamic model more realistic. Issues such as imperfect mixing, dissociation of acid and base reaction and time constants for control valves are highlighted.

4.4 Empirical Modelling for Development of the Modified pH Model

Figure 4:8 shows the MATLAB/Simulink block for the new pH neutralization model that represents the pilot plant. There is an additional block that is the initialisation block. The purpose of the initialisation block is to make sure that for the first 15 seconds the dynamic response in terms of the pH value stabilises at a certain value which is normally a pH value of 7. This condition actually represents the pH value in the reactor tank before any experiment is performed.



Figure 4:8: MATLAB/Simulink representation of the modified pH model

The investigation will be focussed mainly on the dissociation constants of the acid solution. The simulation work will be based on the two experiments that have been discussed previously. The parameter settings for the simulation work in this experiment will be the same as in Table 4.2.

4.4.1 Investigation of the values of the dissociation constants

As mentioned the investigation was to determine the dissociation constants of the acid solution from the process reaction curve in Experiment 1 (i.e. Figure 4:4). A similar approach to determine the dissociation constant of the acid solution, which is based on the titration curves will be used as a guideline (Bates 1973;Christian 2004b).

Therefore, based on the process reaction curve in Figure 4:4, the graphical approach was used to calculate the dissociation constants as described in (Bates 1973;Christian 2004b).

i. First dissociation constant, K_1

$$pK_1 = -\log K_1$$

$$K_1 = anti \log(-pK_1)$$

$$= 6.31 \times 10^{-4}$$

ii. Second dissociation constant, K_2

$$pK_2 = -\log K_2$$

$$K_2 = anti \log(-pK2)$$

$$= 1.59 \times 10^{-7}$$

Figure 4:9 shows the simulation result obtained for a similar simulation model as that used in the simulation experiment described above but using the modified values of the dissociation constants. As shown, the first 1000s brings the pH down to a pH value of 3. At time t = 1150 sec. the flowrate of the alkaline stream is increased to the average alkaline flowrate of 135.92L/h. All parameters are exactly the same as in Table 4.2 for Experiment 1. The dissociation constants used in this simulation work are $K_1 = 6.31 \times 10^{-4}$ and $K_2 = 1.59 \times 10^{-7}$. As shown in Figure 4.9, the dynamic response from the simulation based on the modified pH model has a similar pattern to the dynamic response from the pH neutralization pilot plant itself (Figure 4:4). It has two equilibrium points which are at pH values of 6.8 and 3.2. The dynamic response reaches a pH value of 8 at a time which is approximately 360s after the application of the step change of alkaline flowrate. This time (i.e. 360s) is almost the same as the time found in the actual experiment for the pilot plant for the pH to reach a value of 8 (Figure 4:4). Thus the modified pH model has shown very encouraging results when compared with the behaviour of the real pilot plant for the step test experiment.

Figure 4:10 shows the simulated dynamic response from the modified model for the second experiment. As shown in the figure the dissociation constants have made significant improvement as compared to the previous simulated response shown in Figure 4:7. However the dynamic response in Figure 4:10 is not exactly the same as the response from the actual experiment (i.e. Figure 4:5). The next section will evaluate in detail the performance of this modified model which was based on this figure (Figure 4:10). This will indicate whether the response of the developed model is similar to the response from the pilot plant or otherwise and will be used to assess whether the model has the accuracy required for the planned control system design application.



Figure 4:9: Dynamic response from the modified pH model – Experiment 1



Figure 4:10: Dynamic response from the modified pH model – Experiment 2

4.4.2 Evaluation of the Modified Model

The evaluation of the modified pH model is very important in order to ensure that the developed model is able to provide an adequate dynamic response in comparison with the actual dynamic from the pilot plant. Several issues of model accuracy and external validation for control system design have been highlighted by Murray-Smith in his papers (Murray-Smith 1998;Murray-Smith 2006).

Murray-Smith has also suggested a few methods on external validation in which will provide a good indication of the closeness of the developed model with the actual system (Murray-Smith 1998). One of the suggested methods that provides more quantitative information than is possible from a graphical comparison involves Theil's Inequality Coefficient (TIC).

The equation of the TIC is defined as follows:-

$$TIC = \frac{\sqrt{\sum_{i=1}^{n} (y_i - z_i)^2}}{\sqrt{\sum_{i=1}^{n} y_i^2} + \sqrt{\sum_{i=1}^{n} z_i^2}}$$
(4.16)

This equation involves comparison of two time series; the measured response from the actual plant, y_i and the corresponding response from the developed model, z_i . Thus the numerator of the equation is actually the sum of the squares of the error values representing the difference between the actual value and the simulated value. As explained in the paper the main advantage of this method is that the calculated value of TIC ranges between zero and unity. If the TIC value is close to zero it will indicate that the response of the developed model is very similar to the response from the pilot plant. However if the value is close to one it will show that the dynamic of the developed model is significantly different from the actual response.

Figure 4:11 shows a comparison between the first model and the modified model. It may be seen that there are distinctly different dynamic responses for the three cases presented. This first dynamic response (i.e. Figure 4:11(a)) is the response from the first model that was developed. This is exactly the same as the dynamic response shown in Figure 4:7.

Simulation results shown in Figure 4:11(b) were based on the modified pH model and was obtained for the same set of condition as in Figure 4:11(a). All of these simulation results correspond to the experimental record shown in Figure 4:11(c) and represent the response to a periodic test input.



Figure 4:11: Dynamic responses of the model for the original and modified configurations

As shown in the Figure 4:11(a) the pH response fluctuates in the range between pH value 4 and pH value 10 from the start of the simulation. This transient does not adequately represent the actual dynamic response from the pH neutralization pilot plant. The impact of the new value for the dissociation constant can be observed by comparing Figure 4:11(a) and Figure 4:11 (b). The new response obviously shows a significant improvement in terms of the overall pattern of the dynamic response. The overall pattern and shape is quite similar to the dynamic response from the experiment. However, in the first 150 seconds the pH value increases rapidly unlike the actual response from the pilot plant.

Thus this initial behaviour of the simulation indicates the main differences between the model and the actual dynamic behaviour from the pilot plant. As shown in the figure, the first significant difference is the initial high peak for the pH response. At the 50th second the peak for the response is approximately at a pH value of 8.4. This does not correspond to the actual dynamic response from the pilot plant around that time, as shown in Figure 4:11(c), where the response at t=50 s is only slightly above a pH value of 7 and thus is very close to the initial value.

Figure 4:12 shows the distribution of error for this simulation. This plot represents the difference between dynamic responses in Figure 4:11(c) and Figure 4:11(b). As mentioned previously, in this simulation work actual measured data (i.e. the actual measured values for the concentrations of acid and alkaline as well as the flowrate for both streams) obtained from the pilot plant are used as input time histories in simulating the behaviour of the pilot plant. The overall pattern of the dynamic response from the modified pH model is quite similar in most respects to the response obtained from the pilot plant. Table 4.3 shows the summary of the performance of the modified pH model from a quantitative perspective. A total of 500 samples were considered in the analysis of these simulation results. The data obtained in the actual experiment act as the true values or expected values that the modified pH model needs to match.



Figure 4:12: Distribution of error



Descriptions	Pilot Plant	Modified pH Model	
Min pH Value	6.83	7.18	
Max pH Value	9.73	9.63	
Min Error	-1.44		
Max Error	0.54		
Average Absolute Error	0.5		
TIC Value	0.036		

As shown in the table the minimum pH value in the reactor tank from the experiment is a pH value of 6.83 which is lower than the simulated minimum value of 7.18. However the highest pH value for the actual pilot plant is pH value 9.73 and for the modified model the corresponding pH value is 9.63. This, together with the graphical results (i.e. Figure 4:12) shows that the error between the actual pilot plant and the modified pH model is higher in the initial part of the response, especially for the first 150s of the experiment. However the error decreases in the later part of the experiment.

As given in the table the error indicates the difference between the true value and the value from the simulation results. As shown in the table, the modified pH model produces error values that range from -1.44 to 0.54. These two values provide the range of the accuracy of the developed model.

The actual value from the pilot plant at this minimum and maximum error is 7.33 and 9.23 respectively. The accuracy of the pH model is determined by using the following equation. This will show the ability of the pH model to match the actual value from the actual experiment.

$$Accuracy(\%) = \left(1 - \frac{|Error|}{\text{True Value}}\right) \times 100\% \tag{4.17}$$

As shown in the table (i.e. min error and max error values) the modified pH model is able to produce a level of accuracy between 80.35% and 94.15%.

As mentioned at the beginning of this section the objective of this exercise is to develop a pH neutralization model that can represent the dynamic behaviour of the neutralization pilot plant with 80% accuracy. It appears, therefore, that the objective has been achieved.

Further evidence to support the conclusion that the modified model is adequate comes from analysis of the TIC measure. As explained at the beginning of the section, the TIC value gives a good indication of the performance of any developed linear or nonlinear dynamic model. As given in the table, the TIC value for the modified pH model is 0.036. This value is very much closer to zero than to a value of one which supports the observation that the dynamic response from the developed model is similar overall to the dynamic response from the pilot plant. As suggested by Murray-Smith in his paper (Murray-Smith 1998), a TIC value that is smaller than 0.3 generally will give a level of agreement between the developed model and the actual transients that is adequate for applications such as control system design. The TIC value provides a quantitative measure of model performance that can be useful in further model optimisation and tuning.

Generally, the modified pH model has demonstrated adequate performance compared with the actual pilot plant data. Thus, in general terms, the development of the nonlinear dynamic model for the pH plant has been achieved. The simulation results demonstrate behaviour that is quite similar to the actual pilot plant, taking into account the uncertainties in measured quantities and model parameters.

However there are still some improvements that can be made to the modified pH model in order to increase the accuracy of the pH model. As highlighted the dissimilarity at initial response suggests that the model could be modified and enhanced further. The discrepancy between the initial behaviour of the system and model are suggestive of some issues in terms of imperfect mixing or valve characteristics. Some additional experimental work to investigate the efficiency of the mixing process, the transport delays of the controlled stream and also the movement of the actual control valve need to be carried out.

If there are significant findings that suggest additional dynamics need to be incorporated with the pH model there should be a further stage of model refinement and optimisation. It is believed that with these additional representations and more rigorous external verification and evaluation, the developed pH model will be able to represent the behaviour from the pilot plant accurately.

Some preliminary work on the effects of imperfect mixing has been carried out. The general idea of the approach for the imperfect mixing model development was based on previous work by Bar-Eli & Noyes (Bar-Eli & Noyes 1986). However the dynamics of the imperfect mixing model were represented by a simple first order lag and pure time delay instead of a more complex form of mathematical representation developed-- in the paper. The first order lag with pure time delay was chosen to represent the imperfect mixing characteristics as this form of model structure had previously been found to be useful in representing complex behaviour in terms of the dynamics of a helicopter rotor (Black & Murray-Smith 1989;Bradley, Black, & Murray-Smith 1989). The successful use of simple dynamic elements of this kind to represent modelling uncertainties in the helicopter application led directly to consideration of its use in representing the uncertainties of the mixing process. It is consistent also with one of the simpler forms of lumped-parameter model structure suggested in the paper by Bar-Eli and Noyes referred to above. The response of the pH model with an additional block representing imperfect mixing was inconclusive in the absence of further experimental evidence. In addition, measures of goodness of fit between the simulation results and the corresponding experimental time history were not significantly different from the response without this additional block. Further optimisation of the parameters representing the imperfect mixing process was not attempted in the absence of additional experimental data as it was not believed that this was justifiable on the basis of the available data sets from the pilot plant.

CHAPTER FIVE

5.0	DEVELOPMENT OF A CONVENTIONAL PROPORTIONAL PLUS	
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5.0 DEVELOPMENT OF A CONVENTIONAL PROPORTIONAL PLUS INTEGRAL (PI) CONTROLLER FOR THE PILOT PLANT

As an introduction this section will provide an overview of the Proportional Plus Integral and Derivative type of controller (PID controller) in this type of process application although, in the specific case of this pilot plant, the development process led to a decision to use a Proportional Plus Integral (PI) controller and to dispense with the Derivative component. In reaching such a decision it is of considerable interest and importance to understand fully the impact of each individual control action on the behaviour of the controlled system. The PID form of controller has been used successfully in the process industries since the 1940s and remains the most widely used algorithm today for a very wide range of applications. The success of this type of controller is due to the fact that the PID control algorithm is very simple in structure, the controller is relatively easy to design for most applications and has properties that make it much more straightforward to understand in simple physical terms than many other forms of controller. It therefore provides a kind of standard against which the performance of other forms of controller may be compared.

In the simplest forms of PID controller there are three adjustable control parameters that influence the control performance and, in most cases, PID control algorithms are able to provide a reasonably good performance when the adjustable control parameters have been properly tuned. However the control performance also depends on the nature of the process. Processes having significant nonlinearities are, inevitably, more difficult to control than processes with more linear characteristics using the PID algorithm because parameter values of the controller that are optimised for one part of the operating range may be completely inappropriate for some other operating point. For such cases a simple PID controller is very often unable to provide a satisfactory level of control performance and in applications involving significant nonlinearity in the process plant some non-zero tolerance level needs to be defined for the steady-state error and a range of acceptable dynamic performance has to be considered.

5.1 Overview of the PID Controller

Generally a PID controller has three control terms; Proportional, Integral and Derivative. The proportional term is a simple gain factor and provides a means of influencing the rate of adjustment of the manipulated variable. For most process applications the proportional control action has a very straightforward effect on the performance of the controller, especially in terms of the influence of this term on the overshoot and rise time of the output response to a step change of reference. This control action is capable of reducing the offset error but it does not provide a zero offset in typical process applications involving a Type 0 plant transfer function.

The second term in the PID controller is the integral action term. The main advantage of this control action is its influence on the final steady state error value, although it adjusts the manipulated variable in a slower manner than pure proportional action and the integral action can have a destabilising effect in terms of the dynamic response of the closed-loop system. Integral action is capable of bringing the steady state output value to the desired set point with zero offset for a plant that shows linear behaviour and may be described by a Type 0 transfer function.

In the PID controller one important issue that arises with the integral action is the phenomenon of "Integral Windup". This problem is associated with saturation effects and occurs when the integral action continues to integrate the error (in a positive or negative direction) but the manipulated variable is unable to control the process variable. This is because the control valve or other form of actuator reaches a hard limit at one end or the other of its travel (0% or 100% in the case of a control valve). There are many different anti-windup strategies which have been suggested in order to avoid this situation. As mentioned in a number of papers (Bohn & Atherton 1994;Bohn & Atherton 1995), there are three commonly used methods or schemes that can reduce or prevent the integral windup problem.

The first scheme involves clamping the integrator output at specific a minimum and maximum value. This scheme is normally referred to as a "Limited Integrator" approach. The saturation values usually correspond to the hard limit of the actuator. The main idea of this simplest scheme is that the integrator will stop integrating when the integrator output reaches the limit of the acceptable range.

The second scheme involves switching off or resetting the input to the integrator when the control signal for the actuator reaches the saturation value. The scheme is called "Conditional Integration" and requires an additional feedback loop to track the control signal. The third scheme is a classical approach called "Tracking Anti-Windup". The structure of this approach is quite similar to the second scheme involving another extra feedback loop that will track the output signal. The general idea of this scheme is that it will track the difference between saturated and unsaturated control signal and reduce the input signal to the integrator accordingly. The two papers mentioned above discuss a software package that has been developed in the SIMULINK/MATLAB environment to investigate the performance of these four different anti-windup implementations for PID controllers. Some simulation results on the capability of each scheme have also been presented and it can be concluded that the limited integrator approach is a satisfactory method, provided the integrator elements of the controller allow implementation of this form of limiting

The final control term is the derivative term. This control action will have no direct influence to the final steady state value of error. However, properly tuned, it can provide rapid correction based on the rate of change of the controlled variable. In many situations the derivative term is omitted because it tends to increase the effect of measurement noise and can thus degrade the overall performance of the controller. In cases where there is no derivative term the PID controller is reduced to a PI controller having only the proportional and integral terms and thus has only two principal parameters for adjustment. For PID and PI controllers inappropriate tuning of the adjustable parameters can result in instabilities within the controlled process.

Many previous researchers have used the performance of a PI controller as a benchmark against which the performance of other forms of controller for the pH neutralization process can be compared. In this research, the PI controller is again used as a reference against which other forms of control can be compared. This section describes the procedures followed in attempting to tune a PI controller for the pH neutralization pilot plant. Based on the performance of this controller some objectives will be outlined for more advanced types of controller (such as a Fuzzy Logic Controller).

Figure 5:1 shows the MATLAB/SIMULINK representation of the PI controller for the pH neutralization pilot plant. As shown in the figure there are two controller gains; the Proportional Gain and the Integral Gain which represent the first two control terms that have been discussed previously.



Figure 5:1: MATLAB/Simulink representation for the PI controller

Since the research is not focusing on the investigation of integral windup phenomena, the first anti-windup approach (i.e. the use of Limited Integrators) has been chosen and the other approaches have not been applied. As described above, the use of limited integrators is the simplest approach to overcome the problem of windup and involves setting low and high saturation limits on the integral action. Thus, when the output reaches either of these the limiting value, the integral action is turned off to prevent integral windup. As shown in the Figure 5:1 the MATLAB/Simulink environment includes an integrator function which has an option of limiting and allows upper and lower limits to be set by the user. The output of the integrator is determined for three different conditions. The first condition is when the output integral is less than or equal to the Lower saturation limit and the input is negative. For that case the output is held at the Lower saturation limit. The second condition is when the output integral is between the Lower saturation limit and the Upper saturation limit. The output for this situation is simply given by the integral of the input. The third condition is when the integral is greater than or equal to the Upper saturation limit. For this application involving the pH neutralization process pilot plant the limited integrator in the PI controller of Figure 5:1 was set to 0 for the lower limit and 100 for the upper limit. These values represent the fact that the position of a valve cannot be any more open than fully open (100% opening) and also cannot be driven in a negative direction beyond the fully closed condition (0% valve opening).

5.2 Simulation work on the PI form of Controller

Figure 5:2 shows the MATLAB/SIMULINK representation of the complete pH neutralization plant simulation model including the controller block with PI control. As shown in the diagrams there are two function blocks; Con1 and Con2. These blocks convert the conductivity value for acid and alkaline into an equivalent concentration value.

The CV121 block in the figure represents the control valve movement for the alkaline stream. A first order transfer function is used to provide a linearised representation of the movement of the control valve for flow values between 80L/h and 350L/h. There is no model representation for the control valve that is controlling the acid stream as the actual measured flow values will be utilised throughout the computer simulation exercise. The main function of the scaling block is to change the units of the error into a percentage so that the PI controller reacts correctly according to the value of the error.



Figure 5:2: MATLAB/Simulink representation of the pilot plant for the modified model, with a PI controller

5.2.1 Practical implementation of the PI controller

The classical approach and method most widely used in practice for establishing appropriate values for the control parameters of a PID controller is the Ziegler-Nichols tuning method (Marlin 2000). Although the approach is a proven method it may, especially in the case of highly nonlinear systems, require an modified trial-and-error procedure to find the most appropriate parameter settings. In such cases the tuning procedure often produces an implementation which gives a performance that is far from ideal in some parts of the operating range of the system.

The steps involved in this tuning approach may be described in terms of the following sequence of operations. Firstly the Proportional gain must be set to a minimum value and the other parameters (i.e. Integral and Derivative terms) should be set to give zero action. The Proportional gain should then be gradually increased until oscillations start to appear in the measured closed-loop system response. The gain should then be adjusted so that the oscillations are maintained with constant amplitude. The value of gain that is used to achieve this condition is termed the ultimate proportional gain (Gu) and the period (Pu) of the oscillation resulting from that gain must be measured.

Based on these two values (i.e. Gu and Pu) and some standard formulae (Table 5:1), all of the controller parameters can be determined. In the Zeigler-Nichols formulae for the closed loop tuning method, as summarised in the table below, the ultimate proportional gain is shown as Gu while Pu is the period of the closed loop system response using that particular ultimate proportional gain value.

Type of Controller	Р	PI	PID
Proportional, K_P	0.5Gu	0.45Gu	0.6Gu
Integral, K_I	-	1.2 <i>K_P</i> /Pu	2 <i>K_P</i> /Pu
Derivative, K_p	-	-	K_P Pu/8

 Table 5:1: Ziegler-Nichols tuning formula for a closed loop system

Several experiments were carried out for this PID tuning exercise. Based on the conductivity meters the average value of the concentration for acid and alkaline for those tests was 0.0467M and 0.0504M respectively. This batch of solution was used for the PID tuning process as well as for testing the performance of the controllers. Thus the effect of the concentration of the solution need not be considered further for this whole process.

As explained in the previous paragraph the first step is to find the value of the proportional gain that can produce a maintained oscillation. Figure 5:3 shows the responses in terms of the pH value in the reactor tank during the process of determining the suitable proportional gain. The initial value chosen for the proportional gain was 10, as shown in the first part of the time histories of Figure 5:3. However, this value is not an optimal value. This is because the amplitude of the oscillation decreases over the first 300 seconds for both responses: the pH value and the flowrate for the alkaline stream. After the 300th second the proportional gain was increased to 15. As shown in the figure the amplitude of the responses increases for about 2 cycles and then starts to gradually decrease again. This pattern indicates that the proportional gain should be increased further.



Figure 5:3: PID tuning (Experiment 1)

At the 525th second the value of the proportional gain was increased to 18. As shown in the figure, the responses in terms of the pH value and flowrate both appear to show a constant amplitude of oscillations. This suggests that 18 is the appropriate value for Gu. Figure 5:4 shows the results of the second experiment. This experiment was performed to ensure that the identified proportional gain value (i.e. Gu=18) is reliable and is able to produce the same required response repeatedly.

As shown in Figure 5:4, the amplitude in terms of the oscillatory pH response is quite consistent, with a peak-to-peak value of approximately 1.2. The flowrate for the alkaline stream also shows that it follows the same pattern for each cycle. Generally, these results indicate that the pH neutralization pilot plant is controllable even with a Proportional controller.


Figure 5:4: PID tuning (Experiment 2)

Thus, based on Figure 5:4, the ultimate proportional gain is 18 and the period for the oscillations can be determined from the period of the measured pH response signal, which is approximately 33s. The PI controller parameters can then be calculated as follows:-

Proportional Gain,
$$K_P = 0.45 \ge 18$$

= 8.1

Integral Gain,
$$K_I = (1.2 \times 8.1) / 33$$

= 0.29

The next experiment was performed to check the performance of the PI controller. The settings for the controller parameters are based on the values calculated above. However through a trial-and-error procedure the integral action was subsequently reduced to 0.03 as the controller with the calculated value of integral gain demonstrated an excessively aggressive control action. Although this value of integral gain may not be the optimal value it was used for the experimental investigation and it provided some useful general information about the capabilities of the PI form of controller.

5.2.2 Experimental and Simulation Results – Set-Point Tracking

Experimental Results

Figure 5:5 and Figure 5:6 show the performance of the PI controller with respect to set-point changes. This experiment may be termed Set-Point Tracking and involves a few step changes in the set point of pH over the range of pH values of importance for this pilot plant application. The test results start with a pH set point value of 7 and then the set-point is moved to pH values of 8, 6 and 9 and, finally, back to a pH value of 7. The duration of the experiment is approximately 950s and the concentration for both solutions is exactly the same as in the previous experiment described in section 5.2.1.

As shown in Figure 5.5, the overall performance of the PI controller is not very encouraging. When the set point for the pH is 7 the corresponding process variable from the pilot plant is approximately 6.75. This condition can be seen clearly at the 100th and 900th seconds. Also, there is approximately 20% overshoot when the pH set-point value increases from a pH value of 7 to a pH value of 8. For this particular condition the steady state of the process variable (i.e. the pH value) is still 45% below the target pH value. Typically this problem can be eliminated through further tuning of the integral action (i.e. the integral gain).



Figure 5:5: PI controller performance

However, the inherent nonlinearity of the process remains an important issue and can be seen in the closed-loop behaviour. For example, when the pH value set-point changes from a pH value 8 to a pH value 6 the offset error decreases and the measured output moves closer to the require value. However, the process variable takes quite a long time (approximately 150 seconds) to reach to the target pH value and the corresponding control valve opening for the alkaline flow is at 0% opening. Another interesting situation is observed when the set point for the pH value changes from pH value 6 to pH value 9. In this case the process variable (i.e. the measured pH value) never settles to the desired pH. Instead it oscillates between a pH value of 8 and a pH value of 9.2. As shown in the figure the alkaline flowrate also oscillates between values of 0L/h to 310L/h, approximately. The gain in this process is undoubtedly a function of the operating point and these findings suggest that nonlinearity within the acid-base reaction is the main factor that contributes to this poor control system performance. As shown in Figure 5:5 and Figure 5:6, the 60% valve opening will produce an approximate flowrate of 300L/h. The steady state value for the alkaline flowrate is approximately 110L/h, which corresponds approximately to an opening of 10%. Therefore the operating condition for the control valve is between 8% and 60% opening in order to get a flowrate of 0L/h and 300L/h respectively. These fluctuations in the control valve opening present obvious problems. In addition, it should be noted that the type of valve used in this case is the quick opening type of control valve where even very small movements will provide significant changes in the flowrate. As indicated above, the main reason for this situation is likely to be the inherent nonlinearity of the process.



Figure 5:6: Responses obtained from the system with the PI controller tuned for an operating point involving a pH set value of 8

Generally, a conventional controller like the PI controller operates in a purely corrective fashion so that when the control valve starts to make the corrective action to the pH value the error changes proportionately. In the case of this plant the acid-base reaction process will react differently at different operating points. As explained earlier, the PI controller was tuned at a pH value of 8 and it is believed that because of the nonlinearity of the reaction process the PI controller is unable to provide satisfactory control performance at other set point values

Simulation Results

Figure 5:7 shows the simulation results for the modified model with the PI controller included. The simulation work is based on the simulation model shown in Figure 5:2. The modified model used in this computer-based simulation includes the new dissociation constant values as well as the initialisation block. Data obtained from the above Set-Point Tracking experiment such as the pattern of set point changes, concentrations for both solutions as well as flowrates for the acid streams experiment are used in this simulation work.

As shown in the simulation model the actual data from the pilot plant are set point changes, concentration values for acid and alkaline, and flowrate for the acid stream. The controller parameters (i.e. proportional gain and integral gain) used in this exercise are exactly the same as the one used in the Set Point Tracking experiment. Generally the simulation results for this exercise can be seen to be similar in form to the experimental results shown previously (i.e. Figure 5:5 and Figure 5:6). These results clearly show that the modified pH model produces responses that are very similar in terms of the system behaviour with the PI controller. However the simulated response using the developed process model is slightly slower compared to the responses obtained from the pilot plant itself. This condition can be observed clearly when the pH value set-point changes from pH value 8 to pH value 6. The time taken for the response to reach the set point (i.e. pH value 6) is approximately 130s for the pilot plant itself and 180s for the corresponding simulation involving the modified model.



Figure 5:7: Simulation results of the modified pH model with PI controller

The same situation can also be observed when the set point changes from pH value 6 to pH value 9. At this set point the behaviour from the modified ph model is slightly different from that of the pilot plant. As described previously, the response from the pilot plant never settles to the desired pH value but instead oscillates between a pH value of 8 and a pH value of 9.2. From the simulated results with the modified pH model, the response oscillates at the beginning and continues with a decaying trend. Thus it is believed that the response would eventually settle to its final or steady state value. This condition might be due to the linearization of the control valve (i.e. CV121 block in Figure 5:2) in the simulation model.

Figure 5:8 shows the comparison between calculated values of tuning parameters and the values implemented during the experimental work. As described in Section 5.2.1 the calculated value for integral gain is 0.29 however during the experimental stage the value has been reduced to 0.03. As for the proportional gain the calculated value and implemented value are the same. As shown in the Figure 5:8(a) the pH response for the calculated value of integral gain (0.29) demonstrated slightly higher overshoot and longer settling than for the controller that was implemented experimentally involving the much smaller value of 0.03 for this parameter. In terms of set point offset error the pH response is better compared to the response for the calculated value. However as shown in Figure 5:8(b) the control valve action for the calculated value is slightly more aggressive than the response from the implemented value. This simulation based investigation shows that the optimal integral gain is probably between the calculated value and implemented value.



Figure 5:8: Comparison between calculated and implemented tuning parameters

Further computer based investigation on the effect of each control action has been performed. For this investigation the tuning parameters are given in Table 5:2 and the pH response from the simulation exercise is shown in Figure 5:9. As shown in Figure 5:9 the simulation exercise has been divided into two parts.

Simulation	Proportional Gain	Integral Gain
Sim1	8.1	0.03
Sim2	8.1	0.5
Sim3	8.1	1
Sim4	1	0.29
Sim5	10	0.29
Sim6	20	0.29

 Table 5:2: Tuning parameters for computer based simulation work



Figure 5:9: Further computer based investigation of tuning parameters

The first three simulations (i.e. Sim1, Sim2 and Sim3) were performed to investigate the general effect of the integral term. In this case the proportional gain remains the same as the calculated value (i.e. 8.1) and the integral gain varies over the range given in Table 5:2. Figure 5:9(a) shows that as the integral gain increases the pH response becomes more aggressive and produces poorer control performance, displaying large overshoot values and modified settling times. The last three simulation exercises (i.e. Sim4, Sim5, and Sim6) were carried out to investigate the significance of the other control action which is the proportional term. For this exercise the integral gain varies as shown in Table 5:2. As shown in Figure 5:9(b) the dynamic response from Sim4 is unaccepted because the transient is very slow. As for Sim5 and Sim6, the difference in dynamic response is small although it does suggest that the response for the case of Sim6 is slightly more aggressive.

5.3 Summary

As mentioned earlier, the control performance of the PI controller may be used as a point of reference for other control approaches to the problem of control of the pH neutralization pilot plant. Therefore some control performance objectives have been outlined and these objectives will be used as guidelines in order to achieve improved control performances.

The control performance objectives are as follows: -

1. Peak-response related criteria for process variable

There are two peak-related criteria that are generally used to measure transient performance in control systems; peak overshoot ratio and decay ratio. As shown in the Figure 5:10, peak overshoot is denoted by A whereas the decay ratio can be calculated from B/A.



Figure 5:10: The transient performance measures

A small value for both criteria is usually desired. A value for peak overshoot ratio that appears to be widely accepted in the literature is around 10% and for decay ratio a widely accepted value is 0.25. However, the new control performance objective for the advanced controller is aimed for 0% peak overshoot and zero decay ratio. As shown in the Figure 5:5, in the case of the PI controller, there is approximately 70% peak overshoot ratio when the set point changes from pH value 7 to pH value 8. However the peak overshoot is smaller when the set point changes from pH value 7 to pH value 8 to pH value 6. The decay ratio is very small and can be neglected.

2. Time related criteria

In the case of time related criteria there are two criteria that are widely used to provide some indication of the controller's performance. The first of these is the rise time and the other is the settling time. Rise time is actually the time from initiation of the step change in the set point until the process variable first crosses the new set point level. Usually a short rise time is desired. The settling time is the time for the process variable to reach and remain within 5% of its final value. Again a short settling time is required. It should be noted that the rise time for the PI controller is approximately 50seconds and the settling time is 110 seconds when the set point changes from pH value 7 to pH value 8. As explained earlier, the rise time and settling time for the next set point change (i.e. pH value 8 to pH value 6) are longer, approximately 120 seconds and 180seconds respectively. Since the previous objective is to have zero peak overshoot and decay ratio, this would mean that the settling time would be a crucial time related performance indicator. Based on this result it is sensible to specify the target for the settling time as below 100seconds.

3. Steady state error (Offset error)

The steady state error indicates how close the process variable is to the desired set point value after all transients have died away. Generally zero offset error is required for all steady state control performance objectives. As shown in Figure 5:5, the offset error (the difference between the process variable and the set-point value) for the PI controller ranges from 0.25 to 0.3. Although the acceptable pH value for the neutralization process in most cases is between pH value 6 and pH value 9, some other applications might involve much stricter requirements in terms of the pH value of the product. Thus the objective for the advanced controller is to provide zero offset error to cater for any process and not only the neutralization pilot plant considered in this application. In practice, external disturbances and measurement noise will contribute to the steady state error and make it impossible to achieve zero steady state error at all times. In such cases the process variable will be unable to provide the exact required set point value. Thus the settling band (that is the difference between the process variable and the set point value) should be specified rather than prescribing a zero steady state error value. For this process the acceptable settling band in terms of pH value is taken as +/-0.1.

4. Robustness of the controller

The final objective for the new controller is its robustness. The controller should be able to react to other disturbances such as concentration and flow variations without any retuning work. In the case of the PI controller it would obviously be necessary to perform some retuning when changes are made to the concentration or the flowrate of the acid. Thus this final objective for the advanced controller is to provide more flexibility when the changes are imposed and avoid the need for controller retuning

CHAPTER SIX

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6.0 ADVANCED CONTROLLER DESIGN, DEVELOPMENT, IMPLEMENTATION AND TESTING

This chapter describes the development, implementation and testing of one specific form of advanced controller which represents the second main research activity, following from the development of the pH neutralization model for the pH neutralization pilot plant. The form of advanced control scheme which has been considered in this research study is a flexible non-model-based intelligent control approach applied to the pH neutralization process using a Fuzzy Logic Controller. The structure of this controller involves a combination of feedforward and feedback control. This chapter is mainly concerned with the development, implementation, testing and evaluation of this form of intelligent controller on the pilot plant.

As mentioned in the literature review, the development of this control strategy (i.e. a Fuzzy Logic Controller) is based on Mamdani's methodology (Mamdani 1976;Mamdani & Assilian 1975;The Math Works 2000). This approach allows the development of the fuzzy logic system from a basis of some theoretical knowledge together with practical experience gathered from work on the specific system for which the controller is being developed. This has led to careful consideration of the structure for the proposed advanced control scheme using knowledge of the pH neutralization process system and its nonlinearities. Although designed using the Mamdani approach it was found that during the implementation process for the fuzzy logic controllers some final tuning work needed to be performed on site in order to ensure the correct functioning and reliability of the controllers.

The chapter includes important results concerning the experimental testing of the implemented fuzzy logic controller based on the proposed control system structure. Associated investigations of the robustness of the controller involving pilot plant experiments are presented, as well as additional simulation results relating to various aspects of the controller performance.

Further investigations of the chosen form of control system structure used for the fuzzy logic system implementation are included through comparative simulation studies based on use of another control algorithm (in the form of PI control). Deatiled performance comparisons are made with the fuzzy control implementation

6.1 Choice of Control System Structure

This section describes the development of the structure of the proposed advanced controllers and associated sources of information. The first source represents knowledge of the theory of the chemical process involved, such as the characteristic of the acid-base reaction process. Information about the structure of the plant and its measurement systems also contributed much relevant information that was used in designing the controller, especially in terms of the characteristics of the control valve. Knowledge of some of the main parameters of the process is also important. In addition to these sources of information, the first version of the pH neutralization process model was also used to build up a comprehensive understanding of the dynamic behaviour of the pH neutralization plant.

As mentioned in an earlier chapter (i.e. Section 3.3) there are two important input variables that have a major influence on the neutralization process. These are the flowrate for the acid and the concentrations of both solutions. The development of this control strategy was designed to ensure that the system would respond appropriately to these inputs, unlike some previous approaches that have been discussed in Chapter 4 which assume or require that some of the inputs to have constant values (Gustafsson & Waller 1983a;Henson & Seborg 1994;McAvoy, Hsu, & Lowenthals 1972;Mwembeshi, Kent, & Salhi 2001;Wright & Kravaris 1991).

Figure 6:1 shows the block diagram or structure of the overall control system that has been considered in this research. The structure involves a combination of feedback and feedforward control strategies. The feedback control is included to reduce or eliminate the error between the pH value in the reactor tank and the desired value which is set by the operator. Meanwhile, the feedforward control in this structure predicts the required amount of alkaline flow that will provide a satisfactory steady state control performance.





Colour coding of the blocks are as follows: Green – Process Variable, Pink – Pilot Plant, Blue – Controller, Turquoise – Set Point. Note that the dependence of the set point for the flowrate of alkaline on other process variables. This feature is discussed in the text. As shown, there are three dedicated controllers that have three different responsibilities. The figure also shows that there are five process values that are recorded from the pH neutralization pilot plant. The process value from the pH Meter provides the pH value from the reactor tank while the Flow Transmitters and Conductivity Meters provide the flowrate and conductivity readings, respectively, for both the acid and the alkaline. Generally, the main purpose of the flow controllers is to control the amount of each solution flowing into the reactor tank. The pH neutralization controller controls the pH value in the reactor according to the desired value, which is normally a pH value between 6 and 10.

The Flow Controller 1 is assigned to manage the amount of acid flow into the reactor tank. The controller will ensure that the amount of acid flow will be as close as possible to the required set point. As the amount of acid flow increases the amount of alkaline flow will also increase. This will eventually increase the amount of the final product in the reactor tank. The amount of acid flow thus provides important information for determining the set point for the Flow Controller 2 and will also act as a "load" to the neutralization process in the system, depending on the set point for the pH. The amount of the final product from the reactor tank will also depend directly on this flow rate. Therefore it is appropriate to have flow controllers for both the acid and the alkaline flow.

In addition to the amount of acid, the concentrations of both the acid and alkaline solutions are also important for determining the set point for the alkaline flowrate as shown in the block diagram. Theoretically the concentration of both solutions will be a constant value throughout the process as the preparation of the solution is based on a batch process. However, due to practical issues that can arise during the preparation of the solutions, the concentration value is usually not precisely the same as the expected value. In addition to that, the concentration of the solutions might change slightly over a period of time from the original value. This condition might be due to some other reaction in the tank. The alkaline solution is particularly prone to concentration changes as it can precipitate over time. Due to this situation, it is important to monitor the concentration value and use this as a variable in the system rather than just assuming it to have a constant value.

As depicted in the block diagram of Figure 6.1, the set point for alkaline flow will be generated automatically whereas the other set point, for pH, is entered manually. The main idea of this set point calculation block is to compute and predict the required amount of alkaline flow that can neutralise the amount of acid that is flowing into the reactor tank. The calculation is based on the balanced chemical equation for an acid-base process reaction.

$$H_2SO_4 + 2NaOH \rightarrow Na_2SO_4 + 2H_2O \tag{6.2}$$

Based on this equation it can be shown that the required amount of alkaline flow is double the amount of acid flow, for the case where the concentrations of both solutions are the same. Therefore the equation for the set point calculation block can be derived as follows;

> Required amount of Alkaline Flow = $2 \times$ Amount of Acid Flow $\times \frac{\text{Concentrat ion of Acid}}{\text{Concentrat ion of Alkaline}}$

Therefore, the main responsibility of the Flow Controller 2 is to ensure that the acid that is flowing into the reactor tank will be neutralised. This is done by controlling the amount of alkaline flowing into the tank. For this particular situation the pH value in the tank will remain the same as the current value and should be the same as the pH set point value. If there is any pH value variation between the current pH value and the set point value for pH, the pH controller will react and change the set point for the alkaline flow to some other value. When the pH value in the tank follows the pH set point value, the pH Controller will give "zero" output and the Flow Controller 2 will track the set point back to the value determined by the set point calculation block. This control approach can be considered as a form of cascade control. As clearly shown in the diagram, in addition to the output of the set point calculation block, the set point for the Flow Controller 2 also depends on the output variable of the other controller. In this case it is the output from the pH controller. Therefore the pH controller will act as a secondary controller.

As explained in the literature (Marlin 2000), the primary controller will manage or control the process since it is slower than the process in the secondary loop. Obviously, in the case of this system, the response of the pH process is much slower than that of the flow process, thus satisfying the criteria very well. Other criteria that suit well for use of this cascade approach are the causal relationship between the control valve and the two processes. Any changes of opening of the control valve will definitely have an impact on both process values; the pH value and the alkaline flowrate.

6.2 Development and Implementation of the Fuzzy Inference System

A fuzzy inference system is a process that forms the mapping for the input and output variables using a fuzzy logic approach. This process involves several steps. It usually starts with identifying and defining the boundary of the input and output variables involved (i.e. establishing the relevant Fuzzy Set). This first procedure is quite crucial as the result of this will show the pattern of the input and output sets and provides general ideas about how these variables are linked. This information makes it is easier to move on to the next process, which involves identifying the membership functions for the input and output sets. The simplest and most commonly used membership function is the triangular membership function, which is used in this study. The final process is to develop a set of if-then rule statements. Such statements are used to formulate the conditional statements that comprise the fuzzy logic approach.

As shown in the overview of the control strategy, there are two different types of controller; the flow controller and the pH controller. These controllers are actually both designed using a fuzzy logic approach. The design for the flow controller will depend on the characteristics of the valve that is controlling the particular stream or flow. The control valve performance will indicate some of the constraints that need to be considered when designing the fuzzy logic controller. Variables such as the operating range, the flow rate for a given control valve opening and the sensitivity of

the control valve to electrical inputs will determine the performance of the fuzzy logic controller. In the case of the pH controller, the fuzzy inference system is based on other factors. In addition to the control valve characteristics for alkaline flow, the dynamic reaction of the acid-base neutralization process is of crucial importance in the design. Another important criterion, which needs to be taken into consideration, is the reaction rate. This is a measure of how fast the pH value reacts when a specific quantity of reactant has been pumped into the reactor tank.

6.2.1 Fuzzy Inference System for the Flow Controller

As described in Section 3.3.4, the type of valve that controls the acid stream is called an "equal percentage" type whereas the alkaline stream valve is termed a "fast opening" valve. The response for the equal percentage type of control valve is much slower and less sensitive compared with the fast opening type of control valve. Thus, designing the fuzzy inference system for a highly sensitive type of control valve is difficult compared with the corresponding task for the less sensitive type of control valve. However a suitable range has been identified from the control valve characteristic curve so that the designed fuzzy logic controller can be utilised for both the acid and alkaline flow control.

Figure 6:2 shows the characteristics of both control valves involved on the pilot plant and these are described in detail in Section 4.3.3. Referring to the characteristics for the valve that is controlling the acid flow, the selected operating range lies roughly between 60% and 90% valve opening. This will give a flowrate between 50L/h and 150L/h. The minimum acid flow rate should not be less than 50L/h when both solutions have the same values of concentration as the required alkaline flow would otherwise be below 100L/h. This is based on the characteristic curve for the alkaline flow valve which presents difficulties for control of flowrates of less than 100L/h, with an allowance of less than 5% control valve opening. On the other hand, for the upper part of the range, it is not possible to have a flowrate that is more than 150L/h. This is because the required alkaline flow would be more than 300L/h. and the curve for alkaline flow shows that the maximum flowrate of alkaline flow is roughly around 320L/h. The control valve that is controlling alkaline flow will thus provide a flowrate between 100L/h to 300L/h by controlling the control valve opening from 10% to 60%.



Figure 6:2: Control valve characteristics

The input set for the fuzzy logic controller is based on the "error", as shown in Figure 6:3. This error is actually a difference between the set point and the corresponding current value of the relevant process variable. Based on the selected operating range for both control valves, the range for the error that will represent the input set in the fuzzy controller is preferred to be within the range from -100L/h to 100L/h. This range has been selected because the gap between the upper and lower range for acid flow is 100L/h.



Figure 6:3: Simplifed MATLAB/Simulink model representation for the fuzzy logic flow controller

The control valve characteristic curves shows that there is quite a significant change in the flowrate (about 20L/hr) for the acid stream as well as the alkaline stream, for a step change of the control valve opening of around 5%. Therefore it is sensible to choose the output set range for the fuzzy logic controller to correspond to 0% to 2.5% change in valve opening.

It is important to understand the simplified MATLAB/Simulink model before selecting any particular configuration of membership function. This model is used as a basis for the flow controller for the acid as well as for the alkaline stream. Depending on the present error, which is the difference between the set point and the current process value, the fuzzy logic controller will react according. The largest value of error should be 100L/h hence the controller will react with the maximum output involving 2.5% change in control valve opening.

The output from the fuzzy logic controller is termed the manipulated variable which is then sent to the pilot plant as an input signal to the particular control valve. At the same time the present manipulated variable will be stored in the memory block as shown in the diagram. The output from the memory block will also contribute to the variation of the control valve movement or opening. As shown in the arrangement in Figure 6:3, the memory block will act as an accumulator. When the fuzzy logic controller provides a positive value, the value in the memory block will increase and when it is negative, the value in the memory block will decrease. As the error decreases towards zero the process value gets closer to the desired set point. The output value from the fuzzy logic will also move towards a zero value. At this point the value in the memory block will tend towards a steady state. Finally, the manipulated variable that drives the final movement of the control valve would be obtained from the value in the memory block.

Selection of the type of membership function depends, in general terms, on the behaviour of the input and output set. Based on the results of a literature survey, most of the fuzzy controllers used in the past for control of the pH neutralization process have used two types of membership function: triangular and trapezoid (George & Yuan B 1995;Jamshidi, Ross, & Vadiee 1993;Postlethwaite 1994;The Math Works 2000). Such membership functions are also recognised as the simplest and most commonly used types of membership function in many other control applications. Thus, triangular and trapezoid membership functions were also selected for initial investigations in this application. Both sets, input and output, use the same type of membership function.

There are no specific guidelines in selecting the parameter settings for the membership functions in a fuzzy inference system. However, based on the boundaries and the overall control strategy, the chosen configuration of the membership functions for the input set is as shown in Figure 6:4. Figure 6:5 shows the corresponding membership functions for the output set. Usually the tuning process for parameters is not a straightforward procedure and requires understanding the input and output behaviour of the process as well as knowledge of fuzzy logic principles.

As shown in Figure 6:4, there are eleven groups of membership functions that will represent the input set. This figure also shows that the setting for the input range is between -100L/h and 100L/h. As explained in an earlier paragraph, the input set actually represents the error and this is defined simply as:

$$Error = Set Point - Process Variable$$
(6.3)



Figure 6:4: Membership function for input set

A detailed description of the symbols as well, as the actual parameters used in Figure 6:4, is given in Table 6.1. The centre point is when the error is zero and it is clear that the whole range of input can be divided into two regions, one for negative error and one for positive error. The values for the positive error region mirror those of the negative error region.

As mentioned there are no specific rules for configuring the membership function. In this case 11 sets of membership functions have been chosen which were mainly based on the control valve characteristic and some trial-and-error procedures. During this exercise it was observed that grouping the membership function in the central part of the input range, as shown in Figure 6.4, will ensure that control effort is focused on the specific targeted control range. Thus, when the error lies between -20L/h and 20L/h the membership functions are very close to each other in order to provide a region in which the response is highly sensitive. This is to ensure that the fuzzy controller will provide a good response with zero steady state error as well as minimum overshoot. Meanwhile the range between 20L/h and 100L/h and also between -20L/h and -100L/h will contribute to the overall system performance by ensuring a reasonably fast rise time, which is another important measure of performance.

Symbol	Descriptions	Туре	Parameters		neters	
NVL	Negative Very Large	Trapezoid	-100	-100	-80	-40
NL	Negative Large	Triangular	-60	-40	-20	
NM	Negative Medium	Triangular	-30	-20	-10	
NS	Negative Small	Triangular	-15	-10	-5	
NVS	Negative Very Small	Triangular	-10	-5	0	
Z	Zero	Triangular	-5	0	5	
PVS	Positive Very Small	Triangular	0	-5	-10	
PS	Positive Small	Triangular	5	10	15	
PM	Positive Medium	Triangular	10	20	30	
PL	Positive Large	Triangular	20	40	60	
PVL	Positive Very Large	Trapezoid	40	80	100	100

Table 6.1: Membership function description and parameters for input set

Figure 6:5 shows the arrangement of membership functions for the output set. There is a one-to-one relationship between the input set and the output set and there are also eleven groups of membership function for the output set. As shown in the figure the output set range is from -2.5% to 2.5% valve opening. A detailed description of the symbols as well, as the actual parameters used in Figure 6:5, is given in Table 6.2.

Since the range for the output set is considerably smaller than that for the input set the arrangements of the membership functions are quite consistent. However, as shown in Figure 6:5, there is no concentrated region unlike the arrangement of the membership function for the input set where the concentrated region is at the centre. As in the case of the membership functions for the input set there are also two distinct regions, for positive valve opening and the negative valve opening. The positive valve opening will provide a response for the positive error region whereas the negative valve opening will react appropriately for the negative error region.



Table 6.2: Membership function description and parameters for output set

Symbol	Descriptions	Туре	Parameters			
NVLo	Negative Very Large	Trapezoid	-2.5	-2.5	-2.0	-1.25
NLo	Negative Large	Triangular	-1.65	-1.25	-0.85	
NMo	Negative Medium	Triangular	-1.15	-0.85	-0.5	
NSo	Negative Small	Triangular	-0.75	-0.5	-0.25	
NVSo	Negative Very Small	Triangular	-0.5	-0.25	0	
Zo	Zero	Triangular	-0.15	0	0.15	
PVSo	Positive Very Small	Triangular	0	0.25	0.5	
PSo	Positive Small	Triangular	0.25	0.5	0.75	
РМо	Positive Medium	Triangular	0.5	0.85	1.15	
PLo	Positive Large	Triangular	0.85	1.25	1.65	
PVLo	Positive Very Large	Trapezoid	1.25	2.0	2.5	2.5

The choice of parameters for the membership function is also crucial. These parameters will determine whether the output from the fuzzy logic controller is too sensitive to the input set, which then produces a high level of ripple in the output, or are too insensitive and lead to a very sluggish output response. Thus the key performance index of the fuzzy logic controller will also depend on these parameters.

Table 6.3 shows that the relationship between the input set and the output set of the fuzzy logic controller. These if-then rule statements are quite straightforward since this is a one-input one-output case. As shown in Figure 6:3 there is only a single input and a single output for the fuzzy logic flow controller.

No	Statement	Error (L/h)	Statement	Manipulated Variable (% Control Valve Opening)
1	IF	NVL	THEN	NVLo
2	IF	NL	THEN	NLo
3	IF	NM	THEN	NMo
4	IF	NS	THEN	NSo
5	IF	NVS	THEN	NVSo
6	IF	Z	THEN	Zo
7	IF	PVS	THEN	PVSo
8	IF	PS	THEN	PSo
9	IF	PM	THEN	PMo
10	IF	PL	THEN	PLo
11	IF	PVL	THEN	PVLo

Table 6.3: If-then-rules statements for the fuzzy logic controller

Figure 6:6 is a two-dimensional curve that represents the mapping from the input set to the output set. This curve provides an indication of how the fuzzy logic controller will behave or respond when there is a difference between the set point and the measured value from the flow transmitter.

The diagram provides an indication of how the if-then rule statements work. Basically, when the value of error is positive (that is when the value of the process variable is below the set point), the opening action of the control valve should be increased. This action is also in the positive direction, as indicated in Figure 6:6. On the other hand, when the value of error is negative (indicating that the process variable is above the set point), the opening action of the control valve should be decreased. This action is thus in a negative direction as shown clearly in the Figure 6:6. The overall form of the controller is seen to be approximately linear for error values between -60 and 60 L/h. The main objective for this flow controller is to provide zero error with zero action for the manipulated variable.

As shown in Figure 6:6, each side of the response (i.e. Positive and Negative errors) can be divided into three regions which correspond to the control valve action. At the positive error side, the first region is when the error is bigger than 40L/h where fast and large control action is required. The second region is between 20L/h and 40L/h in which the control action is slightly lower than the first region. In the last region the range of error is between 0L/h and 20L/h. In this region the control action is the slowest but just enough to provide some amount of flow. The region was designed so that the transient will not produce unwanted overshoot. As shown in the figure, there is a flat area between these regions. This is mainly to make sure that the flowrate does not change too rapidly from one region to another. Since the flow process is a fast response process this flat area will help to avoid transients provide ensure a more consistent flowrate before the next control action takes place.



Figure 6:6: The response of the fuzzy logic controller in terms of the manipulated variable as a function of the error

6.2.2 Fuzzy Inference System for the pH Controller

As explained earlier, at the beginning of this chapter, the pH controller will also be responsible for establishing the set point of the flow controller which determines the alkaline flow. In addition to the auto-calculated value, the set point for the flow controller will also depend on the variation of the pH value in the reactor tank with the desired pH set point.

Figure 6:7 shows the MATLAB/Simulink representation of the overall system for control. Generally the idea of the control approach adopted is that when the current pH value is below the desired value the Fuzzy Logic pH Controller will provide a new set point for the Fuzzy Logic Flow Controller. The new value for the set point will depend on the difference between the pH value in the reactor tank and the desired pH value. The difference is called "pHerror", as shown in the figure.

The range for this variable is within the range from -5 to 5 and this is matched to the controllable range for the pH value for the neutralization process which involves pH values between 6 and 10. Thus the input set for the pH Fuzzy Logic Controller represents the pHerror and is in the range from -5 to 5.

The output set for the controller will correspond to the flowrate of the alkaline stream. The range for the output set is configured to be between -100L/h and 100L/h, which is exactly the same as the input set range for the Fuzzy Logic Flow Controller. The saturation block that comes before the Fuzzy Logic Flow Controller will limit the error to the range from -100L/h to 100L/h. This block will prevent any value to the fuzzy controller being missed if the error value lies beyond this range. Thus, if the value is over 100L/h the input signal to the controller will be limited to 100L/h.



Figure 6:7: MATLAB/Simulink representation for the overall pH controller

As shown in the figure there is a saturation block (denoted Saturation1 in the diagram) before the signal is sent to the actuator (i.e. control valve). This is a normal practice to ensure that the amount of signal to the actuator is within the appropriate range. In this case it is between 0% and 100% control valve openings

This condition will occur when there are variations in both the pH value and the alkaline stream at the same time. Since these variations are inter-connected the controllers will react accordingly and bring the error down to zero. Figure 6:8 shows the membership functions for the input set for the pH controller and the detailed description of the symbols and the exact parameter settings used are given in Table 6.4. Unlike the input set for the flow controller there are nine groups of membership functions that will represent the input set for the pH controller. This is because of the smaller range of the input set compared to the range of the input set used for the flow controller. Thus fewer membership functions are needed to cover the range. A further reason for using a smaller number of membership functions for the pH process is that the dynamics of this process are significantly slower compared to the flow process. Therefore it is less sensitive and requires a smaller number of membership functions.

As in the flow controller the number of membership functions is increased towards the middle point of the range. The mid condition is positioned between -1 and 1 as shown in Figure 6:8. This may also be seen from the figures in Table 6.4. This critical range will determine the smoothness of the settling condition and to ensure that the zero offset for the steady state is achievable. However the overall system performance of the fuzzy logic controller will depend on the combination of membership function for the input and output sets.



Figure 6:8: Membership function for the input set for the pH fuzzy logic controllers

Symbol	Descriptions	Туре	Parameters			
NVLph	Negative Very Large	Trapezoid	-5.0	-5.0	-4.0	-2.0
NLph	Negative Large	Triangular	-3.0	-2.0	-1.0	
NMph	Negative Medium Triangu		-2.0	-1.25	-0.5	
NSph	Negative Small	Triangular	-1.0	-0.5	0	
Zph	Zero	Triangular	-0.5	0	0.5	
PSph	Positive Small	Triangular	0	0.5	1.0	
PMph	Positive Medium	Triangular	0.5	1.25	2.0	
PLph	Positive Large	Triangular	1.0	2.0	3.0	
PVLph	Positive Very Large	Trapezoid	2.0	4.0	5.0	5.0

Table 6.4: Membership function descriptions and parameters for the input set

Figure 6:9 shows the membership functions for the output set of the pH controller and the detailed descriptions are given in Table 6.5. The parameter values in this case were determined from the results of experiments that were designed to establish facts about the process such as the values of flowrate needed to increase or decrease the pH to a specific value and provide a reasonable time response.

As in the case of the input set membership functions, there are also nine groups of membership functions in the output set for pH control. As shown in the figure, the triangular shape of the membership function in the middle of the range is very narrow. This is to cater for small variations of the pH error for conditions below a pH value of 0.5. When this condition occurs the pH controller will then make a small step change of the set point which will then make the control valve react accordingly. If this membership function were too wide it would contribute to poor control performance through introducing features in the response such as a large overshoot, unwanted oscillations or a ripple under nominally steady state conditions. In contrast with this membership function in the middle of the range, the rest of the triangular membership functions are all similar in form and are evenly distributed.



Figure 6:9: Membership function for outputs set for pH fuzzy logic controller

Symbol	Descriptions	Туре	Parameters			
NVLph _o	Negative Very Large	Trapezoid	-100	-100	-60	-45
NLpho	Negative Large	Triangular	-50	-40	-30	
NMpho	Negative Medium	Triangular	-35	-25	-15	
NSpho	Negative Small	Triangular	-20	-10	0	
Zpho	Zero	Triangular	-0.05	0	0.05	
PSpho	Positive Small	Triangular	0	10	20	
PMpho	Positive Medium	Triangular	15	25	35	
PLpho	Positive Large	Triangular	30	40	50	
PVLpho	Positive Very Large	Trapezoid	45	60	100	100

 Table 6.5: Membership function descriptions and parameters for output set

The relationship between the input set and the output set of the pH Fuzzy Logic Controller is given in Table 6.6. Again, the if-then rule statements for the pH controller represent a straightforward process since this is a one-input one-output case as shown in the table. From the result of this fuzzy inference system, a two-dimensional curve that represents the overall input and output response of the controller is obtained and is shown in Figure 6:10.

No	Statement	Error (L/h)	Statement	Manipulated Variable (% Control Valve Opening)
1	IF	NVLph	THEN	NVLph _o
2	IF	NLph	THEN	$NLph_{o}$
3	IF	NMph	THEN	NMph _o
4	IF	NSph	THEN	$NSph_{o}$
5	IF	Zph	THEN	Zph _o
6	IF	PSph	THEN	$PSph_{o}$
7	IF	PMph	THEN	PMpho
8	IF	PLph	THEN	PLpho
9	IF	PVLph	THEN	PVLpho

Table 6.6: If-then rule statements for the fuzzy logic controller

As shown in the figure, positive and negative regions can be divided into three specific ranges or regions with three different controller responses. For the positive part of the range, the first region is when the error in the pH value lies between pH value 0 and 0.8. In this region the output or action from the pH controller involves a flow of less than 20L/h. This small flowrate requires less than 0.8% opening of the control valve. Although this region and the associated control valve movement is very small it is of critical importance as it will determine the steady state condition of the system. Thus this region can be called as the "settling region". Towards the upper end of the range two-thirds of the positive region can be termed the "fast response region". This condition occurs when the pH error is larger than 2. For differences between the pH set point and the process variable of this magnitude, an immediate action involves a pH error of between 1 and 2. This is known as the "transition region" which has lower gain and provides a form of "cushion" between the fast action region and the slow action region.



Figure 6:10: The response of the pH fuzzy logic controller

6.3 Simulation and Experimental Results

The main idea of this section is to discuss the feasibility and reliability of the control strategy shown in Figure 6:1. This section also describes the performance of the developed fuzzy logic controllers when applied to the pH neutralization pilot plant. A number of experiments performed to investigate the robustness of the system are discussed. Practical implementation issues are highlighted as well as the benefits obtainable using these controllers. In addition, some results obtained from computer-based simulations based on the modified pH model are also presented in this section. These simulation results allow conclusions to be reached concerning the accuracy and reliability of the modified model and some limitations in the control system performance across the whole of the operating range of the system.

6.3.1 Experimental Results from the pH Neutralization Pilot Plant

This section describes in detail some of the experiments that have been performed during this investigation. All of these results are based on the control strategy described previously. In order to verify the reliability and performance of the fuzzy logic controller several types of experiments and testing have been performed. Each experiment gives specific information about different aspects in terms of the capability of fuzzy logic control in general, and more especially the benefits and limitations of the specific approach adopted for the control strategy in this application.

The first experiment considered involved "set-point change" testing. The objective of this experiment is to observe the control performance of the fuzzy logic controllers when a set point change has been introduced. The experiment was based on 0.05M H_2SO_4 mixed with 0.05M NaOH. These values were chosen because they are typical values for a neutralization process of this kind. The flow controller set point for the acid stream was set at 80L/h and two step-changes were made for the pH value in the reactor tank. The first change was made from pH value 7 to pH value 10 and the second set-point change was a change in the negative direction from pH value 10 to pH value 7.

The experiment was successfully performed and the results are shown in Figure 6:11. The figure shows the five process variables that were recorded from the pilot plant, as explained earlier. Figure 6:11(a) shows the response from the pH meter in the reactor tank and **h**is variable provides a useful indication of the overall performance of the controllers. At a glance the performance of the fuzzy logic controllers appear very good.


Figure 6:11: The step response experiment for changes of the pH set point.

The uppermost record, (a), shows the measured and set pH values while the lower traces, (b) and (c), show the flow rates and conductivity measurements for both acid and alkaline.

The figure shows that the approach that was implemented has produced a control system that successfully reacted to the set point changes. The first set point change was at 295 seconds and the second change was made at 600 seconds. The response took less than 100 seconds to reach the steady state values in each direction. The transient responses were also very encouraging as there was zero offset and a very small overshoot. Figure 6:11(b) and (c) show the other process variables, the flowrate and conductivity value for both solutions. As shown in Figure 6:11(b), the control valve that is controlling the alkaline stream has responded appropriately to the set point changes. At the steady state condition the flowrate was fluctuating between 130L/h and 150L/h with an average flowrate value of 140L/h.

As explained previously, the set point for alkaline flow is a dynamic value and is dependent on the other process variables. Thus the response shown in the figure was an expected and acceptable behaviour. The figure also shows that the fuzzy logic controller for flow control in the acid stream has reached the required set point value of 80L/h within a few seconds. In order to obtain more insight concerning the capability and performance of this flow controller at the steady state condition, data from the 100th second to the 900th second has been analysed using statistical methods and the results are shown in Table 7.0. As shown in the table, the average flowrate for the acid stream under steady state conditions is 79.96L/h and most of the time the value of the flowrate has a steady value of 79.75L/h. The difference between the set point for acid and these actual values is less than 0.5L/h. This is a significant achievement in a process of this kind.

As shown in Table 6.7, the average values from the conductivity meter for acid and alkaline are 24.23mS and 12.34mS respectively. These values correspond to average concentration values for acid of 0.0497M and for alkaline of 0.0586M. The concentration value for acid is very close to the set up value, which is 0.05M. However the true concentration value for alkaline is slightly above the target value. This discrepancy was found in every experiment and thus each test will have a different combination of concentration values.

D	Flowrate for	Conductivity (mS)			
Descriptions	acid (L/h)	Acid	Alkaline		
Mean	79.96	24.23	12.34		
Median	79.97	24.23	12.34		
Mode	79.75	23.81	12.31		
Standard Deviation	0.98	0.11	0.12		
Minimum	76.47	24.22	11.77		
Maximum	83.4	24.59	12.73		

Table 6.7: Descriptive statistical values for the process variable for the pH set-point change experiment

The performance of the conductivity meters can also be evaluated based on the information given in Table 6.7. The average conductivity value and the standard deviation value for the acid are 24.23mS and 0.111mS respectively. The average conductivity value for the alkaline is 12.34mS with a standard deviation value of 0.123mS. These results show that the values are close to each other and are very consistent. It also indicates that the conductivity meters can provide reliable and precise data. Therefore the auto-calculation set point for the alkaline stream will also be reliable and consistent. Based on these average values obtained from the flow transmitter for acid and also from the conductivity meters, the set point for alkaline flow can be calculated as follows:-

Set Point for Alkaline
$$= \frac{2 \times 79.96L/h \times 0.0497mS}{0.0586mS}$$
$$= 135.63L/h$$

It should be noted that this set point value is generated when there is no error in the pH value at the reactor tank.

Figure 6:12 shows in detail how the control approach works. All responses in the figure are based on the same experiment as described above. The set point for alkaline flow was gradually increased at the beginning of the experiment and settled at an average value of 134.48L/h. As shown, there was zero pH error at the beginning of the experiment and this continued until the 295th second. The difference between expected value and the actual average value is about 1.15L/h. Therefore the accuracy of the auto-calculation block is about 99.15%. This result is also very encouraging and shows that all of the process variables are reliable and accurate.



Figure 6:12: Additional response from the set point experiment

When a step change from pH value 7 to pH value 10 was performed at the 295th second, the pH error was transiently increased to 3. As shown in the figure, the set point for alkaline flow increased to a maximum of about 210L/h at this time. This additional flow, 75L/h, was from the pH fuzzy logic controller. Once the pH value reached the set point, which in this case is 10, the set point for alkaline flow was brought back to the steady state value for that set point. On the other hand, when the pH error was moving in the negative direction at the 600th second, the set point for the alkaline flow was also moving towards a negative value which decreased to around 80L/h. Once again, when there was no error between the pH set point and the desired pH value the set point for the alkaline flow settled at the average set point flowrate of 134.48L/h.

As shown in Figure 6:12, the manipulated variable for the control valve also varies between 28% and 30% control valve opening at the steady state condition. According to the control valve characteristic for the alkaline stream these values correspond to 130L/h and 150L/h. An additional 10% was added (approximately) during the set change from pH value 7 to pH value 10 to increase the flowrate to 220L/h. The control valve reacted immediately by maintaining the opening at the steady state range although some fluctuations could be observed. For the case of the step down change, the response for the control valve opening is different. This is due to the constraints of the control valve. As shown in the figure and explained in an earlier paragraph, the new set point for the alkaline steam is 80L/h. In order to reach this value the control valve must vary within a range from 5% to 10% opening. It is not an easy task for the controller to operate with such a small movement of the control valve behaviour is to be expected.

The next test or experiment involved a set point tracking test. This experiment was performed to test the robustness of the fuzzy logic controller for a series of a random set point changes. Although the target pH value for the specific neutralization process considered in the current application is always 7 some other processes might involve control with other solutions at different pH values. Thus this test will determine whether the fuzzy logic controller can provide good responses at different set points.

The experiment was performed successfully and the results are shown in Figure 6:13. These results were obtained after 2500seconds and there were eight set point changes in the pH value. The initial set point for the pH value is 7 and the final required pH value is also 7. The minimum set point value is a pH value of 6.5 and the highest set point value was pH value 10. The average value for the conductivity was 22.7mS and 10.93mS for acid and alkaline respectively. These values agree with the concentration value. In the case of acid the concentration value was 0.0495M and for alkaline it was 0.0519M.

The set point for the fuzzy logic flow controller for acid was 70L/h. Based on the results shown in the figure data were taken for more detailed analysis from the 250th second to 2500th second. Over this time interval the actual flowrate of the acid stream ranges between 69L/h and 71L/h. The average flowrate value was found to be 70L/h which was exactly the same value as the set point for the fuzzy logic flow controller. The standard deviation of the samples was very small. The statistical summary indicates that the flow controller successfully controlled the flowrate of the acid stream with a negligible offset. Therefore, once again, the results show that the flow fuzzy logic controller for the acid stream was capable of providing a good control performance as required.



Figure 6:13: Set point tracking test results

As shown in the figure the results from the testing are very promising. The pH controller reacts to the set point changes immediately and the responses for all the step changes are broadly similar in form. However it is worth pointing out that the response for the step change from pH value 6.5 to pH value 7.5 at t = 1500 seconds is slightly slow compared with the other responses. This might be due to the process gain or acid-base reaction activity in this region. As mentioned earlier, this pH neutralization process involves an acid-base reaction between sulphuric acid and sodium hydroxide. Sulphuric acid falls within a group of diprotic acids and one of its attributes is that it has two equilibrium points. The first point is between pH value 6 and pH value 7 and the other point is between pH value 7 and pH value 8. Based on the acid-base titration curve shown in Section 4.4 (i.e. Figure 4:4) and the explanation relating to Table 4.1, these two regions have a slightly reduced value of process gain. Thus the response shown in the figure is understandable and was to be expected.

The flow rate for the alkaline stream for the steady state condition ranges between about 130L/h and 150L/h. The response of this stream was expected to fluctuate slightly since the type of control valve was "fast opening", meaning that the flow rate changes significantly when there is a very small change of control valve opening. Thus the fluctuation or variation of acid stream was acceptable considering that the movement of the control valve was very small.

The third experiment involved "Load Change" tests. In these tests the flow rate for the acid stream acts as a load or demand for the entire system. The aim of this experiment is to observe the response of the fuzzy logic pH control system when a load disturbance occurs. The expected response from the fuzzy logic pH controller is an immediate and appropriate control action to maintain the pH value at the desired set point (i.e. the pH value of 7) regardless of the changes in the acid stream. The experiment was carried out successfully and the results suggest that the system performed very well, as shown in Figure 6:14.



Figure 6:14: Responses obtained from a load disturbance experiment

Based on the average conductivity value, the concentration values for acid and alkaline were 0.0486M and 0.0496M respectively. As shown in the figure, a series of random set point changes in the acid flow rate were imposed at 200-second intervals, ranging from 50L/h to100L/h. From the responses shown in the figure, it may be seen that the flow controller for the acid stream reacted in a satisfactory and appropriate fashion for these set point changes.

As explained previously, the flowrate of the acid stream is one of the variables that will determine the set point for the alkaline stream. As shown in the figure, the flowrate for the alkaline stream also reacts in response to the set point changes of the acid stream. The responses are satisfactory in terms of their form and show that the control valve for the alkaline stream is properly controlled and managed. As the result of this control valve movement the response in terms of the pH value in the reactor tank is also very satisfactory as shown in the figure.

Once again, a set of data has been collected (i.e. from the 100th second to 1100th second) and analysed using the same statistical methods as before. The results are given in Table 6.8. The average pH value during the experiment is found to be a pH value of 7.03. That is a very encouraging result and shows that the controller is able to control the pH value with a high level of accuracy at the required set point despite the disturbance in the acid stream.

The maximum pH value is 7.25 and the minimum pH value is 6.89. These values occur at 1048th and 1102nd second respectively and differ from the set point pH value of 7. This may be due to the magnitude of the step change (80L/hr to 50L/hr) introduced to the process just before this time. In this case the flow controller takes about 10seconds to reach and settle to the new set point. Meanwhile the flowrate for the alkaline stream needs approximately another 10seconds to reach and settle at its new set point value. Thus this 20seconds of delays causes a significant amount of alkaline to reach the reactor tank. This additional amount of alkaline generates a slightly higher pH value than the average pH value. As shown in the figure the pH controller immediately takes an appropriate action to recover from the excess alkaline by bringing the alkaline flowrate down. Because of this recovery action there is a slight overshoot which takes the pH value to its lowest value (6.89). However, it should be noted that this is still within an acceptable range (as discussed in Section 5.3). This form of transient can be improved further with some minor adjustments to the fuzzy logic pH controller. Generally, the results for this experiment are acceptable.

The fourth experiment involves a test that is similar to that used in the load changes experiment, but with a different type of disturbance. As in the previous experiment, a change of concentration of the acid solution provides the basis for the disturbance for the whole reaction process, but with a concentration decrease in this case. The expected outcome will be the same as in the previous experiment and the test involves investigation of the capability of the controller to maintain the pH value at the required value in the presence of the disturbance.

In this experiment the concentration of acid is decreased while the concentration of alkaline will be kept to a constant value. The method used to decrease the concentration was by filling in the tank with more water (i.e. a dilution process). At the same time the acid solution was stirred manually to ensure as near perfect mixing as possible in the solution. The expected response from the alkaline stream involves a reduction of flow rate. This is because the concentration of the alkaline solution becomes larger compared to the concentration of acid. Based on the balanced chemical equation, the new condition requires a smaller amount of alkaline solution for neutralization. As the result the auto-calculated set point for alkaline flow will also decrease in order to reduce the alkaline flowrate.

The experiment was carried out successfully and the responses from all five process variables were recorded as shown in Figure 6:15 below. The average flowrate for the acid stream was 70L/h and the average conductivity value for the alkaline stream was 12.5mS (i.e. 0.0594M). The initial conductivity value for acid was 22.5mS and then it decreased to 21.5mS, 20.5mS, 18.5ms and finally it settled at 16.55mS as shown in the figure. These values represent concentrations of acid of 0.0462M, 0.0441M, 0.042M, 0.0379M and 0.0339M respectively.

As explained in the previous paragraph, the flow rate for the alkaline stream will decrease when the concentration of the acid decreases. This form of transient can be seen clearly in the figure. The initial flowrate of alkaline is approximately 150L/h and it then decreases to its final value which is approximately 100L/h. This result shows that the pH controller is able to control the pH value in the reactor at different combinations of concentration value for acid and alkaline solutions. In addition to this, it is noted that each experiment mentioned above will involve a different combination of concentration values. All of the results from the experiment indicate a satisfactory performance.



Figure 6:15: Responses obtained from the concentration disturbance experiment.

As shown in the figure the pH fuzzy logic control managed to control the pH value at the required value (i.e. a pH value 7) very effectively. Again samples from the data are taken for statistical analysis from the 100th second onwards and a summary of the results is given in Table 6.8. From this statistical summary it may be seen that the average value for the pH value is 7.026 which is a very encouraging performance. In addition, the maximum pH value for this experiment is 7.12 which is better than in the previous experiment and is well within the acceptable range. These results show that the type of control scheme shown in Figure 6:1 is capable of producing very reliable responses and can handle disturbances effectively.

	pH Value			
Descriptions	Load	Concentration		
2 to the priority	Changes	Changes		
	Experiment	Experiment		
Mean	7.03	7.026		
Median	7.028	7.023		
Mode	7.04	7.04		
Standard Deviation	0.044	0.043		
Minimum	6.89	6.9		
Maximum	7.25	7.12		

 Table 6.8: Statistical results for the concentration disturbance experiment

The final experiment is similar in nature to the previous set-point tracking experiment but involves larger changes applied at regular intervals In the previous set-point tracking experiment the set point of the pH values was changed in a more random way for values from pH 6 to pH 10. In this additional experiment the set point variation has a square wave-form. The initial pH value is 7 and the amplitude of the square wave is 1.5 with a period of 600s. The concentration values for acid and alkaline are 0.0487M and 0.0496M respectively. The average flowrate for the acid stream is 69.99L/h. The purpose of this experiment is to observe the performance of the pH controller in tracking a large and continuous step in terms of the set point change.

The experiment was carried out successfully and all responses are shown in Figure 6:16. The response from the pH meter is very encouraging. The pattern for the first cycle is very similar to the corresponding pattern of the second cycle. The flow rate of the alkaline stream has the expected form and the transient responses are almost exactly the same for each cycle of the set-point changes.



Figure 6:16: Responses from the experiment involving large changes of set point

As explained previously, in the development of fuzzy inference system for the pH controller the expected response from the controller can be divided into three regions, as may be seen from Figure 6:10. These are the fast response region, the transition region and the settling region. The control actions associated with these different regions can be seen clearly in Figure 6:16. For example, when the step change is from pH value 7 to pH value 10 the pH error has an initial value of 3. This value of error falls rapidly due to the fast response control action. As shown in the figure the flowrate of alkaline increases rapidly to give a maximum flowrate of approximately 225L/h. As the flowrate increases the pH value also rises very rapidly from pH value 7 to pH value 8. However the rate of change of pH reduces as the pH moves from pH value 8 to pH value 9. This is because the control action is in a transition region. The flowrate for the alkaline flow is then approximately 170L/h.

Finally when the current pH value gets closer to the target value, with pH error values less than 0.8, the alkaline flowrate settles to a more or less steady value with some minor fluctuations. This situation shows that the control action is in a steady condition appropriate for the new set value. The pH value is then close to the target value and is trying to reach a steady state condition.

6.3.2 Computer-based Simulation Results for the Fuzzy Logic Controller

This section discusses some dynamic responses obtained from computer-based simulation work. All of the results shown in this section are based on the performance of the fuzzy logic controller with the modified pH model. This model is in actual fact the final version of the modified model (referring to information in Section 4.5.3), which includes the new set of dissociation constant values as well as the additional part for initialisation purposes. As mentioned earlier, the main goals for this exercise are to evaluate the reliability of the model as well as to investigate some benefits and limitations of the fuzzy logic approach.

Selected experimental data have been chosen to assist in this investigation such as the value of conductivity for both solutions, flowrates for acid as well as set point values in the reactor tank. There are four simulation results that represent the same four experiments which have been presented and discussed in the earlier section (i.e. the experimental results).

The first simulation result, shown in Figure 6:17, is based on the configuration for the set point change experiment. The actual response from the pilot plant for this exercise is shown in Figure 6:11. As explained earlier, the idea of this experiment is to observe the control performance of the fuzzy controllers when a set point change has been introduced.



Figure 6:17: Simulation of the set point change experiment

As shown in the figure, for the first step change, which is from pH value 7 to pH value 10, the simulation result shows a response that is similar to the experimental result. However, at the second step change (from pH value 10 to pH value 7) the dynamic response in the simulation shows a different transient behaviour, particularly from pH value 8 to pH value 7. This might be due to the variation of the process gain for different parts of the range of pH value. As explained in Section 4.4 (referring to the explanation for Figure 4:4), the process gain for the region from pH value 8 to pH value 6 to pH value 8 is lower than the process gain for the region from pH value 8 to pH value 10. However, as shown in Figure 6:17, the transient takes a much longer time to reach the new set point at pH value 7 compared with the transient results obtained from the pilot plant. The result suggests that the acid-base reaction process from the modified pH neutralization process model is slightly slower than the actual reaction in the pilot plant in this part of the operating range.

Some modifications have been made in order to consider the above-mentioned problems in more detail. These changes are intended to improve the dynamic response of the model between pH value 6 and pH value 8. Figure 6:18 shows the new structure of the controller. As shown in the figure, there is an additional input to the pH fuzzy logic controller that represents the critical region (i.e. from pH value 6 to pH value 8). There is also an additional output from the controller that reacts to the additional input. The main idea of this new configuration is that whenever the set point of the pH value is set within the critical region the total value of the manipulated variable, MV will depend on the second output (i.e. the additional output) from the pH controller. The function of the additional control valve opening from the second output is to make the system more sensitive through more aggressive control valve movements. However, if the set point of the pH value occurs outside this region, the pH controller will only respond to the first input set, which is the pH error. For this condition the second output from the fuzzy logic controller will always be zero. This shows that outside the critical region the pH controller will utilise the same configuration as that used in the experimental work on at the pilot plant. For the fuzzy logic flow controllers, the configuration remains the same as that being used in the experiment on the pilot plant.



Figure 6:18: The new structure of the controller

Figure 6:19 shows the membership functions for the additional input while Figure 6:20 shows the membership functions for the additional output for the pH controller. There is a single membership function for the additional input, which indicates the critical set point pH value. However there are six triangular shapes of membership functions for the additional output.



Figure 6:19: Membership function for the additional input set



Figure 6:20: Membership function for the additional output set

Table 6.9 provides the detailed description of the controller and the actual parameter values used for the membership functions for both the additional input and the output. The investigation of parameters values for the membership functions was mainly based on the performance of the modified pH model. Some titration curves from the modified model and also the performance of the pH controller shown in Figure 6:17 were used as guidelines. Once the structure of the new pH controller was identified the final choice of the parameters for the membership function was based on a trial and error approach.

Additional Input								
Symbol	Descriptions		Туре	Parameters				
CReg	Critical Region		Trapezoid	6	6	7	8	
	Additional Output							
Symbol	Descrij	ptions	Туре	Parameters				
CNLph _o	Critical Large	Negative	Triangular	-100	-95	-90		
CNMpho	Critical Medium	Negative	Triangular	-60	-35	-15		
CNSph _o	Critical Small	Negative	Triangular	-30	-18	0		
CPSpho	Critical Small	Positive	Triangular	0	18	30		
CPMph _o	Critical Medium	Positive	Triangular	15	35	60		
CPLpho	Critical Large	Positive	Triangular	80	90	100		

Table 6.9: Membership function descriptions and parameters for the additional input and output sets

Apart from the additional input and output there are also four additional membership function that have been added to the previous input set (i.e. pH error) of the pH controller. Table 6.10 provides the description of the new configuration of membership function for the input set. As given in the table, the additional membership functions are highlighted as CNSph, CNVSph, CPVSph, and CPSph. The main purpose of the additional membership functions is to make the fuzzy logic controller more sensitive to the pH error (that is to the difference between the set point and the process variable).

Symbol	Descriptions	Туре	Parame ters			
NVLph	Negative Very Large	Trapezoid	-5.0	-5.0	-4.0	-2.0
NLph	Negative Large	Triangular	-3.0	-2.0	-1.0	
NMph	Negative Medium	Triangular	-2.0	- 1.25	-0.5	
NSph	Negative Small	Triangular	-1.0	-0.5	0	
CNSph	Critical Negative Small	Triangular	-0.6	-0.3	-0.1	
CNVSph	Critical Negative Very Small	Triangular	-0.3	-0.1	0	
Zph	Zero	Triangular	-0.5	0	0.5	
CPVSph	Critical Positive Very Small	Triangular	0	0.1	0.3	
CPSph	Critical Positive Small	Triangular	0.1	0.3	0.6	
PSph	Positive Small	Triangular	0	0.5	1.0	
PMph	Positive Medium	Triangular	0.5	1.25	2.0	
PLph	Positive Large	Triangular	1.0	2.0	3.0	
PVLph	Positive Very Large	Trapezoid	2.0	4.0	5.0	5.0

Table 6.10: New configuration for the first input set for the pH controller

Table 6.11 shows the rules for the new configuration of the pH fuzzy logic controller.

No		pH Error (L/h) as		Critical Set Point		Manipulated Variable (% Control Valve Opening)	
		Input 1		as Input 2		Output 1	Output 2
1	IF	NVLph		-	THEN	NVLph _o	-
2	IF	NLph		-	THEN	NLpho	-
3	IF	NMph		-	THEN	$\mathbf{NMph}_{\mathrm{o}}$	-
4	IF	NSph		-	THEN	$NSph_{o}$	-
5	IF	Zph		-	THEN	Zph_o	-
6	IF	PSph		-	THEN	PSpho	-
7	IF	PMph		-	THEN	PMph _o	-
8	IF	PLph		-	THEN	PLpho	-
9	IF	PVLph		-	THEN	PVLph _o	-
10	IF	NVLph	AND	CReg	THEN	NVLph _o	CNL ph _o
11	IF	NLph	AND	CReg	THEN	NLpho	CNL ph _o
12	IF	NMph	AND	CReg	THEN	$\mathbf{NMph}_{\mathrm{o}}$	CNL ph _o
13	IF	CNSph	AND	CReg	THEN	$NSph_{o}$	CNMph _o
14	IF	CNVSph	AND	CReg	THEN	$NSph_{o}$	CNSpho
15	IF	PMph	AND	CReg	THEN	PMph _o	CPLpho
16	IF	PLph	AND	CReg	THEN	PLpho	CPLpho
17	IF	CPSph	AND	CReg	THEN	PSpho	CPMpho
18	IF	CPVSph	AND	CReg	THEN	PSph _o	CPSpho

Table 6.11: If-then statements for the new fuzzy logic controller

Figure 6:21 shows the dynamic response for the same experiment as before with the modifications made to the configuration of the pH fuzzy logic controller. As shown in the figure the dynamic response is very similar to the actual dynamic response from the plant shown in Figure 6:11. This encouraging result shows that the new configuration is able to provide additional control valve movements within the critical region as required.



Figure 6:21: Simulation of set point change experiment with modified fuzzy logic pH controller

As shown, the controllers are able to respond to the two instances of set point changes. The major difference between the previous pH controller and the new configuration of the pH controller is in terms of the behaviour of the control valve that is controlling the alkaline stream. The control valve movement for steady state conditions is more active at pH value 7 compared to pH value 10. This obvious difference is due to the effect of the new pH fuzzy logic controller.

As shown, the flowrate for the alkaline stream fluctuates more obvious than the previous response as well as the response from the actual pilot plant. This limit-cycle like fluctuation may create an issue in terms of the practicality of this controller for an actual plant application but it should be noted that this fluctuation, which is around 50L/h in peak-to-peak magnitude, corresponds to less than 10% of control valve opening, which is a relatively small movement for a control valve. As mentioned in the literature (Marlin 2000), large and high frequency variations in the control valve movement will reduce the life expectancy of the control valve. Thus it is believed that this behaviour is acceptable. It should be noted this modified pH fuzzy logic controller is used throughout all of the remaining simulation exercises.

The second simulation experiment represents the exact situation that applies for the set point tracking experiment on the pilot plant. The simulation result in this exercise should match the experimental result shown in Figure 6:13. The aim of this exercise is to investigate the robustness of the fuzzy logic controller for a series of random set point changes. The dynamic response for this test is shown in Figure 6:22.

As shown in the figure, the transient responses for changes in pH set point value from the computer-based simulation are very similar to the experimental transient responses shown in Figure 6:13. However there are, inevitably, dissimilarities between these two results. Obviously this is due, in part, to the developed pH process model itself. It seems that the response from the modified pH model is quite slow as compared to the actual response from the pilot plant. This can be observed when the pH value changes from pH Value 9 to pH value 6.6. Thus this result suggests that there are still plenty of room for improvement and further investigation of the pH model. In addition to that the differences may also be due to the linearised transfer functions representing the control valve in the computer-based simulation. Unfortunately, further plant tests with the modified fuzzy logic controller and investigation on pH model validation could not be carried out because further access to the plant was impossible at this stage in the work.



Figure 6:22: Simulation result for set point tracking

For the purpose of comparison, Figure 6:23 shows the response of the same simulation exercise without any modification on the configuration of the pH fuzzy logic controller. As shown in the figure, the responses at the critical region are unsatisfactory. The simulation result shown in Figure 6:22 has demonstrated clearly the effectiveness of the new configuration of the pH fuzzy logic controller within the critical region.



Figure 6:23: Simulation result for set point tracking with single input for the pH fuzzy logic controller (i.e. pH error)

In general these encouraging results suggest (from both experimental results and the computer-based simulation studies) that the fuzzy logic control approach is able to react to the set point changes appropriately and also shows that the modified pH model provides a level of performance that is generally adequate with the modified form of fuzzy control.

The objective for the third simulation is exactly the same as in the load change experiment, which is to investigate the capability of the controllers to handle load disturbances. The dynamic response from the actual pH neutralization pilot plant is shown in Figure 6:14 and Figure 6:21, with the corresponding computer-based simulation results being shown in Figure 6:24. The response from the computer-based simulation exercise confirm that the fuzzy logic controllers are able to provide a good transient response in terms of the pH value despite having a series of flowrate disturbances in the acid stream.



Figure 6:24: Simulation results for the load disturbance test.

Statistical analysis performed for this simulation gives the results shown in Table 6.12. Once again the results show that the fuzzy logic controllers are able to maintain the pH value at pH value 7 with high accuracy and repeatability. These results suggest that the performance from the computer-based simulation is better than the experimental results obtained from the pilot plant (i.e. comparison between Table 6.8 and Table 6.12). However the behaviour of the alkaline stream from the actual pilot plant experiment is more stable and encouraging. As shown in Figure 6.24, the alkaline stream fluctuates aggressively when the set point for acid flow was brought down from 80L/h to 50L/h. This behaviour is mainly due to the control valve characteristic in which as explained previously in Section 3.3.4 there is no flow when the opening control valve is less than 5%. At this particular condition the required alkaline flow that will neutralise 50L/h of acid stream is 100L/h. In order to provide 100L/h of flowrate the control valve opening needs to be controlled between 5% and 10% where the control valve movement is very difficult to manage.

As shown in Figure 6:25, the final simulation result shows the capability of the fuzzy logic controllers when there are disturbances in the concentration of the acid solution. As explained previously, the experimental results for this exercise are shown in Figure 6:15. Again the idea of this exercise is to observe whether or not the fuzzy logic controls are able to maintain the ph value at pH value 7 regardless of the disturbances in the concentration of the acid solution.



Figure 6:25: Simulation results for acid concentration disturbances

As shown in the figure the fuzzy logic controllers are capable of maintaining and controlling the pH value at its set point value. Once again it shows that the fuzzy logic controllers are reliable and able to perform their task within the required performance specification. Table 6.12 also provides a statistical evaluation of the simulation results and shows that the simulation results for this exercise are similar to those obtained for the plant experiments involving flowrate disturbances. It indicates that the controllers provide good control performance in the presence of disturbances in the flowrate and concentration for the acid solution.

The results also indicate the same pattern of behaviour of alkaline flow through this computer-based simulation work where the flowrate is slightly more oscillatory than the actual behaviour of the pilot plant.

	pH Value			
Descriptions	Load Changes Experiment	Concentration Changes Experiment		
Mean	7.00	7.01		
Median	7.00	7.00		
Mode	7.00	7.00		
Standard Deviation	0.019	0.017		
Minimum	6.95	6.99		
Maximum	7.15	7.11		

Table 6.12: Statistical results for the simulation exercises

6.3.3 Computer-based simulation of the feedforward/feedback control strategy using PI controllers

This section discusses some dynamic responses obtained from the computer-based simulation work with the same control structure described in Section 6.1. The only difference from the previous section (i.e. Section 6.3.2) is that the simulation results shown in this section are based on the performance of the PI controller. The simulation exercises were performed based on the modified pH model. The same experimental data used in the previous section such as the value of conductivity for both solutions, flowrates for acid as well as set point values in the reactor tank were utilised in this simulation work. The main objective for this exercise is to evaluate the reliability of the control structure which is the Feedback/Feedforward control described earlier. In addition the investigation will also provide some information on the consistency and performance of the modified pH model.

As explained, the difference between the previous computer-based simulation exercises is that the two fuzzy logic controllers will be replaced by two PI controllers. One PI controller will be handling the flowrate of the alkaline streams and the other controller will be responsible of controlling the pH value. These conventional controllers have been tuned in a traditional way and they have shown individually an acceptable control performance.

As described previously there are four simulation results that represent the same four experiments which have been presented and discussed in the earlier sections (i.e. the experimental results and computer-based simulation for fuzzy logic controllers). The first simulation result, shown in Figure 6:26, is based on the configuration for the set point change experiment. The actual response from the pilot plant for this exercise is shown in Figure 6:11. Figure 6:21 shows the simulation result with the fuzzy logic controller.



Figure 6:26: Simulation of set point change with PI controllers

As shown the figure (i.e. Figure 6:26) the controllers are able to respond to the two instances of set point changes. It shows that the control structure is reliable and able to provide good control performance. However the main difference between the previous simulation results (i.e. with fuzzy logic controllers) is that the transient response of the alkaline stream for the PI controller is more aggressive. This can clearly be seen throughout the simulation. As shown, the frequency of the response is quite high. This is unlike the response from the fuzzy logic controller (i.e. Figure 6:21) where the response in terms of the alkaline flow oscillates with reasonably low frequency. From a maintenance point of view this condition of high frequency movement of the stem with the PI control could produce unwanted vibration to the control valve. This will also increase the amount of routine maintenance required for the control valve in question.

The next simulation result shown in Figure 6:27 represents the set point tracking experiment. As explained, the aim of this exercise is to investigate the robustness of the controllers for a series of random set point changes. As shown in Figure 6:27, the PI controllers managed to track the set point changes appropriately. Thus once again these encouraging results suggest that the feedback/feedforward control approach is reliable. As also shown in the figure, the transient responses for changes in the pH set point value from this simulation are very similar to the simulation transient responses with the fuzzy logic controller shown in Figure 6:23 (i.e. simulation exercise without any modification on the configuration of the pH fuzzy logic controller). These two results (i.e. Figure 6:27 and Figure 6:23) show that the modified pH model is consistent in that it behaves with a similar transient, especially when the pH value changes from pH value 9 to pH value 6.5. The response at this particular set point change shows that the developed pH model is relatively slow when compared with the actual response from the pilot plant. However the fuzzy logic control approach has flexibility in the control design, unlike the PI controller where the control design process is quite rigid and is less able to deal directly with such problems even with new tuning parameters.



Figure 6:27: Simulation result for set point tracking with PI controller

Meanwhile the response for the alkaline stream in Figure 6:27 demonstrates transient performance which is very similar to the previous simulation result in Figure 6:26. The response oscillates roughly between 100L/h and 130L/h with very high frequency when one would expect a steady state condition. The response becomes even worse when the pH value changes from pH value 9 to pH value 6.5 and also from pH value 9 to pH value 7. In practical terms this unwanted response is likely to cause damage to the control valve, especially the parts associated with the stem and seat of the control valve.

The third simulation exercise is the load change experiment. As explained previously, the objective of this investigation is to observe the capability of the controllers to handle load disturbances. The dynamic response for this exercise is shown in Figure 6:28.

The simulation results shown in the figure indicate that the feedback/feedforward control with PI controllers is able to provide a good transient response in terms of the pH value despite having a series of flowrate disturbances in the acid stream. However, a problem similar to that encountered in the other simulation experiments involving the PI controllers can be observed for the alkaline stream where the response oscillates with a very high frequency. Unwanted control valve behaviour is also shown between 1000s and 1200s. A similar situation at the same part of the time range has been explained earlier in Figure 6:24 for the fuzzy logic controller. However the responses found with the PI controllers shown in Figure 6:27 and Figure 6:28 are far more critical as compared to the behaviour with fuzzy logic controllers.



Figure 6:28: Simulation results for the load disturbance with PI controllers

The fourth set of simulation results are shown in Figure 6:29. Once again the results show that feedback/feedforward control strategy with the PI controllers has managed to control the pH value at the required value (i.e. a pH value 7) effectively. Thus, based on all the computer-based simulation results shown for all four experiments it can be summarised that the type of control scheme shown in Figure 6:1 is capable of producing very reliable responses in terms of pH value and can handle disturbances effectively. However throughout these four simulation experiments the results also indicate that the responses from the alkaline stream oscillates with high frequency leading to unwanted control valve activity in some situations. Thus the particular fuzzy logic controllers developed in the course of this work have some potential advantages over PI controllers for the same overall controller structure.



Figure 6:29: Simulation results for acid concentration disturbances with PI controller

6.4 Summary

This final sections of Chapter 6 can be summarised in terms of a few main points. The first involves the successful performance of feedback/feedward control scheme. The performance of this control strategy has been confirmed with the implementation of the control strategy with fuzzy logic controllers on the pilot plant. This combined feedforward and feedback control strategy has also provided very encouraging computer-based simulation results with the fuzzy logic controllers as well as with conventional PI controllers.

The second point concerns the development of the fuzzy logic controller. The chapter clearly reveals the main advantage of this approach to controller development which is its simplicity. As described, the development of the controllers is based on theoretical knowledge of the chemical process and on basic engineering principles. Information about the configuration of the pH neutralization pilot plant and some limited information from the developed pH process model provided additional insight relating to the dynamic behaviour of the system.

This chapter has also provided information about the performance and capabilities of the fuzzy logic controllers used in this application which involves a highly nonlinear system. The fuzzy logic controllers have been tested for a number of different types of experiment with different control objectives. In addition the testing also provides evidence concerning practical issues relating to this new control approach involving a calculated set-point for a flow controller. The results from the experiment on the actual pH neutralization pilot plant are very encouraging which generally indicates that this control approach is workable and feasible. These experimental results also show that the fuzzy logic controller is able to provide a reliable and highly accurate control performance. The computer-based simulation results support the conclusion that the fuzzy logic controller is robust and capable in handling different types of disturbance. The simulation results with PI controllers also showed very encouraging control performance in terms of handling the pH value, although some concerns exist in terms of the control valve activity observed in the simulation studies for this type of controller. The flexibility in control design for fuzzy logic controller has also been demonstrated in this chapter which provide an advantage of these controllers over PI controllers. Unlike the classical control approach (i.e. PI controllers) the ease of adding some additional inputs and formulation or modifications of membership functions can be made in order to handle exceptional control behaviour.

Finally this chapter has shown that the modified pH model shows also similar behaviour to that obtained from the pilot plant. Thus this developed model can be a platform for further investigation of other type of advanced controller. However some further investigation can be made to improve this process model especially on the reaction rate of the pH process.

CHAPTER SEVEN

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7.0 CONCLUSIONS AND RECOMMENDATIONS

The first section of this final chapter reviews the main features and contributions of this research. It provides a summary of the achievements relating to the first objective of the research concerning the development of the pH neutralization model and concludes with discussion of the results achieved in terms of the second objective of the research which is the implementation of the advanced controller. It highlights the main benefits of the feedback/feedforward control scheme using a fuzzy logic control approach as an advanced controller for the pH neutralization process and discusses implementation issues. The section also provides insight obtained from computer-based simulation results for the same control structure (i.e. feedback/feedforward) with a conventional Proportional plus Integral controller. Suggestions for further research which builds upon the developments made during the course of the current work are also made in the final section of this chapter.

7.1 Research Project Conclusions

At this point it is important to consider once again the objectives of this research, as outlined in Chapter 1. As described in the first chapter of this thesis, there were two primary objectives of this research. The first was to develop a dynamic nonlinear pH neutralization process model, based on physical and chemical principles, that can represent the specific pH neutralization pilot plant installed at UTP. The accuracy of this model should be sufficient to allow development of conventional and advanced control systems through simulation for subsequent implementation and testing on the plant itself.

The second goal for this research was to design, develop and implement an intelligent or advanced controller, based possibly on a Fuzzy Logic Control approach, involving use of an appropriate controller structure. In addition to these two main objectives, it was also intended to investigate benefits and limitations of the chosen control algorithms and the type of process model developed during this investigation.
Generally, both the main objectives have been achieved. The developed model of the pH neutralization process is capable of providing dynamic responses that are sufficiently similar to those obtained from tests on the available pH neutralization pilot plant to allow the model to be used as a basis for design and development of control systems. This similarity has been demonstrated both through qualitative graphical comparisons of time histories and by means of quantitative measures such as Theil's Inequality Measure. In terms of the second objective, the control performance obtained from the implementation of the intelligent controller based on fuzzy control principles was very encouraging. The next sub-sections provide more comprehensive discussion and conclusions for each of the objectives.

7.1.1 The pH neutralization process model

As explained above, the first primary objective of this research involved modelling a pH neutralization process for the pilot plant installed at UTP. The main feature of interest in this pilot plant is that it incorporates instrumentation and types of actuators that are currently being used in the process industries. It is believed that, from this point of view, the investigation has provided realistic solutions which may be of direct interest to industry.

The approach adopted for the modelling process is based on the use of physical and chemical principles and fundamental laws, using a conventional mathematical modelling process, coupled with information obtained from preliminary tests carried out on the pilot plant itself in order to obtain estimates of certain parameters which were not known *a priori*. This physico-chemical modelling approach is a rigorous and generally applicable method of deriving dynamic equations for a pH neutralization process using a type of representation based on the concept of a continuous stirred tank reactor (CSTR) model. This was the modelling approach introduced by McAvoy in 1972 for this type of process application.

The pH neutralization process model that was first developed provided a form of dynamic response which was in agreement with most published results in the literature, especially in terms of the simple titration curve experiments. During the model analysis stage, the developed model provided useful insight associated with the theoretical understanding of factors such as the influence of concentration and flowrate on the pH neutralization process. In terms of the initial model verification and validation process, the computer-based simulation results also demonstrated behaviour that is broadly similar to the dynamic characteristics found from tests carried out on the actual pilot plant. However, some important differences were found between responses of the model and system for particular test conditions. Thus, it may be concluded that the first model is satisfactory, reliable and adequate for representation of the actual behaviour of the pH neutralization plant but has some important limitations. Although these results were encouraging and suggested that the developed model could be used to provide a model for the development of various types of intelligent controller, subsequent enhancement of the data acquisition system and the associated user interface made more complex experiments possible. These allowed an improved simulation model to be developed which led to the possibility of further improvements in the performance of control systems implemented on the pilot plant.

Further investigation of the improved model at the formal model validation stage has also been performed successfully. Transients observed in computer-based simulation of the developed model were critically evaluated through comparison with experimental results. This more detailed investigation of the model was feasible using the new and improved system for distributed data collection and control system that was installed on the pilot plant mid-way through the current investigation. This new system offers much more flexibility in terms both of implementation of control schemes and dynamic testing of the system under open-loop conditions. It was observed that the model first developed showed some discrepancies when its responses were compared with the response from the pilot plant. Thus, based on these differences in behaviour and more detailed analysis of the model it was concluded that some assumptions made during development of the first model were unacceptable and needed to be revised. In the re-evaluation of the pH model it has been established that two factors could be changed to ensure that the model provides dynamic responses more consistent with those observed on the plant itself. The first of these related to the values of the dissociation constants. Using the dynamic response from the pH neutralization pilot plant new dissociation constant values were determined from plant observations rather than from theory.

The modified dynamic model of the pilot plant has been compared in detail with the results of experiments on the pilot plant. Detailed investigations were carried out, during the model validation process, where the dynamic response from the pH model was tested and analysed in several ways. Based on graphical evaluation, the dynamic response from the improved model was very similar to the dynamic transient of the pilot plant. In terms of more detailed point by point evaluation within records and statistical analysis, it has been shown that the data from the computer-based simulation are very close to the experimental data. The final evaluation involved a comparison of experimental and model time series using Theil's Inequality Coefficient (TIC). The outcome from the TIC analysis has successfully shown that there is a good agreement between the developed model and the actual transients in the measured responses from the actual plant.

Therefore, in general terms, it may be concluded that the developed pH model with a new set of dissociation constants has successfully demonstrated dynamic performance which is adequate for control system design purposes when compared with the actual pH neutralization pilot plant. Thus the development of the nonlinear dynamic model for the pH plant has been successfully achieved. The simulation results from the computer-based simulation demonstrate behaviour that is very similar to the actual pilot plant, taking into account the uncertainties in measured quantities and model parameters.

The second significant factor related to imperfect mixing. Although representation of imperfect mixing was not incorporated in the final version of the pH model, investigations indicate it is a key factor that needs to be explored further. It was observed that the volume of the reactor tank in the pH neutralization pilot plant is larger than the volume of reactor tank used in most previous reported studies. Thus the initial assumptions in which the acid-base reaction process in the reactor tank is taken to be instantaneous and the tank is assumed perfectly mixed at all times were judged to be inappropriate. It is believed with an additional representation and more experimental work involving rigorous external validation and evaluation of models, a new pH model can be developed which will be able to represent the behaviour of the pilot plant even more accurately.

7.1.2 The implementation of the feedback/feedforward control scheme with the advanced controller

The second main objective of this research concerns the implementation of advanced forms of controller with a feedback/feedforward control structure on the pH neutralization pilot plant. Based on the literature survey, a non-model based type of control strategy has been considered. The controller will not depend too significantly on the developed model, although insight gained from the modelling process undoubtedly provided useful insight in the development of the control schemes considered. Investigation and implementation of the feedback/feedforward control schemes in this research have shown the effectiveness of "correction of error" and "prediction of disturbances" control strategies.

The advanced controller that has been considered and implemented on the pilot plant is based on the fuzzy logic control approach. This advanced control was incorporated within the feedback/feedforward control scheme.. Based on the implementation process of this control approach it can be concluded that the process of developing the fuzzy logic controller was less complicated than the process for many other forms of control algorithm. However, prior to this implementation process it is essential to have a good understanding and working knowledge of the system to be controlled, including information about the capability of the instrumentation and actuators involved, as well as the affect of the main parameters of the system model. It is believed that this research has successfully demonstrated the viability of the feedback/feedforward control structure. In addition to that the fuzzy logic approach has also shown the practicality of its implementation as an advanced control system on this highly nonlinear type of process. Thus this study provided useful insight concerning the use of a fuzzy logic approach to control the nonlinear and time varying processes in general.

A wide range of tests and experiments have been performed successfully on the pilot plant in order to provide insight regarding issues such as control performance, stability and robustness of the feedback/feedforward control structure with the chosen fuzzy logic controller. Generally all the control performance objectives have been achieved successfully. The experimental results were very encouraging and the controlled dynamic responses of the plant with the fuzzy logic controller were judged satisfactory in terms of the initial requirements. In general the controllers were able to handle various types of disturbances. Thus it has been shown that the intelligent controller based on fuzzy logic control principles is capable of providing a good control performance. Through this study, it is also believed that these promising and encouraging results should encourage engineers to give more consideration to the use of this control approach within the process industries. However further experimental investigations relating to the use of conventional control algorithms with the same control structure were not possible because of time limitations in terms of access to the pilot plant.

The investigations on the performance of the feedback/feedfoward control structure also involved computer-based simulation work. An extensive computer-based simulation study was carried out using advanced controllers (i.e. fuzzy logic) and conventional controllers (i.e. PI controllers). Generally, the computer-based simulation results based on the fuzzy logic controllers and PI controllers showed results and control performances similar to those demonstrated in the experimental results. However, the performance in terms of the control valve activity suggested that the advanced control system structure based on combined feedforward and feedback principles with fuzzy logic controllers was capable of giving an overall control performance which was generally better than that for the same controller structure with a conventional PI control algorithm. The simulation work supported the fact that the fuzzy logic approach was able to provide more flexibility in handling a specific control problem and also offers fewer complications in terms of control system design and development. In conclusion, the fuzzy logic control approach with combined feedforward and feedback controller structure has been shown to be capable of providing good control performance in terms of set-point tracking, disturbance rejection, stability and robustness.

7.2 Summary of the Main Contributions

One of the main contributions of the research reported in this thesis is the development of a form of process model that can be applied to real plant involving industrial actuators and industrial measuring devices and instrumentation. This model has a generic form and has been implemented using widely used simulation tools. This makes the simulation model modifiable for other plant. External validation tests carried out using the pilot plant at UTP have provided useful evidence about the strengths and weaknesses of the model and have demonstrated its suitability as a nonlinear dynamic model for use in the design of conventional and advanced forms of a controller.

The development, implementation and testing of the feedback/feedforward control scheme with fuzzy logic control principles on the actual pH neutralization process pilot plant represents the second important contribution. It is believed that there are few previous published examples involving pilot plant implementation. Most previously published work on advanced forms of control applied to pH neutralization processes have either involved simulated processes or relatively small laboratory bench-top rigs that do not involve industrial actuators or instrumentation systems.

It has been demonstrated, from tests on the pilot plant and through simulation studies, that the fuzzy controller has performance advantages in terms of tracking, disturbance rejection and robustness compared with a conventional proportional plus integral controller with the same control structure.

7.3 Recommendations for Future Research

As part of the key contribution of the research, the outcome from the research study has also suggested and established some areas of work for other researchers to consider. Thus this section presents some suggestions and recommendations for future research.

This research study has shown that there is a need to improve the widely used pH neutralization process model so that it will provide dynamic behaviour similar to that found in the existing types of pH process plant used in industry. The current investigation suggests that adapting the pH neutralization process model to fit the practicalities of a specific plant is not a trivial undertaking, especially when factors such as imperfect mixing are significant.

A rigorous study on how to incorporate the more practical elements of the pH neutralization process plant within an improved form of modular and generic simulation model is necessary. In the initial investigation it might be useful to reconsider the assumptions made by previous researchers. Thus it is hoped that the results of such an investigation may provide a good platform for a further off-line computer-based simulation study to investigate open-loop and closed-loop dynamic characteristic of specific examples of pH neutralization process plant.

It is also believed that a more accurate pH process model is needed in designing other types of advanced control approach which utilise a process model to provide an accurate and reliable prediction. It is also hoped that developments of this type can help bridge the well known "gap" between theory and industrial practice. As mentioned from the beginning of the thesis, this project involves an acid-base reaction process between Sulphuric acid and Sodium Hydroxide. Thus, an investigation on how different types of acid and alkaline would react and behave with this control approach has to be a further recommendation for future work. Another recommendation would be the use of a buffer solution in the neutralization process. This would also be another interesting investigation especially from the chemical engineering point of view.

An additional recommendation would be an investigation of the implementation issues of additional types of advanced controller on this particular pH neutralization pilot plant. This is basically to fully utilise the advantages of the pH neutralization pilot plant configuration. As an example, further investigations of other methods based on the Tagaki-Sugeno approach would also be useful.

It would be interesting to find out the differences in terms of control performance, stability, robustness possible with this approach, as well as the implementation issues that arise. Also, based on the literature survey (Postlethwaite 1994;Sing 1997;Sing & Postlethwaite 1996) the use of a fuzzy logic approach to develop a pH neutralization process representation as a model predictor for a model based predictive control approach has been successfully implemented on a small laboratory scale. This provides an interesting area for further modelling, design and experimentation using the pilot plant at UTP to investigate the control performance possible with this type of on-line modelling and control approach. This would again, hopefully, provide information of potential value to industry.

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8.0 **REFERENCES**

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APPENDICES

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9.0 LIST APPENDICES

Appendix I: Recalibration Results

Appendix II: Technical specification of the pH meter

Appendix III: Technical specification of the conductivity meter

Appendix IV: List of I/O of the system and pin assignment for the I/O cards

Appendix V: Layout of user interface for experimental work

Appendix I: Recalibration Results





Appendix II: Technical specification of the pH meter

• Controller

Model : alpha-pH1000 1/4 DIN pH/ORP Controller



VIEW ENLARGED IMAGE

Product Features

- :: Built-In Programmable Limit, Proportional (Pulse Length or Pulse Frequency) ideal for precision process control applications
- :: User-Customization through Advanced Setup Menu offers flexibility in matching the controller's functions to suit individual's specific requirement
- :: Automatic Calibration with Auto-Buffer Recognition e liminates mistakes during calibration
- :: Symmetrical Mode Operation eliminates electronic noise problems when used with solution ground
- :: One-Point Online Calibration without shutting down the line
- :: Hold Relay for use with float switches/flow switches and other controllers as a failsafe function
- :: Two Level Password Protection prevents un authorized tampering with settings
- :: 0 to 2000 Second Time Delay Adjustment on control and alarm delays
- :: Two Galvanically Isolated Scaleable 0-20/4-20 mA Outputs for pH/ORP
- :: Wash Contact Relay controls electrodes cleaning systems at desired duration and frequency
- :: Choice of Glass or Antimony Electrode for general purpose or hydrofluoric acid applications
- :: Adjustable Hysteresis (Dead Band) prevents rapid contact switching near set point
- :: Non-Volatile Memory retains all stored parameters and calibration data even if power fails
- :: Large Dual Display shows pH (or ORP) with temperature simultaneously features clear multiple icons, set points, and status messages
- :: Choice of Temperature Sensor Pt100/Pt1000 with 2-wire or 3-wire temperature input selection
- :: Easy Installation and Wiring with detachable plug-in connectors

Applications

General: Useful for any batch or on-line type application that requires accurate pH or ORP control.

Water Purification/Treatment: Use for batch and on-line control of incoming process water, rinse water treatment, recirculating system and waste water treatment.

Industrial: Ideal for chemical processing, food processing. aquarium, pharmaceutical, hydroponics and waste control industries.

Regulatory: Hook to recorder to document data for regulatory compliance.

• pH Process Electrode

Model: EC100GTSO-05B



Specifications

Product Specification	Description
pH Range	0 to 14
Reference	Annular Teflon, double junction
Reference electrolyte	Saturated KCI, polymerized gel
Operating temperature	0 to 80 °C
Pressure tolerance	6 bars
Temperature sensor	Pt 100
Potential matching pin	Platinum
Material	PPS (Ryton)
Thread	3/4" NPT
Cable	Integral 5m low-noise semi-conductor screened
Connector	BNC
Dimensions: Length (excludes cable)	151 mm
Diameter (external)	26 mm
Weight	650 g

Appendix III: Technical specification of the conductivity meter

• Controller

Model : alpha-CON1000 1/4 DIN Conductivity Controller

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VIEW ENLARGED IMAGE

Product Features

- :: Ten Selectable Conductivity Measurement Ranges in one controller via its IP54 front panel. Highlevel accuracy of ±1% of full scale can be obtained with appropriate cells and correct temperature coefficient
- :: User-Customization through Advanced Setup Menu offers flexibility in matching the controller's functions to suit individual's specific requirement
- :: Choice of Cell Constant (0.01, 0.1, 1.0, 10.0) for accurate control in any solution
- :: Hold Relay for use with float switches/flow switches and other controllers as a failsafe function
- :: Two Level Password Protection prevents un authorized tampering with settings
- :: 0 to 2000 Second Time Delay Adjustment on control and alarm delays
- :: Two Galvanically Isolated Scalebale 0-20/4-20 mA Outputs
- :: Wash Contact Relay controls electrodes cleaning systems at desired duration and frequency
- :: Adjustable Hysteresis (Dead Band) prevents rapid contact switching near set point
- :: Non-Volatile Memory retains all stored parameters and calibration data even if power fails
- :: Line Resistance Compensation against intrinsic cable resistance for longer cable connection
- :: Large Dual Display shows measurement with temperature simultaneously features clear multiple icons, set points, and status messages
- :: Choice of Temperature Sensor Pt100/Pt1000 with 2-wire or 3-wire temperature input selection
- :: Easy Installation and Wiring with detachable plug-in connectors

Applications

General: Use for virtually any batch or online applications where rapid, accurate control. Great for OEM/system integrator.

Industrial: Use in applications involving agriculture, chemical processing, boiler and water heaters, waferfab, microprocessor manufacturing, pharmaceuticals, pulp and paper industries, and bleach manufacturing.

Water Purification/Treatment: Use to treat batches of incoming process water, ultrapure water, boiler and feed water control.

Regulatory: Hook to recorder to document data for regulatory compliance.

Conductivity Process Electrode

Model : EC91346S



Specifications

Product Specification	Description
Conductivity range	Up to 500 mS/cm
Cell constant, k	0.3, 4-Cell
Temperature sensor	Pt 100, 3-wire
Pressure rating	6 bar
Material	Ryton, SS 316
Thread	3/4" NPT
Cable	Integrated 7.6m, 8-wire double-shielded, open
Dimensions: Leng (excludes cable)	th 150.5 mm
Diameter (external)	22.2 mm
Weight	650 g

Appendix IV: List of I/O of the system and pin assignment for the I/O cards

Digital I	nput Card	MM32-Diamond Digital Input
Card No- Pin Assignment	Name	Description
Card A-1	LS100	Limit switch for overflow indication – Reactor Tank
Card A-2	LS110	Limit switch for overflow indication – Discharged Tank
Card B-3	Unused	
Card A-4	P100-Run	Indication for pump status for acid stream -RUN
Card A-5	P100-Trip	Indication for pump status for acid stream –STOP
Card A-6	P110-Run	Indication for pump status for alkaline stream -RUN
Card A-7	P110-Trip	Indication for pump status for alkaline stream –STOP
Card A-8	AG120	Indication for agitator at reactor tank -RUN
Card B-1	AG120	Indication for agitator at reactor tank -RUN
Card B-2	Unused	
Card B-3	Unused	
Card B-4		Unused
Card B-5	Unused	
Card B-6	DCS/XPC	Indication for selector switch for DCS – Plantscape Honeywell System or New Data Acquisition system (MATLAB)
Card B-7		Unused
Card B-8		Unused

Digital Output Card		MM32-Diamond Digital Output
Pin Assignment	Name	Description
1	P110	Pump activation for acid stream
2	P100	Pump activation - alkaline stream
3	AG120	Agitator activation – Reactor Tank
4	AG130	Agitator activation – Cascaded Tank
5	AG140	Agitator activation – Discharged Tank
6	Unused	
7	Unused	
8	Unused	

Analogue Input Card		MM32-Diamond Analogue Input
Card No- Pin Assignment	Name	Description
1	CT100	Measured value from conductivity meter – Acid Tank
2	FT120	Measured value from flowmeter – Acid stream
3	CT110	Measured value for conductivity meter – Alkaline Tank
4	FT121	Measured value from flowmeter – Alkaline stream
5		Unused
6	Unused	
7	AT122	Measured value from pH meter – Reactor Tank
8	AT130	Measured value from pH meter – Cascaded Tank
9	1T140	Measured value from pH meter – Dischanged Tank
10	Unused	
11	Unused	
12	Unused	
13	Unused	
14	Unused	
15	Unused	
16	Unused	

Analogue Output Card		MM32-Diamond AnalogueOutput
Pin Assignment	Name	Description
1	FCV120	Control valve for acid stream
2	FCV121	Control valve for alkaline stream
3	ACV130	Control valve for product
4		Unused



Appendix V: Layout of user interface for experimental work

