Modelling and Control for Industrial Neutralization Water Unit

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Synopsis:

This Master Thesis has been proposed by ELFE company to improve the control strategy of the neutralization water unit in the Ammonia Plant. This project makes a rough description of the Ammonia plant and Demineralization Unit. Demin unit exists in order to provide demineralised water for steam production at heat exchangers. Neutralisation unit is responsible for processing the waste water from regeneration process of demin unit, in order to dispose it in the sea.

Two models are derived. A pilot model of 1 tank and a real 2 tanks model as it already exists at the factory. Both of them are modelled and linearised. Linearisation method around Operating point and inversion of the Non Linear function are used in order to over come the non linearities. Also an observed based PI controller is used to control the models.

Both models and control are implemented with Simulink. The results from the simulations are presented and evaluated.

Acknowledgments

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Special thanks to Sofia Zouda, student at School of Electrical and Computer Engineering at Aristotle University of Thessaloniki, for her corrections and help.

Closing I want to thanks my parents for their love and endless support to me.

List of acronyms

AAU	Aalborg University
ELFE	Hellenic Fertilizers Industry
HCl	Hydrochloric Acid
NaOH	Caustic Soda
OP	Operating Point
pH	power of Hydrogen[4]
PI	Proportional Integral

Preface

This Master Thesis has been proposed by ELFE company in order to investigate possible improvements at control strategy of the neutralization water unit in the Ammonia Plant. This project was proposed by Panagiotis Dagakhs who is working as head engineer of automation and instrumentation department at ELFE company.

The documentation of the project is written in English and is a research report. The parts that exist at this Master Thesis are introduction, modelling, control, implementation, results and conclusion. Also a nomenclature is made for a notation explanation that there is at this project. Reference and documentation are presented at the end of the report.

Contents

Part I

Introduction

This part describes some basic information about the factory.Also an elementary description of the process that will be considered.

Introduction 1

1.1 ELFE Company

Company Presentation

Hellenic fertilizers ELFE is one of the leading corporations at the fertilizing industry in Europe.The facilities are located in Northern Greece near the Kavala city. The PFI Phosphoric Fertilizing Industries was founded in 1961 and started operating in 1965 [2]. In 2000 the 2 most important fertilizing industries in Greece, PFI and Chemical Industries of Northern Greece SA, were merged and formed the biggest chemical industry of Greece. This industry in 2009 was acquired by ELFE SA. Nowadays this company continues to be the only fertilizing company in Greece and one of the biggest in South East Europe. [2]

Figure 1.1: ELFE Factory

The main object of the industry is to produce compound and nitric fertilizers (NPK). It is the biggest factory in Kavala and one of the biggest in Greece. The producing fertilizers are divided at 4 main types:

- **Nitrogenous Fertilizers (N)**

  The main nutrition element is the Nitrogen (N). At this type are included 7 groups of fertilizers

  - Ammonium Nitrate (AN)

  - Calcium Ammonium Nitrate (CAN)
  - Ammonium Sulphate Nitrate (ASN)
  - Ammonium Sulphate (AS)
  - Urea
  - Ammonium Nitrate in combination with trace elements
  - Ammonium Sulphate Nitrate with trace elements
  - Nitrogenous fertilizers with DCD-slow release

- **Compound Fertilizers (NP)**

  The main nutrition are Nitrogen (N), Phosphorus (P) , Sulphur (S). At this type are included 3 groups of fertilizers

  - Fertilizers which contain only the three primary nutrients Nitrogen (N), Phosphorus (P) and sulfur (S).
  - Fertilizers with above three main elements Nitrogen (N), Phosphorus (P) and sulfur (S), plus other secondary nutrients or micronutrients.
  - Fertilizers with three main elements Nitrogen (N), Phosphorus (P) and sulphur (S), which contains nitrification inhibitor DCD.

- **Soluble Fertilizers**

  - Specialized water-soluble fertilizers with high technology, for secure results and buffering capacity of the soil solution.
  - Suitable for cultivation in different substrates and hydroponics because of adequate nutritional capacity and low conductivity.
  - Widely used in greenhouses, horticultural crops, seedbeds, outdoor crops (tomato, cucumber, vegetables, etc.).
  - Water soluble fertilizers are supplying the plants with all the nutrients at different stages of development, ensuring complete nutrition.
  - Fertilizing with water-soluble fertilizers ensures optimal growth without following growth of toxic salts in the soil.
  - They have very high compatibility with most fungicides and insecticides.

Generally the factory is able to produce 50 labels of fertilizers.

1.2 Ammonia Plant

The factory is divided at 7 units

- Ammonia Production Unit
- Production Unit of Nitric Acid and Nitric Fertilizers
- Sulphuric Acid Production Unit
- Phosphoric Acid Production Unit
- Compound Fertilizers Production Unit
- Steam Turbine Generators
- Bag Filling Unit

This thesis is focused at Ammonia unit and more specific at neutralization unit which is as part of demineralization unit.

In order to produce ammonia, Nitrogen (N) and Hydrogen (H) are needed.

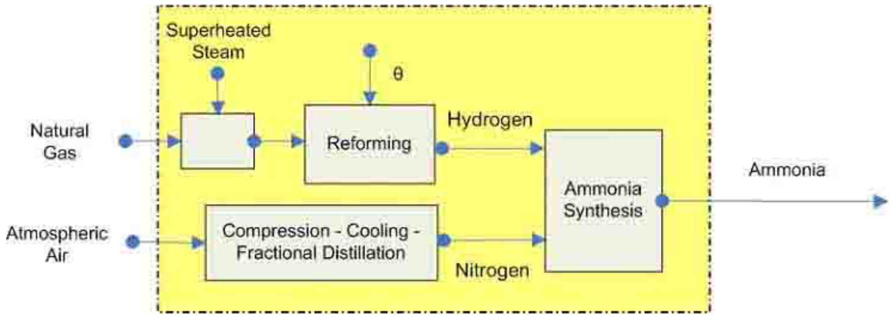

Figure 1.2: Production Diagram for Ammonia

- The **Nitrogen** is obtained from the atmospheric air. These are the steps that are needed
  - **Compressed ambient air**
    The ambient air is compressed at 3 steps. Between these steps the air is chilled with water alternators and the producing water consecrations are removed.
  - **Air Drying** The compressed air is led through a dryer where the moisture and CO_2 are removed.
  - **Nitrogen production** The dry clean air is chilled and it is distilled. The product from this process is pure Nitrogen.

- The **Hydrogen** is obtained from the natural gas. These are the steps that are needed
  - **Steam reforming of the natural gas**

    At this step the natural gas is transformed to Hydrogen , Carbon Monoxide and Carbon Dioxide. This reaction is extremely endothermic so addition of heat is needed. All this process is taking place into the reformer. Reformer is as large reactor with catalyst of nickel and temperature around 1000 degrees of Celsius. The reactions that take place are the following:

    $$\begin{aligned} CnHm + nH_2O &\rightarrow nCO + (n + \frac{m}{2})H_2 - Q_1 \\ CH_4 + H_2O &\rightarrow CO + 3H_2 - Q_2 \\ CO + H_2O &\rightarrow H_2 + CO_2 + Q_3 \end{aligned} \tag{1.1}$$

    The gas that leaves the reformer is a mixture of $C0_2$, CO, H_2O and CH_4
  - **Reforming of the carbon monoxide**

    The reformed gas is leaving the reformer and enters a reactor with catalyst of iron/chrome oxide. There, the carbon monoxide of the reformed gas react with steam and is transformed to Hydrogen and Carbon Dioxide.
    The reaction that take place is the following:

    $$CO + H_2O \rightarrow CO_2 + H_2 + Q_3 \tag{1.2}$$

    Where Q is the temperature.
  - **Purifying the Hydrogen**

    The gas is cooled through water alternators and then enters the Pressure Swing Adsorption Purification Unit (PSA). In this unit the gas is filtered and pure Hydrogen remains.
- Ammonia Synthesis

  The two gases,Nitrogen and Hydrogen, are compressed and heated at proper pressure and temperature. The mixture of hydrogen and nitrogen, syngas, enters into a reactor, where with iron as a catalyst, ammonia is formed. This reaction is extremely exothermic. The ammonia is cooled through water alternators and then chilled in order to be liquid. The reaction that take place is the following:

  $$N_2 + 3H_2 \rightarrow 2NH_3 + Q \tag{1.3}$$
- Ammonia Storage

  Then Ammonia stores in two tanks which are located in the plant.

The produced ammonia is consumed by the production units of nitric acid and fertilizers.

1.3 Demineralization Unit

The majority of the chemical reactions that take place at the Ammonia Unit are exothermic. In order to take advantage this energy, a super high temperature steam is produced.This steam is used to rotate the turbine generator of the factory which produce a significant amount of the energy that it consumed.

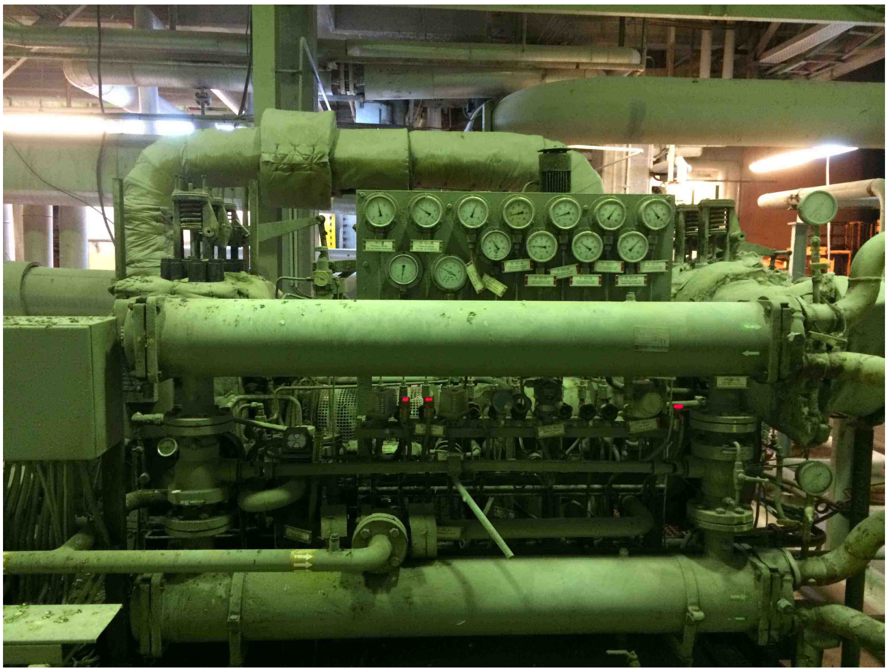

Figure 1.3: Steam Generator

Steam production needs demineralized water. This water comes through heat alternators where steam is produced. This steam is over heated until it reaches 300^oC and $40kg/cm^2$.
As a result of this, a Demineralization unit is established at the factory .The main characteristics of the well water is a high alkalinity ,an amount of up 8ppm suspended solids plus approximately 100ppm CO_2.

First the raw water passes from a sand filter to remove the suspended solids. This filter shall be backwashed automatically as soon as the pressure drop exceeds the maximum allowed value.

Filtered water flows to the dealkalizing filter where all Ca^{++} and Mg^{++} ions related to HCO_3 ions are exchanged against H^+ ions, forming H_2CO_3 which is splitted into CO_2 and water, in the degassifier above the deagassed water pit. Regeneration of this filter is done automatically when the flow meter reaches the set point.

H_2CO_4 is used as regenerant, and is diluted to max. 0.7% strength to avoid precipitation of $CaSO_4$. The dealkalized water flows to a CO_2 degassifier where CO_2 is removed.

Process condensate treatment

Filtration, CO_2 and NH_3 removal

The process condensate contains suspended solids, NH_3, CO_2 and organics, the nature of which is not defined.
First the process condensate is deagassed to remove the excess CO_2.
From the degassifier the condensate is pumped into an anthracite filter where the suspended solids are removed.
Because of the high amount of NH_3, a cation exchanger has been installed to remove the NH_3, by which the size of the demineralization unit and the chemical consumption is minimized.

The end of the operating cycle is determined on conductivity.
Regeneration is carried out downwardly, using HCl.
Introduction of the regeneration starts out automatically when the conductivity exceeds the set point.

Demineralization

Cation-anion exchanger and mixedbed demineralizer

The demin plant consists of one cation exchanger, one anion exchanger and one mixedbed demineralizer.
The mixed dealkilized water/process condensate is pumped from the degassed water pit to the cation and anion exchanger where it is almost completely demineralized.

NH_3, CO_2 and ionogenic organics are removed from the process condensate in the process condensate treatment, but non ionogenic organics pass the demineralization filters and can be found in the demin water.

Since organics may cause a fouling of the resins, there are used acrylic and macro reticular type of anion resins, there are used resistant sensitive to the fouling.

The end of the operating time of the cation/anion exchanger is on high conductivity after the anion exchanger, where by the regeneration will start automatically after exceeding the preset set point.

Both cation and anion exchanger are regenerated counter currently which means a higher regeneration efficiency and better water quality.

After the anion exchanger the demin water is mixed with the turbine condensate and the mixture passes the mixedbed polishing filter, and flows to the denim storage tank.
The mixedbed has a long operation time because of the low saltload, but shall be regenerated automatically as soon as the conductivity exceeds the set point.

1.4 Chemical process description of Demin Unit

General

Exchanged materials are water insoluble grainy substances which possess the faculty to exchange their deposited ions against ions existing in the water. The process, on practice, occurs in filters.

Depending on their origin, they are:

1. Inorganic Exchange Resins
    - natural products: volcanic ashes of the Eifel
    - synthetic products
2. Organic Exchange Resins
    - made from coal
    - made from synthetic resins
        - on a phenolic basis
        - on a styrene basis

In today's water treatment technique, synthetic resins, preferably on a styrene basis, are applied. They can be regenerated with Na^+ and H^+ ions (cationic resins) and with OH ions (anionic resins), it being thus possible to remove cations as well as anions.

Well water pretreatment

Sand filter

The sand filter removes suspended matter, from the raw water and protects the ion exchange resins of the next appartus from fouling by this matter.

Dealkalizing filter V-462

In the dealkalizing filter which is filled with weak-acid cation exchange resin hydrogen cycle (H^+-form) take place ion exchanging.

This cation resin is capable to exchange the present dissolved calcium and magnesium which are combined with bicarbonate into an equivalent amount of hydrogen, according to the following reactions:

$$\begin{aligned} Ca(HCO_3)_2 + RH_2 &\rightarrow RCa_2 + 2H_2CO_3 \\ Mg(HCO_3)_2 + RH_2 &\rightarrow Rmg_2 + 2H_2CO_3 \end{aligned} \tag{1.4}$$

R-indicates one equivalent of the cation exchange resin.

The formed H_2CO_3 carbon acid is unstable and will be splitted up in the CO_2 degassifier according to the reaction

$$H_2CO_3 \rightarrow H_2O + CO_2 \tag{1.5}$$

As soon as the resin become exhausted after preset number at flow meter, due to loading with Ca^{++} and Mg^{++} ions, resin has to be regenerated.

For regeneration HCl is used as regenerant, to be diluted to max.0.7% .

Process condensate treatment

Process condensate filter

The process condensate filter is filled with anthracite instead of sand and removes suspended matter, from the supplied condensate to protect the ion exchange resins of next filters from fouling by this matter.

Anthracite instead of sand is used as filter medium, because sand can be formed Silica (SiO_2) at high process condensate temperature.

Cationfilter process condensate V-465

In the cation filter which is filled with a strong acid cation exchanged resin in the hydrogen cycle (H^+-form) take place ion exchanging.

The cation resin is capable to exchange the present dissolved ammonium which are combined with ions, into an equivalent amount of hydrogen, according to the following reaction.

$$NH_4OH + RH_2 \rightarrow RNH_4 + H_20 \tag{1.6}$$

R-indicates one equivalent of cation exchange resin.

Formed is H_20 so that 95% of the ammonium is held back.

As soon as the resin became exhausted, determined on conductivity, due to loading with ammonium, resin has to be regenerated.
For regeneration HCl is used as regenerant

Demineralization

Cation V-466 - anion filter V-467

The cation-anion filter will demineralize the pretreated water to a a specific electric conductivity under 20μS/cm.

The water flows first through the cation filter, filled with strong acid cation exchange resin and there after through an anion filter, filled with strong base ionexchange resin.

The cation exchange resin in the H^+-form is capable of replacing all cations by hydrogen ions and converting all states to their corresponding acids according to the reactions.

$$\begin{aligned} CaSO_4 + RH_2 &\rightarrow RCa + H_2SO_4 \\ MgCl_2 + RH_2 &\rightarrow RMg + 2HCL \\ Na_2(HCO_3)_2 + RH_2 &\rightarrow RNa + 2H_2SO_3 \\ KCl_2 + RH_2 &\rightarrow RK + HCl \\ Na_2SiO_2 + RH_2 &\rightarrow 2RNa + SiO_2 \end{aligned} \tag{1.7}$$

R-indicates the cation exchange resin.

The effluent of the cation exchanger contains: sulphuric acid, hydrochloric acid, carbonic acid and silicic acid.

It follows that a water containing only anions on passing through a bed of anion exchanger is demineralized.

As soon as resins exhausted, determined on conductivity due to loading with ions from the water, resins have to be regenerated.
Cation resins are regenerated with solution of hydrochloric acid, anion resins with a solution of sodium hydrocyde.
Both chemicals being applied in excess, the formed salts will be disappear to sewer with rinsing water.

Mixedbed filter V-468

The mixedbed filter ion exchanger polishes the water from the cation-anion-filter which is mixed up with turbine condensate and will produce demineralized water with specific electric conductivity under 0.2μS/cm .

The mixedbed is filled with strong acid cation and with strong basic anion resins, thoroughly mixed-up.

Reactions during operation and regeneration of the mixedbed will be the same at those in the cation-anion filter. By regeneration, the resins will be automatically separated before the chemicals enters the filter.

1.5 Neutralization Unit

Regulations for Industrial Waste Water Disposal

The sea area in front of the factory is characterized as area for fishing and all other uses except water supply and bathing. Due to this characterization and according to European and Greek laws for Industrial waste water disposal, the water which is disposed should fulfil the following criteria:

- Not clearly visible floating or settleable solids or sludge deposits, coming from sewage or industrial waste

- pH from 6.5 to 8.5

- Dissolved oxygen of at least 5,0 mg /l

- Not toxic or harmful in general, oil stained, hot or other waste, liable individually or in combination to make these waters unfit for this intended use

As a results of these regulation the chemicals that are used for resins regeneration should be neutralised before their disposal to the sea. So there is a Neutralization Unit at the factory.

General

The system is consisted by the following parts:

- **The mixing pit**

Figure 1.4: Mixing Pit

- **The neutralization pit**

Figure 1.5: Neutralization Pit

- **Supply valves for dosing of caustic soda, hydrochloric acid and mix air**

Operation of the system

Effluents from the filters during regeneration are collected in the neutralization pit. At high level of the neutralization pit the waste water pump is started whereby the effluent is recirculated from the neutralization pit to the mixing pit. The pH of the circulated effluent is measured continuously by an electrode placed in the pressure line of the waste water pumps, until pH has come within preset valves of the connected pH meter where after the circulating valve close

(a) Pumps. **(b)** Valves.

Figure 1.6: Valves and dosing pumps.

and the drain valve opens to discharge the neutralized water to sewer. The pH of the incoming water in the mixing pit is also continuously measured by an electrode in the mixing pit and depending on its value hydrochloric acid or caustic soda from the storage tanks will be dosed. The dosing however can be only take place by running waste water and the pH solution is between the limits, because the limit contacts are blocked when the pump is not running. Mixing air to mixing pit is always supplied as the control panel is in operation. Level in the neutralization pit is indicating by four level switches. When the level is below the lowest level switch the pumps are blocked to prevent them against running dry.

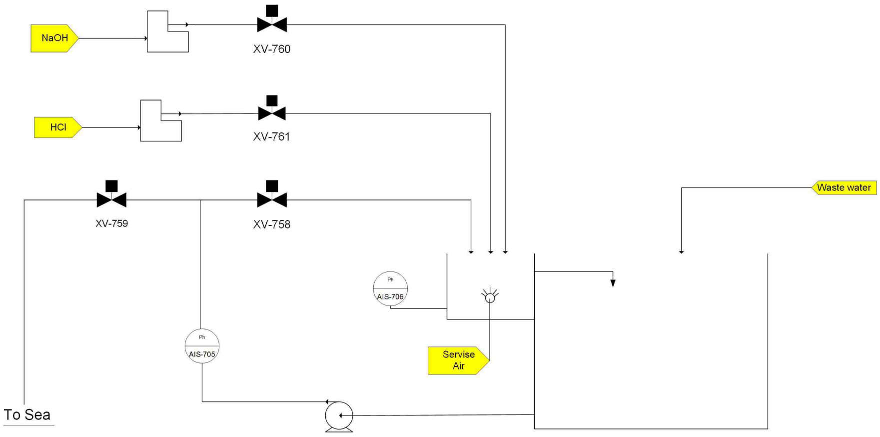

Figure 1.7: Neutralization system

Problem Formulation

2

From the previous chapter the necessity of a neutralization unit is obvious which neutralizes the waste water from the factory before this goes to the sea. This unit should work under the regulation that EU and Greek government dictate [3]. This unit already exists at the factory but it works manually.
The present project will develop a control system that neutralize the waste water from the factory using the existing equipment but it will work fully autonomous.
More analytical, a control system will be designed.The controlled input is the base flow. In order to enabled controlled a signal 4-20mA will be sent from controller to dosing pump which is already established at the unit.The base flow that will be used for of neutralization has the following characteristics.

- It is caustic soda $NaOH$
- The concentration is stable $(0.2 mol/lt)$

The waste water flow will be consider as a disturbance.The characteristics of this disturbance are known.

- It is always hydrochloric acid (HCl)
- The concentration is almost the same every time $(0.1 mol/lt)$
- The characteristics of the waste water flow can be determined from the resin regeneration programme and will be used as a disturbance in the analysis. A flow estimation of the disturbance is the following.

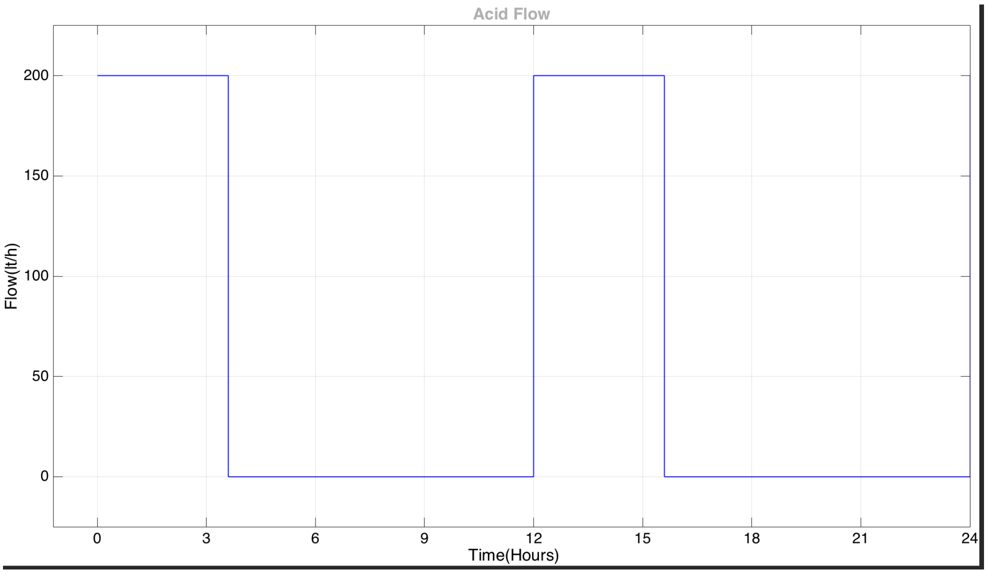

Figure 2.1: Typical Disturbance Flow

The main tasks of the controller are:

- Set the pH value at neutralization pit inside the wish values, in order to be able to dispose it at the sea.
- Finish the neutralization process before another wave of waste water comes into neutralization pit.
- Take into account the dosing pump flow limitation.
- Avoid overshoot (as this is possible) because the controller strategy task is to use only base for the neutralization process

Reading Guide

3

In this report two models of the neutralization process will be formulated. A pilot model of 1 tank and a real system model which consists of 2 tanks. It will be designed a controller using a function which invert the strong non linearity in the measurement and approximate the remaining bilinear system using linearisation. Also linear controllers will be designed using pole-placement for controller and observer in a state space formulation. Both models will be implemented with Simulink along with the controllers. The behaviour will be tested with the characteristic disturbance.

Based on these requirements the poles of the system should be on the negative real axis to avoid overshoot. Also an effect of first order system response is needed. In order to achieve this a dominant pole will be set and the rest of the poles will be set much faster. The choice of the dominant pole is made in relation to the duration of the typical disturbance.

Part II

Main Section

This part includes the Modelling and the Control methods.

Modelling

4

4.1 pH Model

Definition of pH

pH is the negative logarithm of molar concentration of hydrogen ions into a solution.

$$pH = -\log_{10}[H^+] \tag{4.1}$$

It was introduced by the Danish chemist Søren Peder Lauritz Sørensen at the Carlsberg Laboratory in 1909[8]. pH is used to determine the acidity or basicity of a solution. A neutral solution has 7pH. Solutions with pH smaller than 7 are characterised as acid. On the other hand solutions with pH higher than 7 are characterised as base.

Furthermore the acid or base solution can be categorized as strong or weak acid or base depending on the amount of H^+ or OH^- and acid constant. Acid constant determine how much the acid dissociate into H^+ and the acid residue. For strong acids acid constant is so large that it can be considered completely dissociated. For example Hydrochloric acid is a strong acid but acetic acid is a weak one.

Titration Curve

The most popular method to determine the total acidity or basicity of a solution is a Titration curve. The titration curve presents the change at pH versus reagent, for example amount of added base to a solution of acid. The shape of this is mainly depending on the nature of the acid and base. If it is strong or weak acid/base. Another factor that is able to change the shape of the titration curve is the concentration of the reagent that comes into the solution.

The point where the titration curve has the greatest slope is named equivalence point or inflection point[1]. This point varies. If for example there is a strong base, strong acid titration the equivalence point will be at 7pH. On the other hand if, for example, there is a strong acid weak base titration, the equivalence point will be at i.e. 5pH

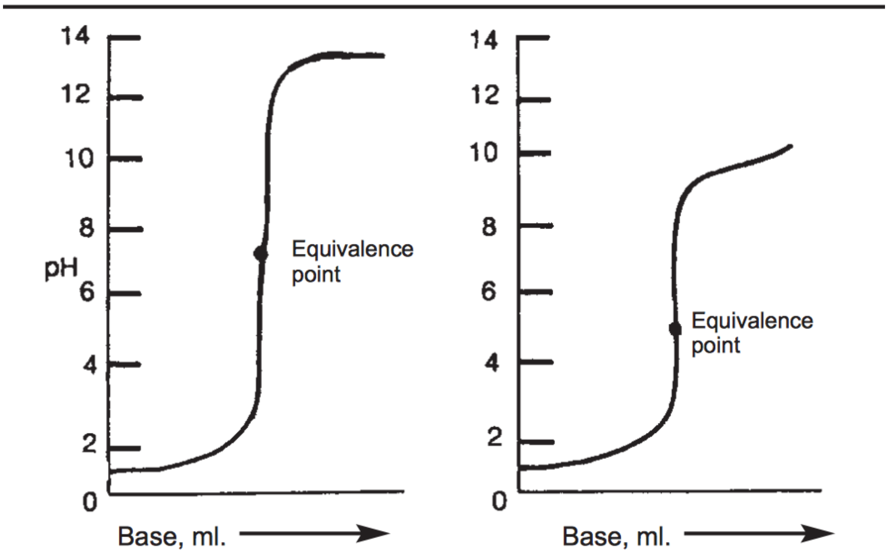

Figure 4.1: Titration Curve [1]

4.2 1 Tank Model

At this section a simple model of 1 tank will be designed. This model will consist of one tank with constant volume, were two flows of acid and base are mixed and neutralized. At following section the model will be expanded at real factory set up.

The main characteristics of this model are :

- The base flow will be considered as a controllable input $NaOH$
- The acid flow will be considered as a disturbance flow HCl
- The concentration of the acid and the base that comes into the solution is always the same.
- The tank is operated with overflow, the flows in and out of the tank are equal. So the volume of the tank is constant.

And assumptions of this model are :

- The solution temperature is always the same.
- The base and the acid which came inside are perfectly mixed.
- The solution remains electrical neutral

Mass Balance Equation

There are a lot of literature about pH model but the most widely accepted [7] is McAvoy model for pH neutralization [10]. This method will be used at this report.

Trying to neutralize a solution, for example hydrochloric acid with soda, the reaction that take place is the following

$$\begin{aligned} HCl + NaOH &\rightarrow H_2O + NaCl \\ H^+ + OH^- &\rightarrow H_20 \end{aligned} \tag{4.2}$$

So product of the neutralization process is water and salt.

The main idea for pH modelling is to calculate X and then transform X to hydrogen ions H^+. and after that from H^+ to pH. X is the difference between molar concentration of hydrogen ions H^+ and hydroxide ions OH^-. Due to the fact that the used chemicals are strong base and strong acid they are considered as completely dissociated.

The solution should remain electrical neutral. So electro neutrility equation is

$$[Na^+] + [H^+] = [Cl^-] + [OH^-] \tag{4.3}$$

Re-arranging the 4.3 X is

$$X = [OH^-] - [H^+] \tag{4.4}$$

A sodium balance equation and acetic balance equation are used in order to calculate X .

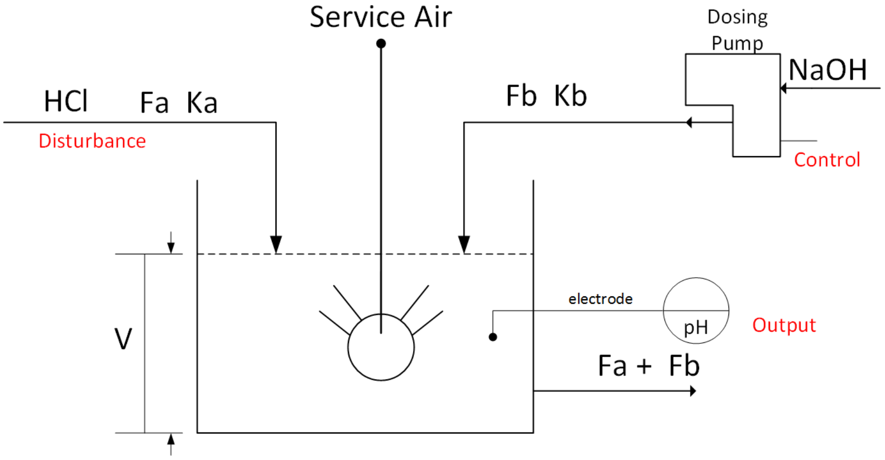

Figure 4.2: 1 tank Model

For the system of one tank these equations are formed as:
Acetate balance equation is

$$V\frac{dH^+}{dt} = F_a H^+_{in} - (F_a + F_b)H^+ \tag{4.5}$$

Sodium balance equation is

$$V\frac{dOH^-}{dt} = F_b OH^-_{in} - (F_a + F_b)OH^- \tag{4.6}$$

Where V is the volume of the solution, F_a is the flow of the acid and F_b is the flow of the base. Subtracting equations 4.5 from 4.6 and using 4.4 on the previous page a balance equation for X is obtained

$$V\frac{dX}{dt} = [OH^-_{in}]F_b - [H^+_{in}]F_a - X(F_a + F_b) \tag{4.7}$$

For simplicity can be written as

$$V\frac{dX}{dt} = k_b F_b - k_a F_a - X(F_a + F_b) \tag{4.8}$$

Where k_b is molar concentration of hydroxide ions and k_a is molar concentration of hydrogen ions. These are measured at units of moles per litre.

From X to pH

The related measurement that is available at the system is pH. So a relationship between X and pH should be defined.

Using the equation 4.4 on the preceding page

$$\begin{aligned} X &= [OH^-] - [H^+] \\ [H^+] &= -X + [OH^-] \end{aligned} \tag{4.9}$$

$[OH^-]$ is also related to $[H^+]$ with

$$[OH^-] = \frac{K_W}{[H^+]} \tag{4.10}$$

Where K_W is the self ionisation constant of the water and it is equal with

$$K_W = 10^{-14}$$

Replacing equation 4.10 at 4.9

$$\begin{aligned} H^+ &= -X + [OH^-] \\ [H^+] &= -X + \frac{K_W}{[H^+]} \\ [H^+]^2 + X[H^+] - K_W &= 0 \end{aligned} \tag{4.11}$$

Solving this second order polynomial two solutions are obtained. Discarding the unrealistic one the relationship between X and $[H^+]$ obtained

$$[H^+] = \frac{-X}{2} + \sqrt{\frac{X^2}{4} + K_W} \tag{4.12}$$

And using equation 4.1 on page 21 pH is calculated.

From pH to X

The control strategy is to design the controller using an approximate linearised balance equation base in equation 4.8 on the facing page and invert the strongly non linear relationship [5] which occur from the transformation of X to pH 4.12 and 4.1 on page 21.

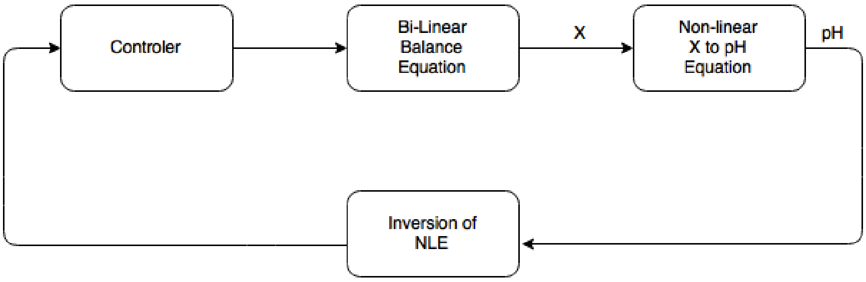

Figure 4.3: Block Diagram of the control strategy

As a result of that a relation between pH and X should be calculated.

To transform pH to $[H^+]$ an inversion of equation 4.1 on page 21 is used

$$[H^+] = 10^{-pH} \tag{4.13}$$

To transform $[H^+]$ to X an inversion of equation 4.12 is used

$$X = \frac{K_W - [H^+]^2}{[H^+]} \tag{4.14}$$

Linearisation around OP

The last term on the right hand site of the equation 4.8 on the preceding page is bi-linear.

$$V\frac{dX}{dt} = k_bF_b - k_aF_a - X(F_a + F_b) \tag{4.15}$$

So this equation needs to be linearised.

The method of the linearisation around operating point is chosen. The operating point is $7pH$ or $\bar{X} = 0$ due to the fact that the task is to neutralize the solution. Also $\bar{F_a}$ is known because the characteristics of the disturbance are known. The choice of the OP should be close to the steady state point. So solving the equation 4.8 on page 24 for F_b and using $\bar{F_a}$ and $\bar{X}$, the $\bar{F_b}$ is derived.

Now the linearisation can proceed

- $X = \bar{X} + X^{\Delta}$
- $F_b = \bar{F_b} + F_b^{\Delta}$
- $F_a = \bar{F_a} + F_a^{\Delta}$

Where $\bar{X}$ is the operating point steady state value and X^{Δ} is the difference from operating point.
Also due to the fact that at steady state $\frac{dX}{dt} = 0$

$$0 = k_b\bar{F_b} - k_a\bar{F_a} - \bar{X}(\bar{F_a} + \bar{F_b}) \tag{4.16}$$

Replacing these relationships at 4.8 on page 24

$$\begin{aligned} V\frac{d(\bar{X} + X^{\Delta})}{dt} &= k_b(\bar{F_b} + F_b^{\Delta}) - k_a(\bar{F_a} + F_a^{\Delta}) - (\bar{X} + X^{\Delta})(\bar{F_b} + F_b^{\Delta} + \bar{F_a} + F_a^{\Delta}) \\ V\frac{d(X^{\Delta})}{dt} &= \underbrace{k_b\bar{F_b} - k_a\bar{F_a} - \bar{X}(\bar{F_a} + \bar{F_b})}_{=0} - (\bar{F_a} + \bar{F_b})X^{\Delta} + (k_b + \bar{X})F_b^{\Delta} \\ &- (k_a - \bar{X})F_a^{\Delta} - \underbrace{X_{\Delta}(F_a^{\Delta} + F_b^{\Delta})}_{\approx 0} \end{aligned} \tag{4.17}$$

So the linearised equation is

$$V\frac{d(X^{\Delta})}{dt} = -(\bar{F_a} + \bar{F_b})X^{\Delta} + (k_b + \bar{X})F_b^{\Delta} - (k_a - \bar{X})F_a^{\Delta} \tag{4.18}$$

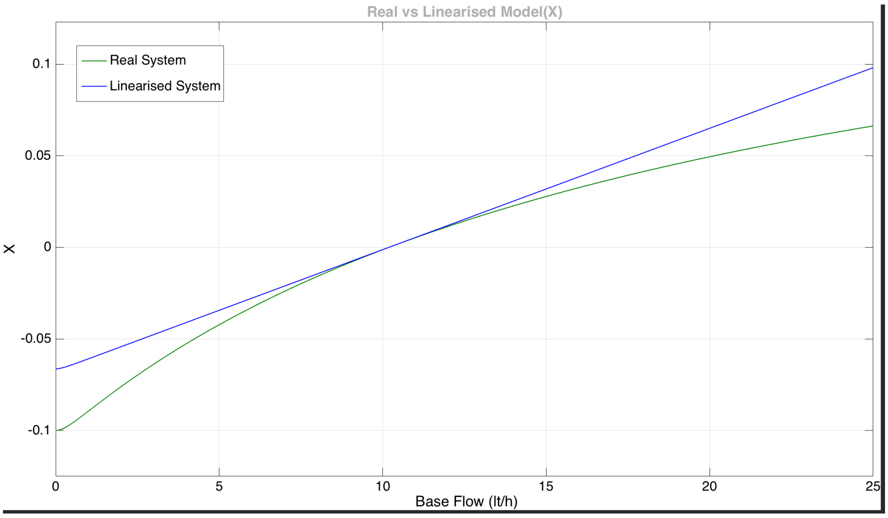

Figure 4.4: Difference between Linearised and Real System

Figure 4.4 shows the steady state relationship between F_b and X as calculated using the bi linear relationship 4.8 on page 24 and linear approximation with $\bar{X} = 0$ 4.18 on the facing page.

State Space model of 1 tank system

Dividing 4.18 on the preceding page by V the state space equations are obtained

$$\begin{aligned} \dot{X^{\Delta}} &= -\frac{(\bar{F_a} + \bar{F_b})}{V} X^{\Delta} + \frac{(k_b + \bar{X})}{V} F_b^{\Delta} - \frac{(k_a - \bar{X})}{V} F_a^{\Delta} \\ y &= X^{\Delta} \end{aligned} \tag{4.19}$$

The system is formulated as

$$\begin{aligned} \dot{X^{\Delta}} &= AX^{\Delta} + B_C F_b^{\Delta} + B_D F_a^{\Delta} \\ y &= CX^{\Delta} \end{aligned} \tag{4.20}$$

Where

- $A = -\frac{(\bar{F_a} + \bar{F_b})}{V}$
- $B_C = \frac{(k_b + \bar{X})}{V}$
- $B_D = -\frac{(k_a - \bar{X})}{V}$
- $C = 1$

4.3 2 Tanks Model

At this section the real unit of neutralization will be modelled. As it is described at previous chapter this unit consist of

- 2 tanks
  - Mixing Pit
  - Neutralization Pit
- 2 pH meters one at mixing pit (AT-1) and one at the output of neutralization pit(AT-2)
- 1 pump which recycle the water between 2 tanks or dispose water to the sea
- 2 valves which control if the water recycle or goes to the sea
- And a dosing pump which controls the flow of base

The main characteristics of the model are

- The base flow is considered as a controllable input and it is dropped into mixing pit $NaOH$
- The acid flow is considered as disturbance and it is dropped into neutralization pit HCl
- As an output of the system will be considered the pH at the output of neutralization pit (AT-2)
- The volume of the mixing pit (V_1) is constant
- The pump recycles the water between 2 tanks until both of the following are fulfilled
  - AT-2 is between 6.5pH and 9 pH
  - There is no flow of acid

  Then the flow from second tank stops to go at the first tank and is be disposed in the sea
- The volume of the neutralization pit (V_2) varies but it is not measurable. There is only a level switch which deactivates the pump when the level goes under a certain point.

The assumptions that have been made are the same as 1 tank model which are

- The solution temperature is always the same.
- The base and the acid which came inside are perfectly mixed.
- The solution remains electrical neutral
- Density of the solution is independent from X

Mass Balance equations for 2 Tanks Model

The same method of modelling as 1 tank model will be used. Due to the fact that this model consists of 2 tanks, 2 balance equations for X_1 and X_2 will be developed. Also a third differential equation is needed because of the fact that the volume of the Neutralisation pit (V_2) varies.

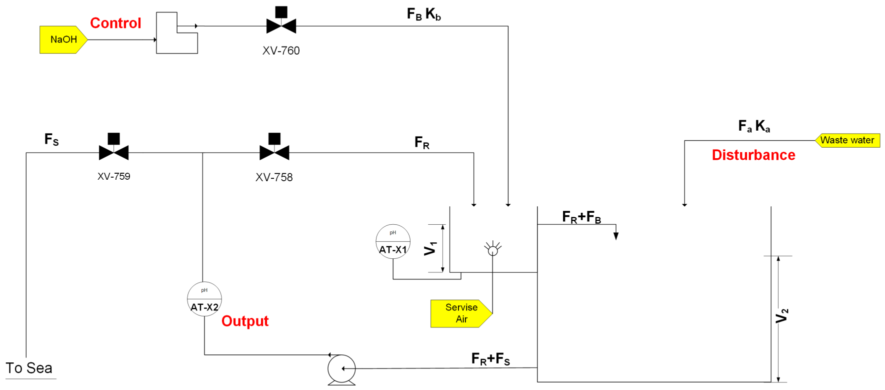

Figure 4.5: 2 tanks Model

1^{st} Tank X balance differential equation is

$$V_1 \frac{dX_1}{dt} = k_b F_b + X_2 F_R - X_1(F_b + F_R) \tag{4.21}$$

Where X_1 and X_2 is the difference of molar concentration between H^+ and OH^- in mixing pit and at the output of neutralization pit, accordingly. V_1 is the volume of mixing pit which is constant and F_R is the flow from the pump when it recycles the water which is also constant.

2^{nd} Tank Mass balance differential equation is

$$\frac{dV_2 X_2}{dt} = X_1(F_b + F_R) - k_a F_a - X_2(F_S + F_R) \tag{4.22}$$

Where F_S is the flow from the pump when it disposes the water in the sea

2^{nd} Tank Mass Balance equation which uses volumes with the assumption that density is constant.

$$\frac{dV_2}{dt} = F_b + F_a - F_S + \underbrace{F_R - F_R}_{=0} \tag{4.23}$$

The 2^{nd} Tank Mass balance differential equation 4.22 on the preceding page should be written as

$$\frac{dV_2}{dt}X_2 + \frac{dX_2}{dt}V_2 = X_1(F_b + F_R) - k_aF_a - X_2F_S \tag{4.24}$$

and if the 4.23 is used to replace the 1^{st} term at the left hand site $\frac{dV_2}{dt}$

$$V_2\frac{dX_2}{dt} = X_1(F_b + F_R) - k_aF_a - X_2F_R - (F_b + F_a)X_2 \tag{4.25}$$

So the equations 4.21 on the preceding page , 4.25 and 4.23 describe the real neutralization unit.

Linearisation around OP

The same method of linearisation will be used. In the linearised equations it turns out that only the OP value of the V_2 appears in the equation 4.25. Therefore the equation 4.23 is not use in the controller design. The value of V_2 should be chosen close to the steady state point where the acid is getting neutralized. This is assumed to be suitable since we do not want overshoot and in particular this could be harmful if it appears when the disturbance pulse of acid is about to stop. This value is found through simulations.

The equation 4.23 will be embedded at 4.22 on the preceding page as it is already written at 4.25. So only the 4.21 on the preceding page and 4.25 will be linearised.

Also the controller works only when the solution is recycled. Controller will be turned off when the solution goes to the sea. As a result of that the F_S term is not usable for the controller design. So F_S and F_R will be replaced by F_T.
After these assumptions the equations for linearisation are

$$V_1\frac{dX_1}{dt} = k_bF_b + X_2F_T - X_1(F_b + F_T) \tag{4.26}$$

and

$$V_2\frac{dX_2}{dt} = X_1(F_b + F_T) - k_aF_a - (F_T + F_b + F_a)X_2 \tag{4.27}$$

The values for $\bar{X_1}$, $\bar{X_2}$, $\bar{F_a}$, and $\bar{F_b}$ are derived in the same way as they derived at the 1 tank model.

For the equation 4.26 on the facing page

- $X_1 = \bar{X_1} + X_1^\Delta$
- $X_2 = \bar{X_2} + X_2^\Delta$
- $F_b = \bar{F_b} + F_b^\Delta$
- k_b, V_1 and F_T are constant

Where $\bar{X_1}$ is the operating point steady state value and X_1^Δ is the difference from operating point.
For steady state the equation 4.26 on the preceding page is

$$0 = k_b\bar{F_b} + \bar{X_2}F_T - \bar{X_1}(\bar{F_b} + F_T) \tag{4.28}$$

Replacing these equations at 4.26 on the facing page

$$\begin{aligned} V_1\frac{d(\bar{X_1} + X_1^\Delta)}{dt} &= k_b(\bar{F_b} + F_b^\Delta) + (\bar{X_2} + X_2^\Delta)F_T - (\bar{X_1} + X_1^\Delta)(\bar{F_b} + F_b^\Delta + F_T) \\ V_1\frac{d(X_1^\Delta)}{dt} &= \underbrace{k_b\bar{F_b} + F_T\bar{X_2} - \bar{X_1}(\bar{F_b} + F_T)}_{=0} - (\bar{F_b} + F_T)X_1^\Delta + F_TX_2^\Delta \\ &+ (k_b - \bar{X_1})F_b^\Delta - \underbrace{X_1^\Delta F_b^\Delta}_{\approx 0} \end{aligned} \tag{4.29}$$

So the linearised equation is

$$V_1\frac{d(X_1^\Delta)}{dt} = -(\bar{F_b} + F_T)X1^\Delta + F_TX_2^\Delta + (k_b - \bar{X_1})F_b^\Delta \tag{4.30}$$

For the equation 4.27 on the preceding page

- $X_1 = \bar{X_1} + X_1^\Delta$
- $X_2 = \bar{X_2} + X_2^\Delta$
- $F_b = \bar{F_b} + F_b^\Delta$
- $F_a = \bar{F_a} + F_a^\Delta$
- k_a, V_2 and F_T are constant

For steady state the equation 4.27 on page 30 is

$$0 = \bar{X}_1(\bar{F}_b + F_T) - k_a\bar{F}_a - (F_T + \bar{F}_b + \bar{F}_a)\bar{X}_2 \tag{4.31}$$

Replacing these equation at 4.27 on page 30

$$\begin{aligned} V_2\frac{d(\bar{X}_2 + X_2^{\Delta})}{dt} &= (\bar{X}_1 + X_1^{\Delta})(\bar{F}_b + F_b^{\Delta} + F_T) \\ &\quad - (\bar{X}_2 + X_2^{\Delta})(\bar{F}_b + F_b^{\Delta} + \bar{F}_a + F_a^{\Delta}) - (\bar{X}_1 - k_a(\bar{F}_a + F_a^{\Delta}) \\ V_2\frac{d(X_2^{\Delta})}{dt} &= \underbrace{\bar{X}_1(\bar{F}_b + F_T) - k_a\bar{F}_a - (F_T + \bar{F}_b + \bar{F}_a)\bar{X}_2}_{=0} + (\bar{F}_b + F_T)X_1^{\Delta} \\ &\quad - (F_T + \bar{F}_b + \bar{F}_a)X_2^{\Delta} + (\bar{X}_1 - \bar{X}_2)F_b^{\Delta} - (k_a + \bar{X}_2)F_a^{\Delta} \\ &\quad + \underbrace{X_1^{\Delta}F_b^{\Delta} - X_2^{\Delta}F_b^{\Delta} - X_2^{\Delta}F_a^{\Delta}}_{\approx 0} \end{aligned} \tag{4.32}$$

So the linearised equation is

$$V_2\frac{d(X_2^{\Delta})}{dt} = (\bar{F}_b + F_T)X_1^{\Delta} - (F_T + \bar{F}_b + \bar{F}_a)X_2^{\Delta} + (\bar{X}_1 - \bar{X}_2)F_b^{\Delta} - (k_a + \bar{X}_2)F_a^{\Delta} \tag{4.33}$$

State Space model of real system

Dividing 4.30 on the preceding page and 4.33 by V_1 and V_2 respectively, the state space equations are obtained

$$\begin{aligned} \dot{X}_1 &= -\frac{(\bar{F}_b + F_T)}{V_1}X_1^{\Delta} + \frac{F_T}{V_1}X_2^{\Delta} + \frac{(k_b - \bar{X}_1)}{V_1}F_b^{\Delta} \\ \dot{X}_2 &= \frac{(\bar{F}_b + F_T)}{V_2}X_1^{\Delta} - \frac{(F_T + \bar{F}_b + \bar{F}_a)}{V_2}X_2^{\Delta} + \frac{(\bar{X}_1 - \bar{X}_2)}{V_2}F_b^{\Delta} - \frac{(k_a + \bar{X}_2)}{V_2}F_a^{\Delta} \end{aligned} \tag{4.34}$$

The system is formulated as

$$\begin{aligned} \begin{bmatrix} \dot{X}_1{}^{\Delta} \\ \dot{X}_2{}^{\Delta} \end{bmatrix} &= A\begin{bmatrix} X_1^{\Delta} \\ X_2^{\Delta} \end{bmatrix} + B_cF_b^{\Delta} + B_dF_a^{\Delta} \\ y &= C\begin{bmatrix} X_1^{\Delta} \\ X_2^{\Delta} \end{bmatrix} \end{aligned} \tag{4.35}$$

Where,

- $$A = \begin{bmatrix} -\frac{(\bar{F}_b + F_T)}{V_1} & \frac{F_T}{V_1} \\ \frac{(\bar{F}_b + F_T)}{V_2} & -\frac{(F_T + \bar{F}_b + \bar{F}_a)}{V_2} \end{bmatrix} \tag{4.36}$$

- $$B_c = \begin{bmatrix} \frac{(k_b - \bar{X}_1)}{V_1} \\ \frac{(\bar{X}_1 - \bar{X}_2)}{V_2} \end{bmatrix} \tag{4.37}$$

- $$B_d = \begin{bmatrix} 0 \\ -\frac{(k_a + \bar{X}_2)}{V_2} \end{bmatrix} \tag{4.38}$$

- $$C = \begin{bmatrix} 0 & 1 \end{bmatrix} \tag{4.39}$$

Control

5

In this chapter the control system for both one and two tank model will be designed.

As it is already described at previous chapter, the control strategy that is presented at the following system, is to Linearise the bilinear Mass Balance equation and invert the non linearities which occur from the transformation of X to pH.

According to the figure 5.1, the first block bi-Linear Dynamic equation will be represented by the linearised approximation when designing the controller. The next block represents the Non Linear Static Element which are the functions 4.12 on page 25 and 4.1 on page 21 . In order to overcome this non linearity the inversions of 4.12 on page 25 and 4.1 on page 21 are calculated as 4.14 on page 25 and 4.13 on page 25 accordingly.

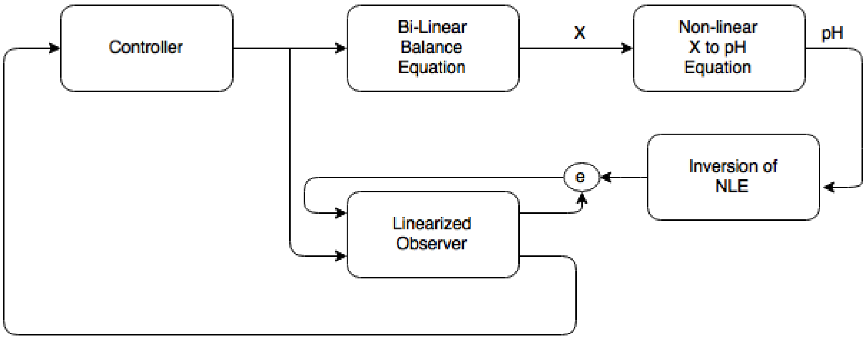

Figure 5.1: Block Diagram of the whole System

More analytical the closed loop system for both one tank and real system consists of:

- A bilinear system
- A Non Linear static element which is inverted
- An observer of the linearised version of system
- PI controller, with reference signal

A reason that the observer is used, is to handle potential noise that might occurred due to inversion or measurement. Also a switch that turns off the controller is used for the real system.

5.1 Controller of 1 tank model

First of all the design specification for the controller should be set. These are the requirements

- No steady state error
- The settling time should be as fast as this is possible
- Avoid overshoot as this is possible

Open Loop System

As it is described at 4.18 on page 26 the open loop system is the following.

The system is formulated as

$$\begin{aligned} \dot{X^\Delta} &= AX^\Delta + B_C F_b^\Delta + B_D F_a^\Delta \\ y &= CX^\Delta \end{aligned} \tag{5.1}$$

Where

- $A = -\frac{(\bar{F_a}+\bar{F_b})}{V}$
- $B_C = \frac{(k_b+\bar{X})}{V}$
- $B_D = -\frac{(k_a-\bar{X})}{V}$
- $C = 1$

This linearised 1^{st} order system is used for the controller design.

Controller Design

A controller rearrange the poles positions so that the system will be stable and fulfils the requirements. An integral control is used in order to avoid the steady state error. Also an observer gain L is used, so that $A + LC$ is stable with the desired eigenvalues. The entire systems poles will be consisted by the eigenvalues of the integral feedback $A_e + B_e F_e$ where and of the observer $A + LC$. Where A_e,B_e and F_e are the extended matrices for the integral control. Based on separation theorem that poles of the closed loop are the poles of the observer and the poles of the system as if the feedback was directly from states [9].

The observable matrix is a scalar because the system is a first order system.

$$O = C \tag{5.2}$$

Also *the observable canonical form* T is a scalar for the same reason.

$$T = O^{-1} \tag{5.3}$$

Observer gain

The observer gain L can be calculated through the following steps [9]:

- Open loop polynomial. $det(\lambda I - A) = \lambda + \alpha$
- Desired observer polynomial. $det(\lambda I - (A + LC)) = \lambda + \alpha_{obs}$

$$\begin{aligned} L_o &= \alpha - \alpha_{obs} \\ L &= TL_o \end{aligned} \tag{5.4}$$

Using the rule of thumb the observer pole is set a bit faster than the system pole.

Integral feedback

For the integral control the equations of the system become [9]:

$$\begin{aligned} \dot{x_e} &= A_e x_e + B_e u \\ y &= C_e - x_e \\ y &= Cx \end{aligned} \tag{5.5}$$

for which a state feedback $u = F_e x_e$ has been designed, where:

$$\begin{aligned} A_e &= \left(\begin{array}{c|c} A & 0 \\ \hline C & 0 \end{array} \right) \\ B_e &= \left(\begin{array}{c} B \\ \hline 0 \end{array} \right) \\ C_e &= \left(\begin{array}{c|c} C & 0 \end{array} \right) \\ F_e &= \left(\begin{array}{cc} F & F_I \end{array} \right) \\ x_e &= \left(\begin{array}{c} x \\ x_I \end{array} \right) \end{aligned} \tag{5.6}$$

The extended state feedback F_e was found using the Matlab command

$$F_e = -place(A_e, B_e, [poles])$$

The minus in front of place is use because a positive feedback is chosen.

The system poles are setted considering the controller requirements that have been setted. The poles that have been chosen can be found at B.1 on page 81.

5.2 Controller for Real Model

The design specifications for the controller have been specified at chapter 2 on page 15.

The main tasks of the controller are:

- Set the pH value at neutralization pit inside the wish values in order to be able to dispose it at the sea.
- Finish the neutralization process before another wave of waste water comes into neutralization pit.
- Take into account the dosing pump flow limitation.
- Avoid overshoot (as this is possible) because the controller strategy task is to use only base for the neutralization process

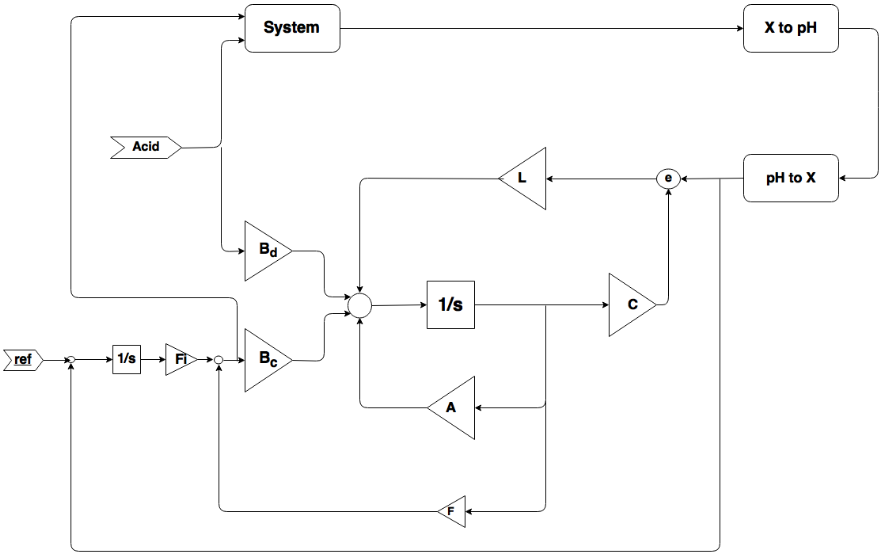

Figure 5.2: Observer based PI Controller

Due to a lack of measurement for flow of acid F_a an estimation of it is fed at the observer. This estimation is based in the fact that the flow of acid, when it exist, has certain value.

Open Loop System

As it is described at 4.34 on page 32 the open loop system is the following.

The system is formulated as

$$\begin{aligned} \left[\begin{array}{c} \dot{X_1}^{\Delta} \\ \dot{X_2}^{\Delta} \end{array} \right] &= A \left[\begin{array}{c} X_1^{\Delta} \\ X_2^{\Delta} \end{array} \right] + B_c F_b^{\Delta} + B_d F_a^{\Delta} \\ y &= C \left[\begin{array}{c} X_1^{\Delta} \\ X_2^{\Delta} \end{array} \right] \end{aligned} \tag{5.7}$$

Where,

- $$A = \left[\begin{array}{cc} -\frac{(\bar{F_b}+F_T)}{V_1} & \frac{F_T}{V_1} \\ \frac{(\bar{F_b}+F_T)}{V_2} & -\frac{(F_T+\bar{F_b}+\bar{F_a})}{V_2} \end{array} \right] \tag{5.8}$$

- $$B_c = \left[\begin{array}{c} \frac{(k_b-\bar{X_1})}{V_1} \\ \frac{(\bar{X_1}-\bar{X_2})}{V_2} \end{array} \right] \tag{5.9}$$

- $$B_d = \left[\begin{array}{c} 0 \\ -\frac{(k_a+\bar{X_2})}{V_2} \end{array} \right] \tag{5.10}$$

- $$C = \left[\begin{array}{cc} 0 & 1 \end{array} \right] \tag{5.11}$$

This linearised 2^{nd} order system is used for the controller design.

Controller Design

The same control strategy is used as at 1 tank Model

The observable matrix is

$$\begin{aligned} O &= \left(\begin{array}{c} C \\ CA \end{array} \right) \\ det(O) &= -0.33 \neq 0 \end{aligned} \tag{5.12}$$

So the system is observable.

Matrix O is used in order to compute *the observable canonical form* T for the system. This matrix is used in order to determine the observer gain L. The derivation of the matrix can be seen as:

$$\begin{aligned} t_2 &= O^{-1} \left(\begin{array}{c} 0 \\ 1 \end{array} \right) \\ t_1 &= A \cdot t_2 \\ T &= \left(\begin{array}{cc} t_1 & t_2 \end{array} \right) \end{aligned} \tag{5.13}$$

Observer gain

The observer gain L can be calculated through the following steps [9]:

- Open loop polynomial. $det(\lambda I - A) = \lambda^2 + \alpha_1 \lambda + \alpha_1$
- Desired observer polynomial. $det(\lambda I - (A + LC)) = \lambda^2 + \alpha_{obs,1} \lambda + \alpha_{obs,1}$

$$\begin{aligned} L_o &= \begin{pmatrix} \alpha_1 - \alpha_{obs,1} \\ \alpha_2 - \alpha_{obs,2} \end{pmatrix} \\ L &= TL_o \end{aligned} \tag{5.14}$$

Using the rule of thumb the observer poles are set a bit faster than the system poles.

Integral feedback

For the integral control the equations of the system became:

$$\begin{aligned} \dot{x_e} &= A_e x_e + B_e u \\ y &= C_e - x_e \\ y &= Cx \end{aligned} \tag{5.15}$$

for which a state feedback $u = F_e x_e$ has been designed, where:

$$\begin{aligned} A_e &= \left(\begin{array}{c|c} A & 0 \\ \hline C & 0 \end{array}\right) \\ B_e &= \left(\begin{array}{c} B_c \\ \hline 0 \end{array}\right) \\ C_e &= \left(\begin{array}{c|c} C & 0 \end{array}\right) \\ F_e &= \begin{pmatrix} F & F_I \end{pmatrix} \\ x_e &= \begin{pmatrix} x \\ x_I \end{pmatrix} \end{aligned} \tag{5.16}$$

The extended state feedback F_e was found using the Matlab command

$$F_e = -place(A_e, B_e, [poles])$$

. The minus in front of place is used because a positive feedback is chosen. The poles that have been chosen can be found at B.1 on page 81.

The system poles are placed considering the controller requirements that have been set. As a result of that, one pole is placed close to the zero as a dominant pole and the other poles are placed much more faster(at least 10 times). The position of the dominant pole is chosen so that the settling time of the response is smaller than the duration of typical disturbance. Due to this placement the system response looks like a 1^{st} order system response.

Controller evaluation

In order to evaluate the controller design, the close loop transfer function from disturbance to X_2 should be derived.

The close loop is consisted by

- System
- Controller
- Observer

Formulating these in one system

$$\begin{aligned}\begin{bmatrix}\dot{X}_1\\X_2\\X_i\end{bmatrix}=\overbrace{\begin{bmatrix}A&0\\C&0\end{bmatrix}}^{A_e}\begin{bmatrix}X_1\\X_2\\X_i\end{bmatrix}+\overbrace{\begin{bmatrix}B_c\\0\end{bmatrix}}^{B_e}\left(\begin{bmatrix}0&0&F_i\end{bmatrix}\begin{bmatrix}X_1\\X_2\\X_i\end{bmatrix}+\underbrace{\begin{bmatrix}F_1&F_2\end{bmatrix}}_{F}\begin{bmatrix}\hat{\mathbf{X_1}}\\\hat{\mathbf{X_2}}\end{bmatrix}\right)+\\+\begin{bmatrix}B_d\\0\end{bmatrix}F_d\end{aligned}\tag{5.17}$$

$$\begin{aligned}\begin{bmatrix}\dot{\hat{\mathbf{X_1}}}\\\hat{\mathbf{X_2}}\end{bmatrix}=[A]\begin{bmatrix}\hat{\mathbf{X_1}}\\\hat{\mathbf{X_2}}\end{bmatrix}+[B_d]\left(\begin{bmatrix}0&0&F_i\end{bmatrix}\begin{bmatrix}X_1\\X_2\\X_i\end{bmatrix}+\underbrace{\begin{bmatrix}F_1&F_2\end{bmatrix}}_{F}\begin{bmatrix}\hat{\mathbf{X_1}}\\\hat{\mathbf{X_2}}\end{bmatrix}\right)+\\-L\left(C\begin{bmatrix}\hat{\mathbf{X_1}}\\\hat{\mathbf{X_2}}\end{bmatrix}-C\begin{bmatrix}X_1\\X_2\end{bmatrix}\right)\end{aligned}\tag{5.18}$$

Combining equitation 5.17 and 5.18 in a state space system

$$\begin{aligned}\dot{x_{cl}}&=A_{cl}x_{cl}+B_{cl}u\\y&=C_{cl}x_{cl}\end{aligned}\tag{5.19}$$

Where

$$\begin{aligned}
A_{cl} &= \begin{bmatrix} A_e + B_e \begin{bmatrix} 0 & 0 & F_i \end{bmatrix} & B_e F \\ B_c \begin{bmatrix} 0 & 0 & F_i \end{bmatrix} - LC & A + B_c F + LC \end{bmatrix} \\
B_{cl} &= \begin{bmatrix} B_d \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \\
C_{cl} &= \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \end{bmatrix} \\
x_{cl} &= \begin{bmatrix} X_1 \\ X_2 \\ X_i \\ \hat{\mathbf{X_1}} \\ \hat{\mathbf{X_2}} \end{bmatrix}
\end{aligned} \tag{5.20}$$

Finally the transfer function is

$$G_{d_{cl}} = C_{cl} \left(sI - A_{cl} \right)^{-1} B_{cl} \tag{5.21}$$

The poles and zeros locations are presented at the following graph

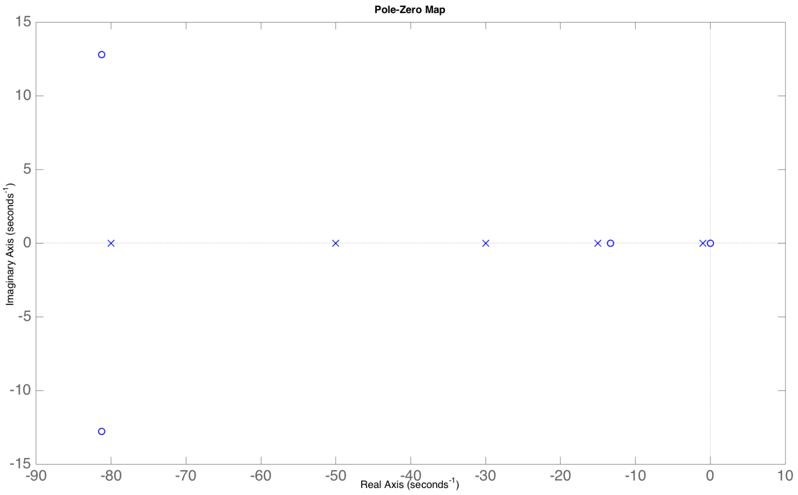

Figure 5.3: Poles and Zero locations

It can be observed that the poles have the desired position.

Also a step response with a step amplitude $200l/h$ of the transfer function is simulated.

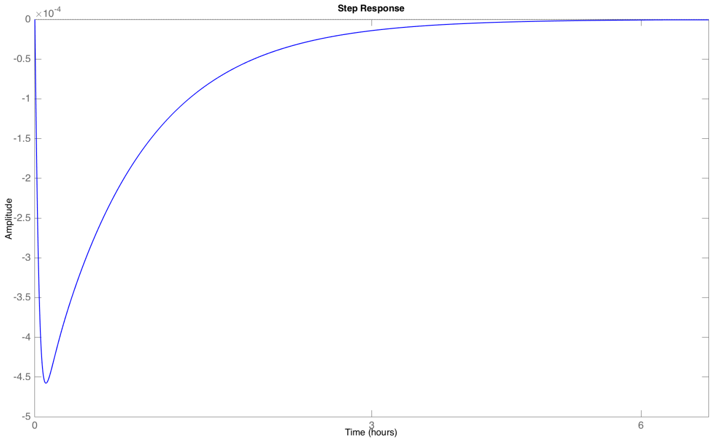

Figure 5.4: Transfer function step response

According to figure 5.4 it is clear that the system response has indeed an effect of a first order response. This effect is a result of poles position choice. Also there is no oscillation as it was expected because the poles have only real part. Additionally it is obvious that there is not a steady state error as a result of the integral control. Furthermore it is clear that the solution is neutralised before the pulse of acid finish.

Controller stop

During the simulations it was observed that the solution pH has an overshoot when the disturbance pulse stops. In order to handle this, a 'controller stop' was designed because tank 1 contained a great deal of base which was of no need if the fluid in tank 2 was approximately neutral and acid flow becomes zero. This switch turns off the controller when the pH is between the limits and the acid flow stops. Here is the response of the system with Controller Stop.

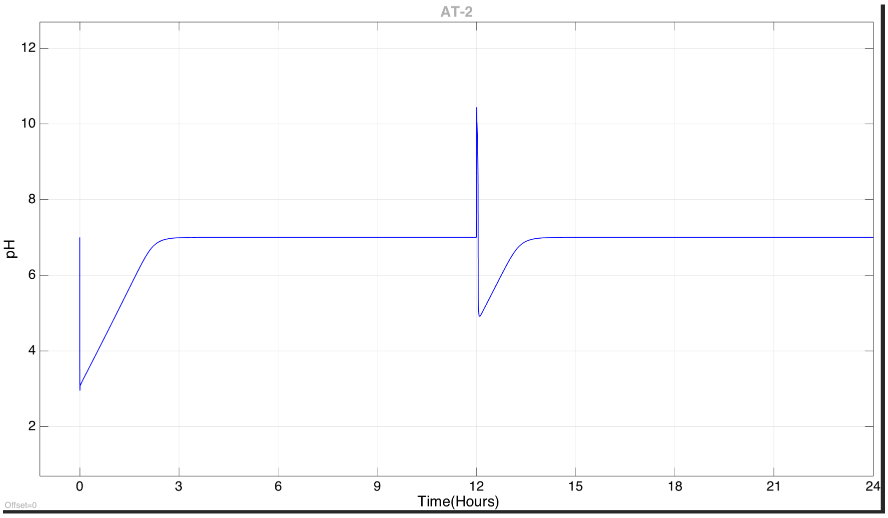

Figure 5.5: Response of the system with Controller Stop

And without Controller Stop.

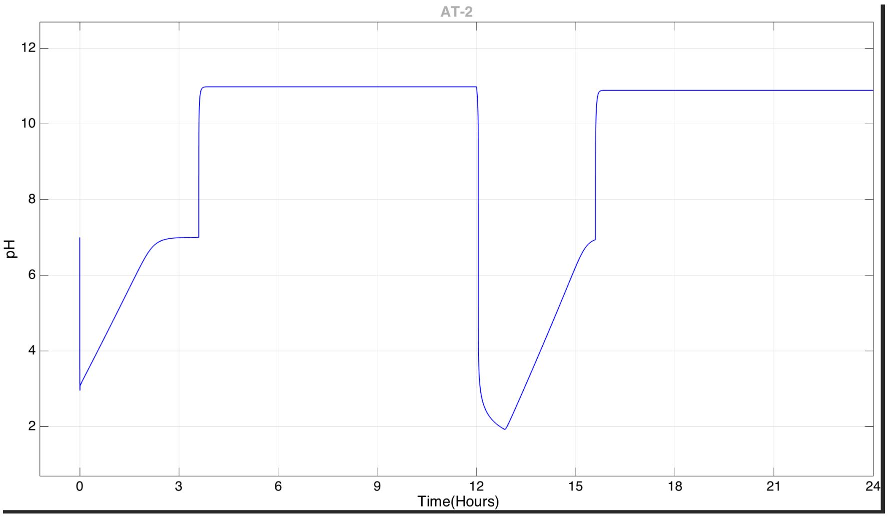

Figure 5.6: Response of the system without Controller Stop

The necessity of the switch is obvious.

Implementation 6

The implementation of the system has been done with Simulink. Three simulations will be developed

- 1 tank model with PI controller and observer
- Real model with PI controller and observer
- Real model with PI controller and observer which use both X_1 and X_2.
- Real model with PI controller without observer

These models implement the equations that have been derived from modelling.

The measurements that are available are

- X_1(Simulate signals)
- X_2 (Simulate signals)
- $pH1$
- $pH2$
- V_2
- F_b
- F_a
- $MassBalance$

6.1 1 tank model implementation

The equation 4.8 on page 24 is implemented in figure 6.1 on the following page

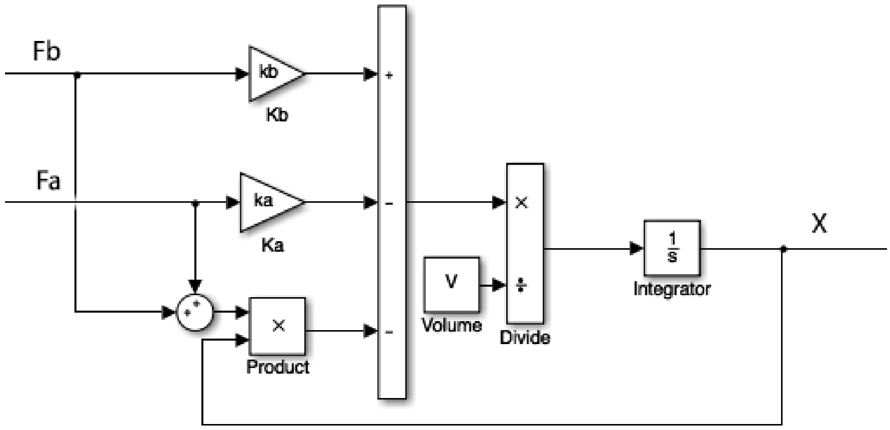

Figure 6.1: 1 tank system implementation

The equations 4.12 on page 25 and 4.1 on page 21 are implemented in figure 6.2

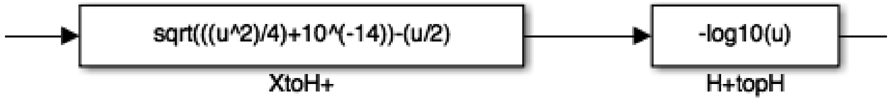

Figure 6.2: Implementation of X to H^+ and from H^+ to pH

The equations 4.13 on page 25 and 4.14 on page 25 are implemented as in figure 6.3 on the facing page

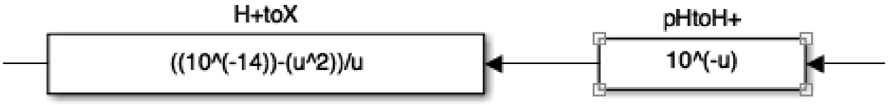

Figure 6.3: Implementation of pH to H^+ and from H^+ to X

The complete simulation is presented at appendix A.1 on page 72.

6.2 Real Model with PI Controller and Observer

The equations 4.26 on page 30 and 4.27 on page 30 are implemented as in figure 6.4

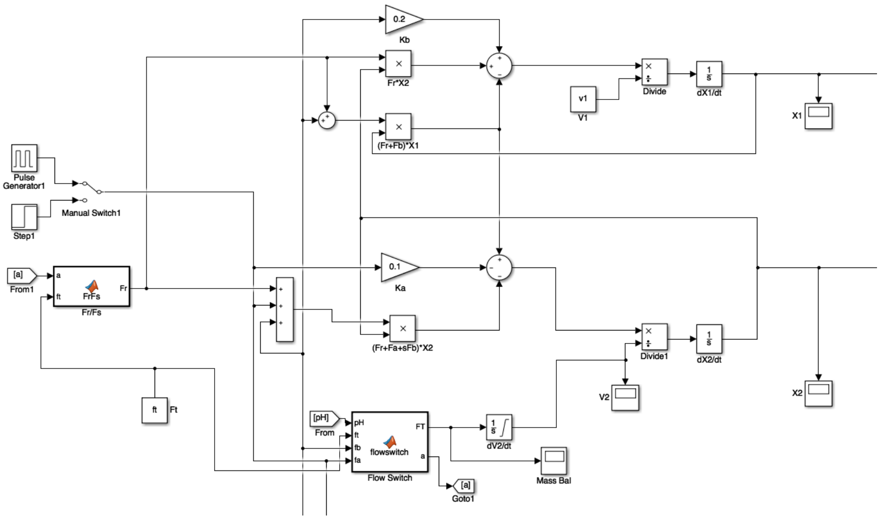

Figure 6.4: Real System Implementation

The embedded blocks *Flow Switch* and *Fr/Fs* are used in order to simulate the pump flow change between recirculation and water disposal to the sea. This switch is done based on the safety regulations which are

- pH inside environmental limits
- There is not flow of acid inside the system

Also there is a low limit at the V_2 in order to protect the pump.

The observer and the controller are implemented as in figure 6.5 on the next page

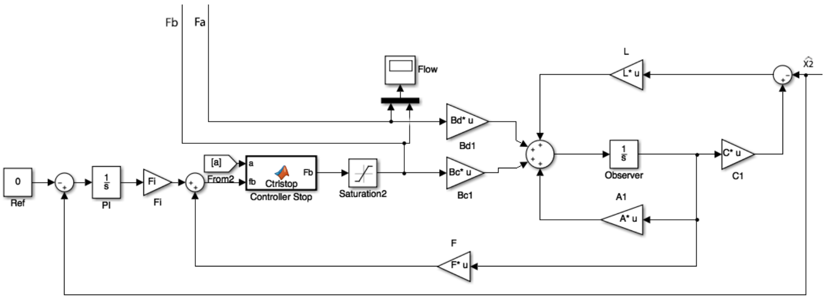

Figure 6.5: PI Controller with Observer

The *Controller Stop* implement the controller switch which turns off the controller as it is explained at 5.2 on page 38.

From X to pH and the inversion of this, are the same as at 6.1 on page 45

The complete simulation is presented at appendix A.3 on page 76.

6.3 Real model with PI controller and observer which use both X_1 and X_2

At this section the same system as in 6.2 on the previous page is used. The difference is that X_1 is also fed at observer. In order to achieve this, C matrix of the Observer became

$$C = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

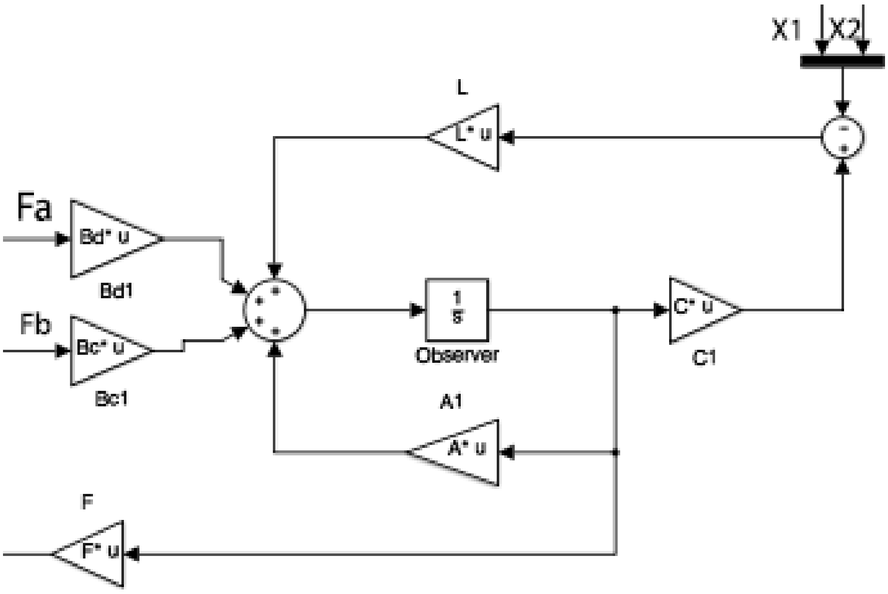

Figure 6.6: PI Controller with Observer which use X_1 and X_2

Everything else is the same.

The complete simulation is presented at appendix A.4 on page 78.

6.4 Real Model with PI controller

At this simulation the observer is removed and the system is tested without observer. This method might be implementable in real life but this version could be affected by noise from measurement or from cable.

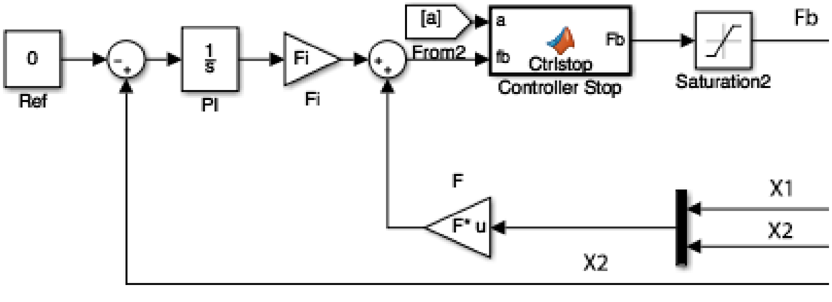

Figure 6.7: PI Controller without Observer

Everything else is the same.

The complete simulation is presented at appendix A.5 on page 80.

Part III

Results

This part present and evaluate the results from simulations.

7

Results

In this chapter, the results of the simulation will be presented.

The results will be separated by the simulation that they have been obtained.

The parameters from simulations can be found at B.1 on page 81

7.1 1 tank model

At this section the results from one tank model will be presented.

Step response

First of all the acid and base flow will be presented.

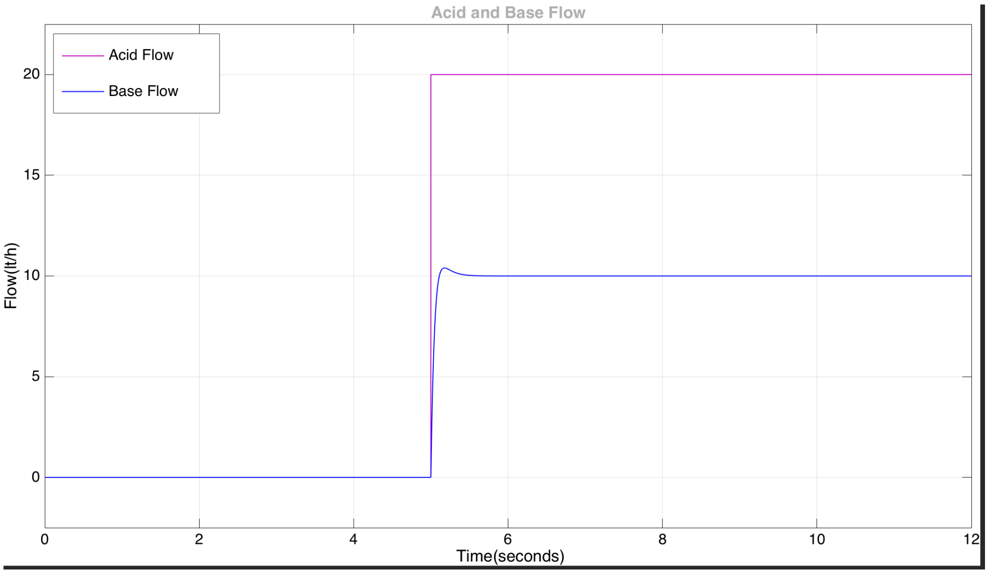

Figure 7.1: Acid and Base flow of 1 tank model

It is observable that the control output performs with a small overshoot but quit fast at the disturbance.

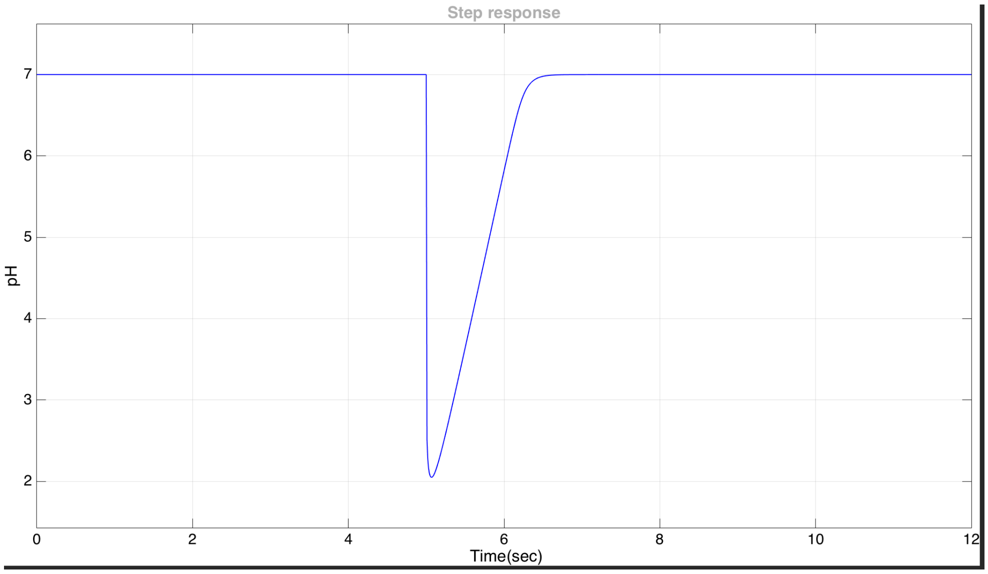

Figure 7.2: pH of 1 tank model

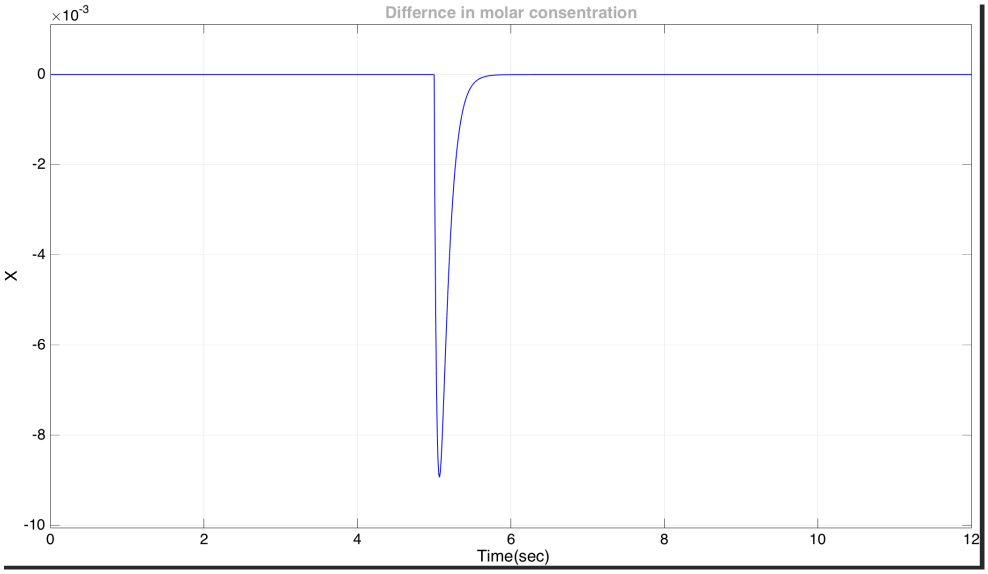

Figure 7.3: X of 1 tank model

According to 7.2 and 7.3 the controller fulfils all the design criteria.

7.2 Real system with observer based PI controller

At this section the real system simulation results will be presented. Two types of input are used

- Step response

- Real Disturbance

Step response

As a disturbance, a step with amplitude of $200lt/h$ is used.

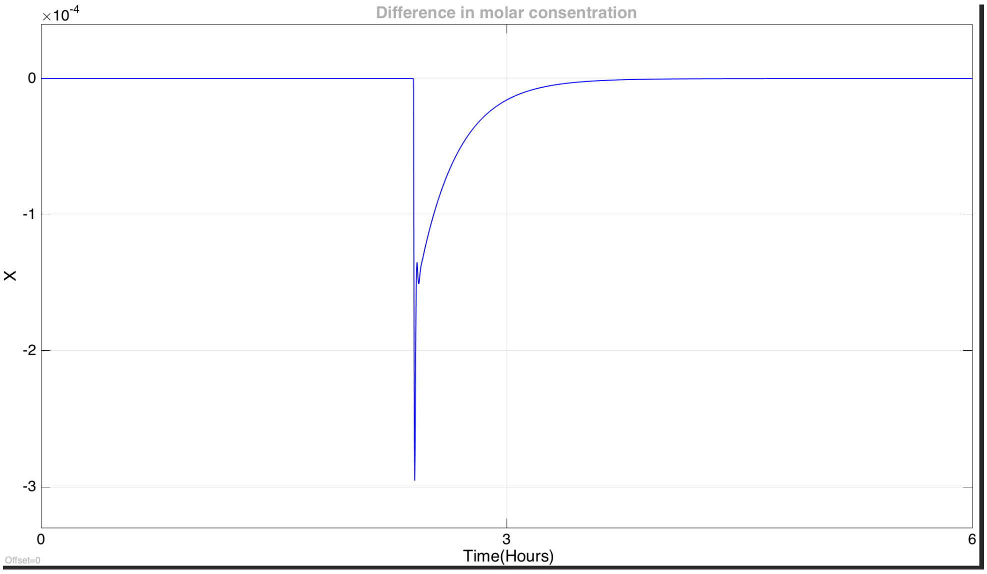

Figure 7.4: Step Response of the Real System

The response of the system is acceptable and fulfils all the design criteria. The difference which is observed from 5.4 on page 43 is normal. The reason of this difference exists, is the fact that the step response of 5.4 on page 43 is done with the linearised model and the simulation is done with real model.

Real Disturbance

First of all the acid and the base flow will be presented.

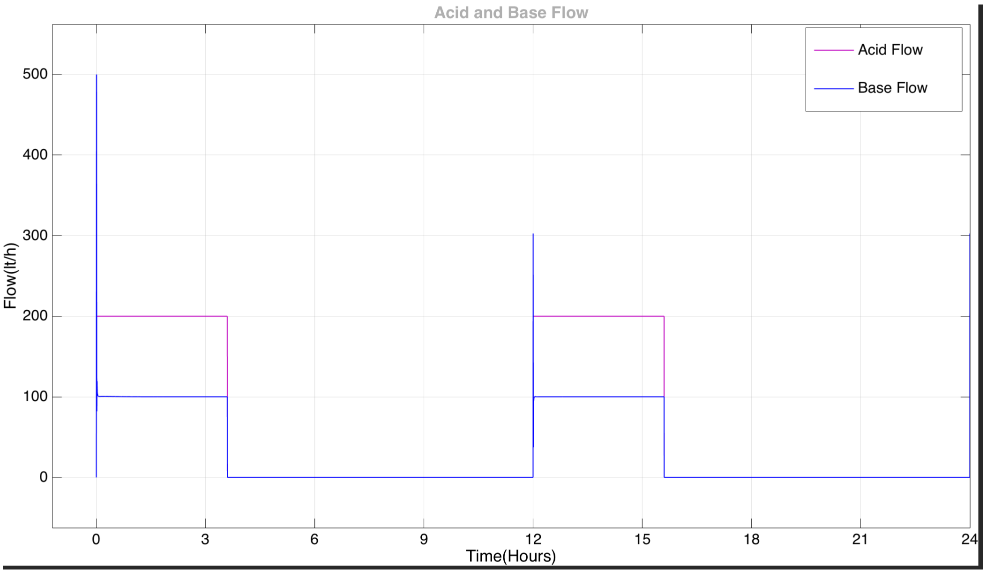

Figure 7.5: Acid and Base Flow

The results are acceptable despite the spikes which occurred due to the controller overshoot. This overshoot appears very early and disappears a long time before the end of the pulse. The dangerous situation appear if there is basic conditions in the second tank when the acid pulse stops.

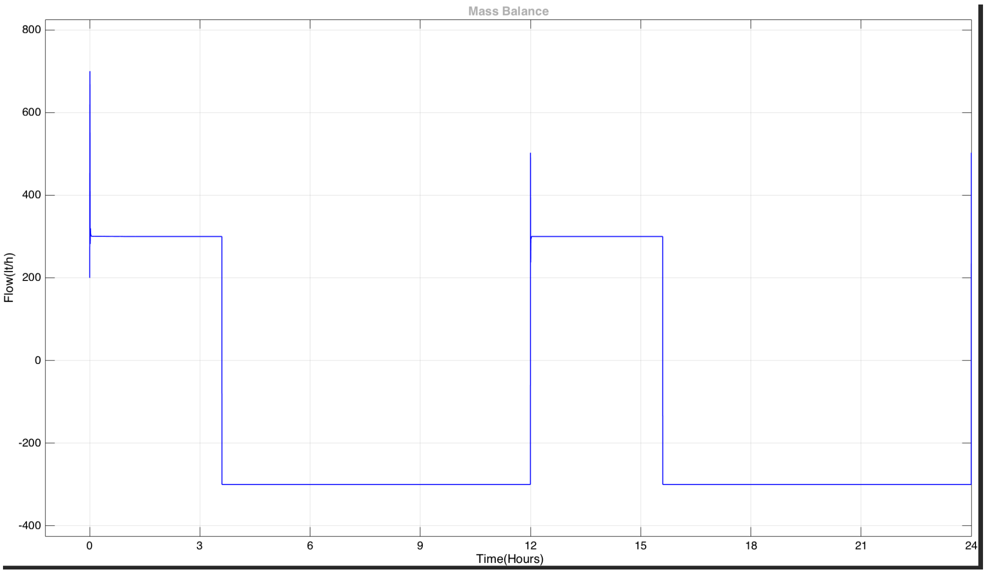

Figure 7.6: Mass Balance of Second Tank

At figure 7.6 is presented how the switch between recirculation and sea disposal, impacts at the mass balance of the second tank.

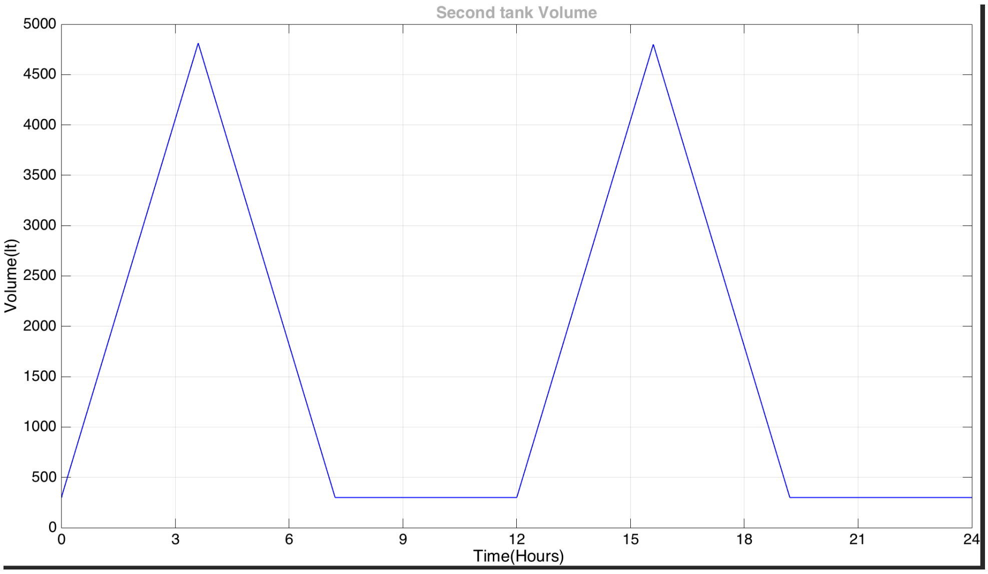

Figure 7.7: Volume of Second Tank

This figure 7.7 shows the Volume of the second tank. The results are acceptable because the tank does not over flow (maximum capacity $10m^3$). Also the low level limitation switch, works and keeps the level over $300lt$.

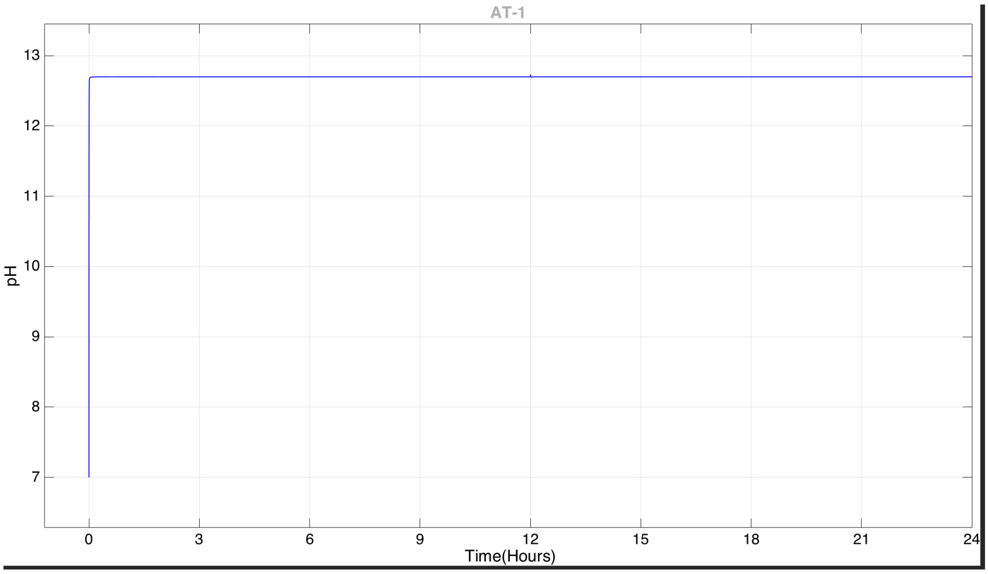

Figure 7.8: AT-1

The pH of the first tank remains always basic. The reason of this fact is the *Controller Stop* and the pump flow change. The *Controller Stop* turns off the controller, when the neutralisation is finished and the acid flow stops. So a big amount of base remains in tank 1 which is unable to be neutralised because there is not a flow between two tanks. The basic condition in tank 1 helps the control at the second pulse of acid because X_1 value from tank 1 to tank 2 has a suitable value when the controller starts.

The difference between molar concentration of H^+ and OH^- is the output of the controller.

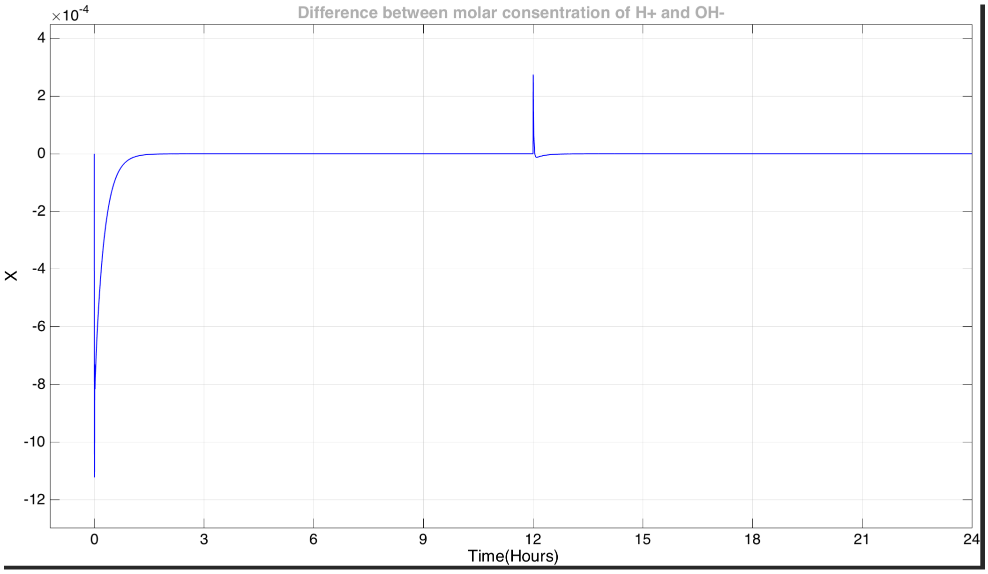

Figure 7.9: Difference between molar concentration of H^+ and OH^- of the second tank X_2

Which is represented as pH

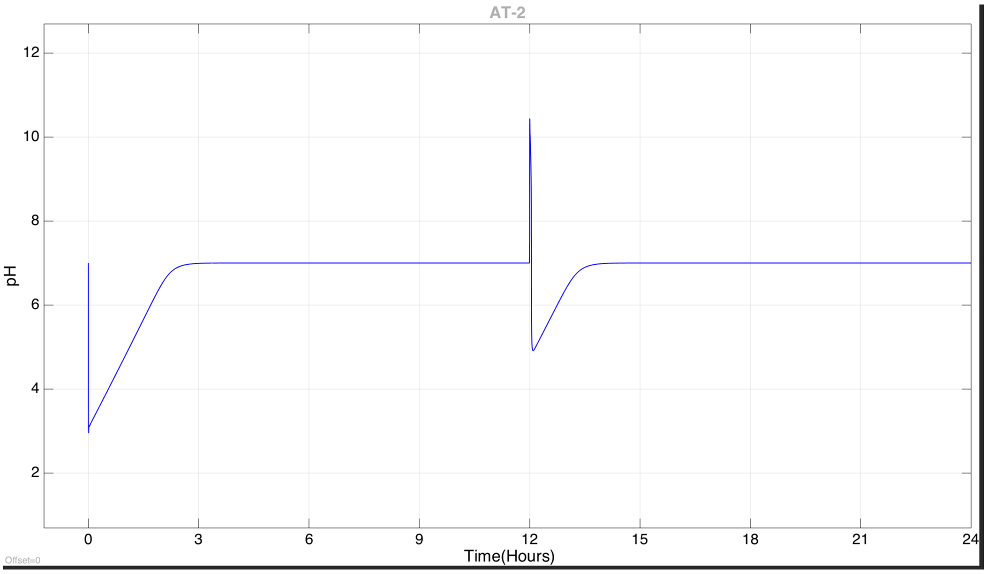

Figure 7.10: AT-2

The results are acceptable because they fulfil the controller requirements. The difference between two working cycles is explained from the fact that the second tank pH, remains basic after the first cycle. Also, the spike in the beginning of the second cycle, is explained by the same reason. Finally in the beginning of the pulse the volume is far from the linearisation point, so the response can not be expected to be exactly like the linearised.

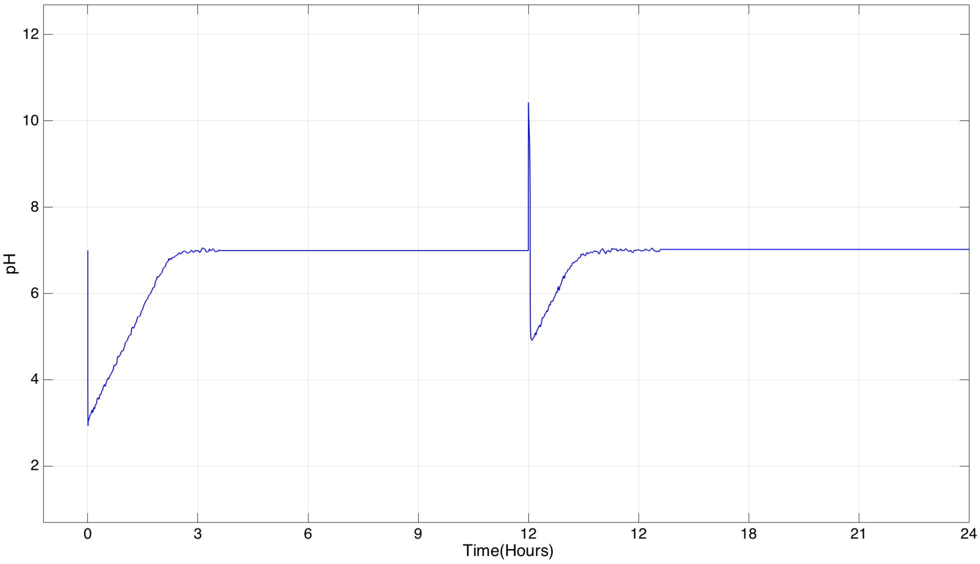

Figure 7.11: AT-2 with noise

Even with noise at the measurement the controller performs very well.

7.3 Real system with observer based PI controller which use both X_1 and X_2

At this section the results will be presented from another version of the controller.

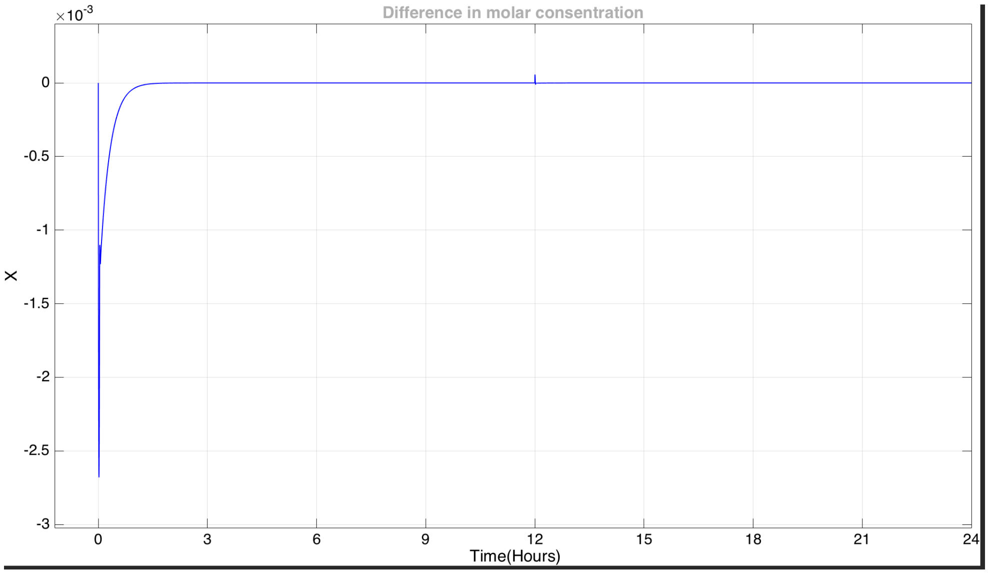

Figure 7.12: X_2 with observer which use both X_1 and X_2

It can be observed that the disturbance is slightly smaller and the controller has pretty much the same performance. The other results are almost the same.

7.4 Real system with PI controller without observer

This version avoid observer.

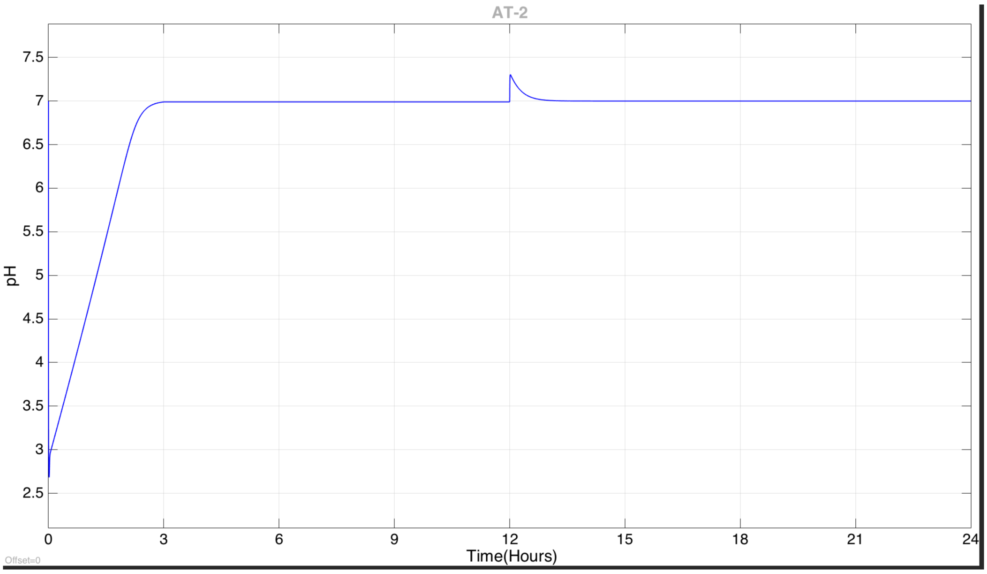

Figure 7.13: pH without observer

It is obvious that the controller performs very good, even without observer. But the observer is necessary because in real conditions the pH measurement, which is used as a feedback, may has noise and delay.

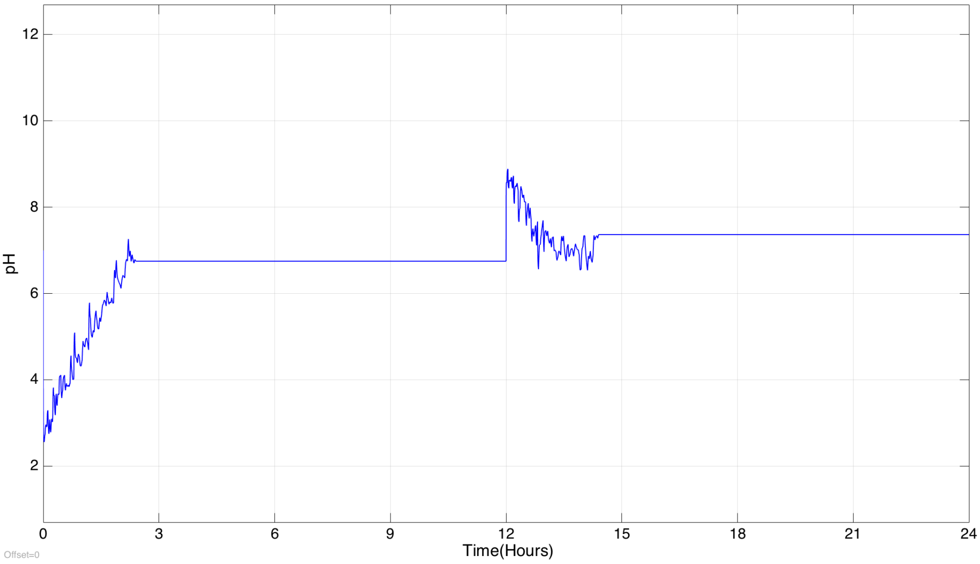

Figure 7.14: pH with noise without observer

Part IV

Conclusion

This part will describe the conclusions and the reflections made working through this Master Thesis.

Conclusion 8

At this master thesis a model and a controller developed for a pH neutralization unit.In order to overcome the non linearities that exist at pH modelling two methods are used.

- Linearisation around operating point for the bi linear differential equation.
- Linearisation through inversion of the non linear static equation.

The control method that is used is observer based PI controller.The controller is tuned through pole placement method.The criteria for poles position are :

- System response like a first order system.
- Settling time is smaller than disturbance pulse.

A controller turn off switch is introduced.The reason for this is to shut off the control signal when the water is disposed in the sea.The utility of the *controller stop* is validated by the results.

The results from the simulation show that the whole process reaches the requirements that have been set.

Perspective

9

This part will discuss further opportunities for studying about pH neutralization

There are plenty methods for pH neutralizations further than the methods that have been tested at this thesis.
The method of feedback linearisation [6] can be used in order to linearise the bi-linear equations.The following block diagram shows the main idea 9.1.

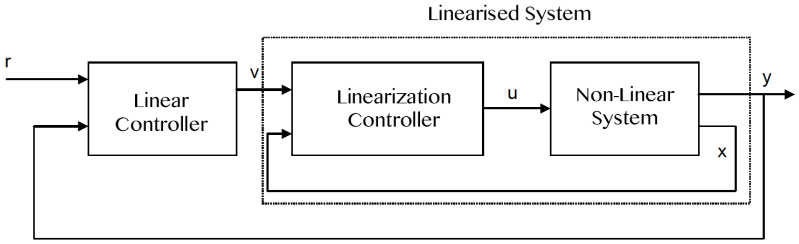

Figure 9.1: Block Diagram of Feedback Linearisation

Generally, a non linear system can be called linearised by feedback, if a controller $u = f(v, y)$ can be found so that the closed loop system which occurs with input v and output y is linear.
Feedback linearisation is based on the complete knowledge of the system model and the precise measurement of the states as well. Usually there is not a full knowledge of the system. The occurring modelling errors can be, under circumstances, viewed as disturbances. It is a design matter of the outer control loop to make the system robust against disturbances.

Furthermore more complex control methods can be used such as Linear Quadratic control.

Part V

Appendices

Appendix A

A

A.1 1 tank PI Controller with Observer Full Simulink Model

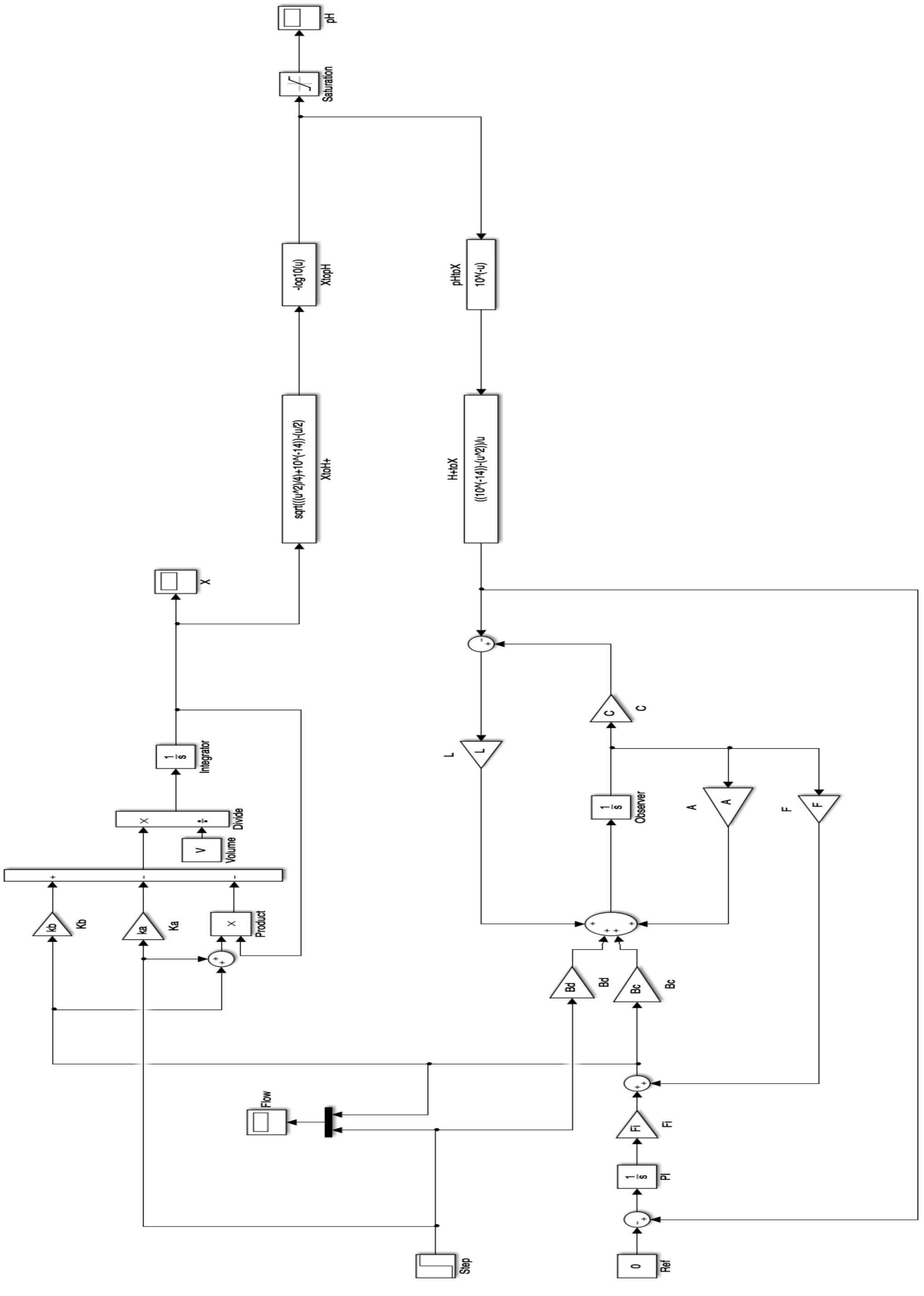

Figure A.1: 1 tank PI Controller with Observer Full Simulink Model

A.2 PI controller with observer which use both X_1 and X_2 Full Simulink Model

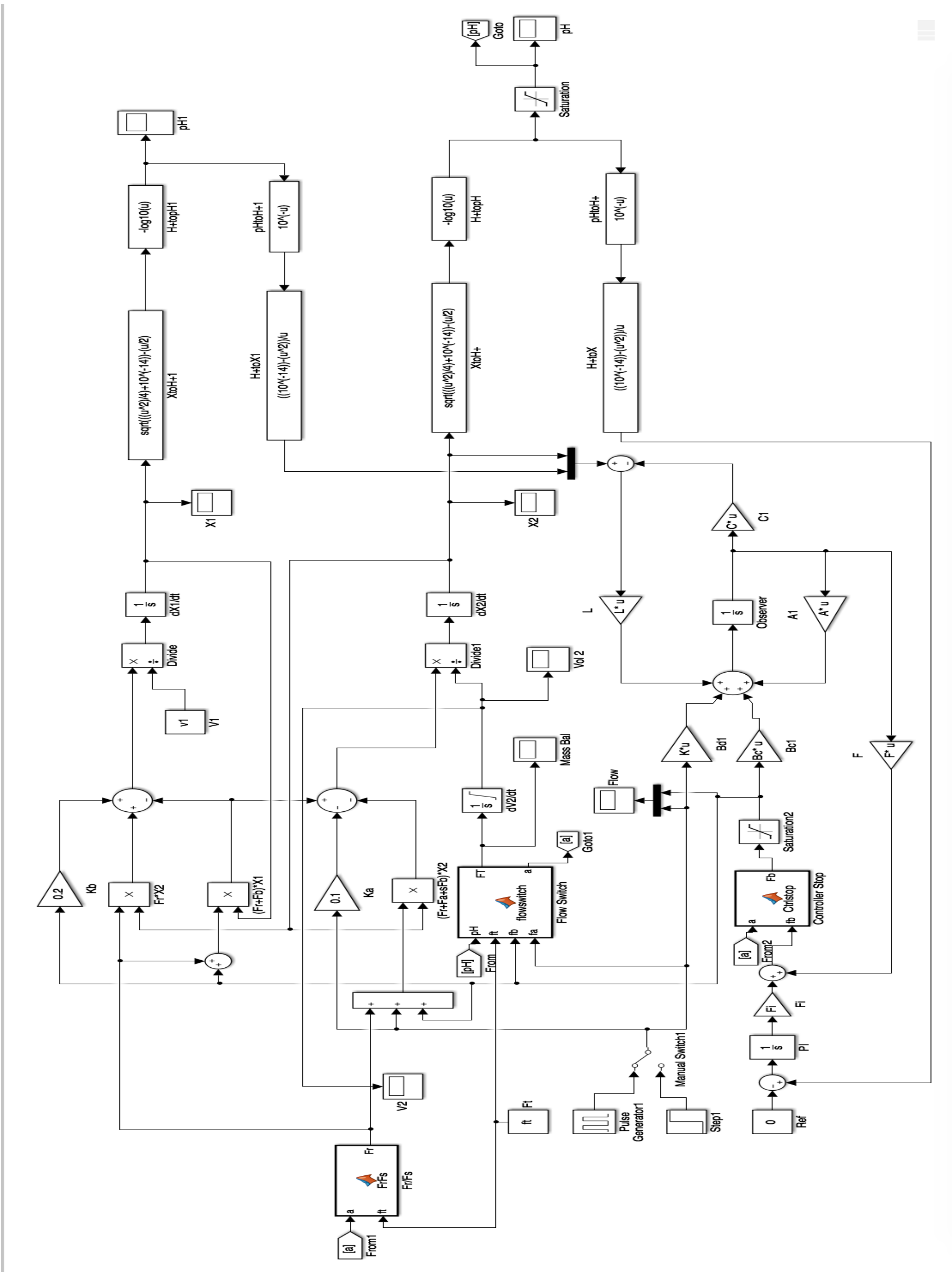

Figure A.2: PI controller with observer which use both X_1 and X_2 Full Simulink Model

A.3 PI Controller with Observer Full Simulink Model

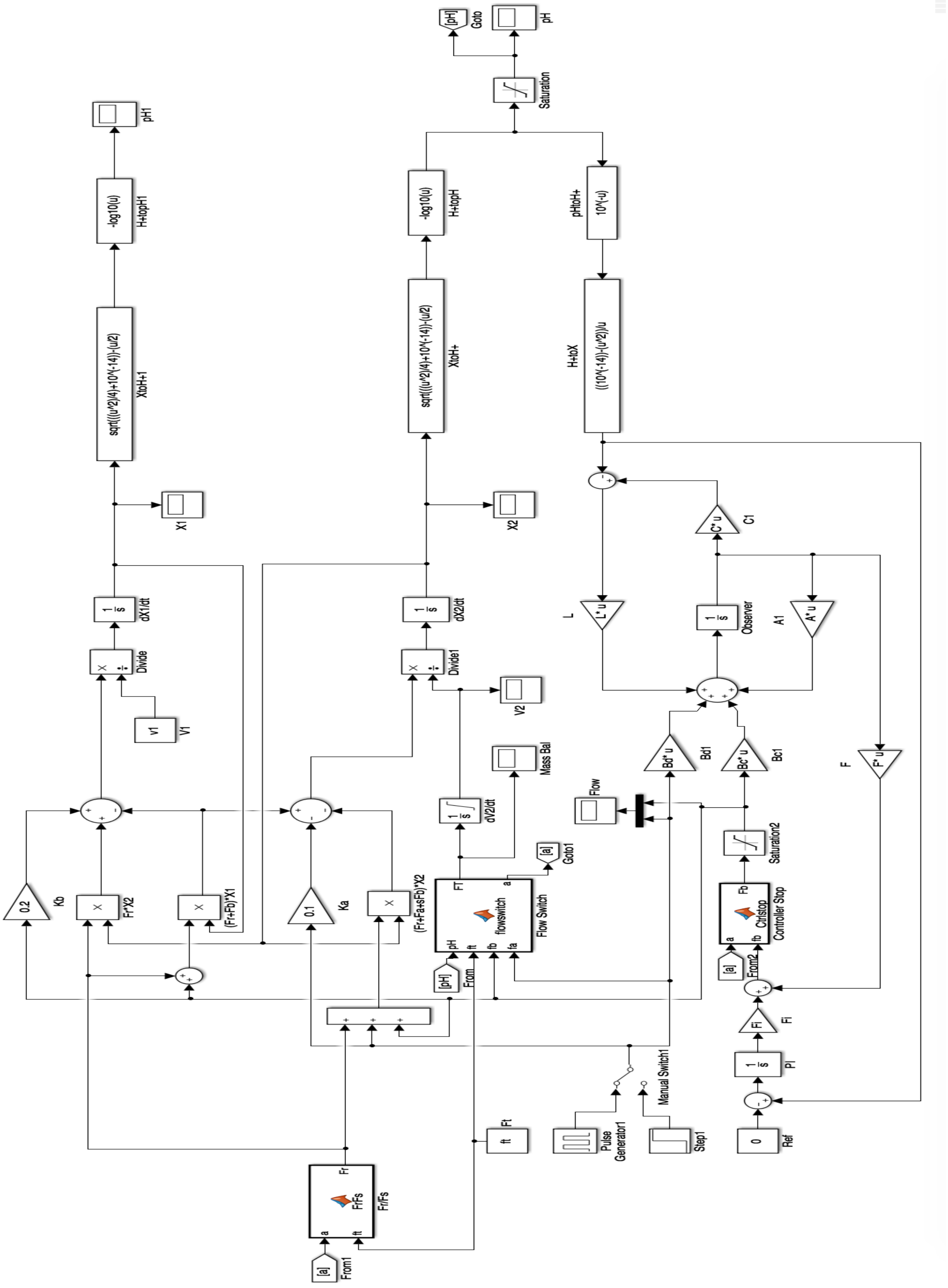

Figure A.3: PI Controller with Observer Full Simulink Model

A.4 PI controller with observer which use both X_1 and X_2 Full Simulink Model

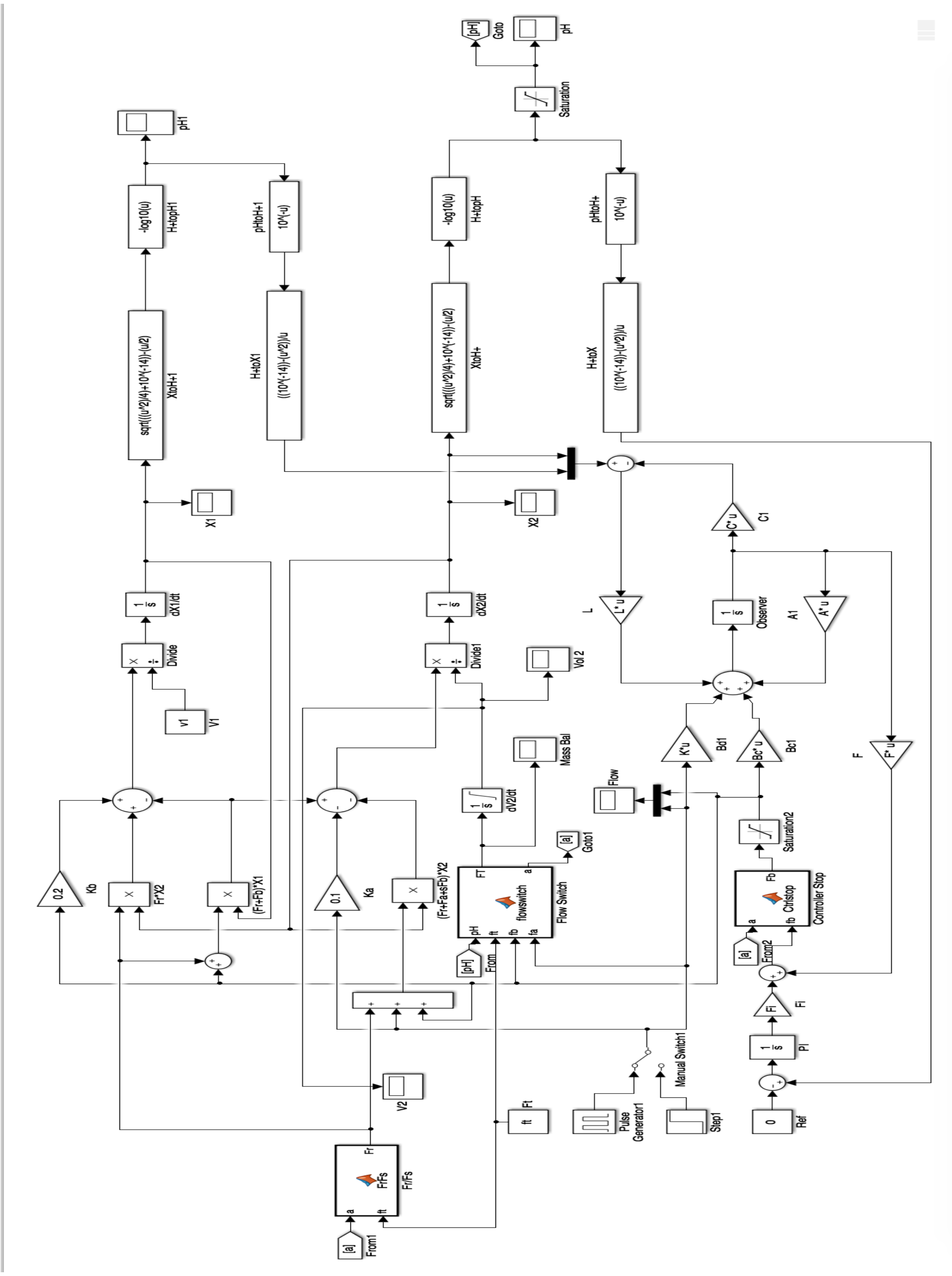

Figure A.4: PI controller with observer which use both X_1 and X_2 Full Simulink Model

A.5 PI controller without Observer Full Simulink Model

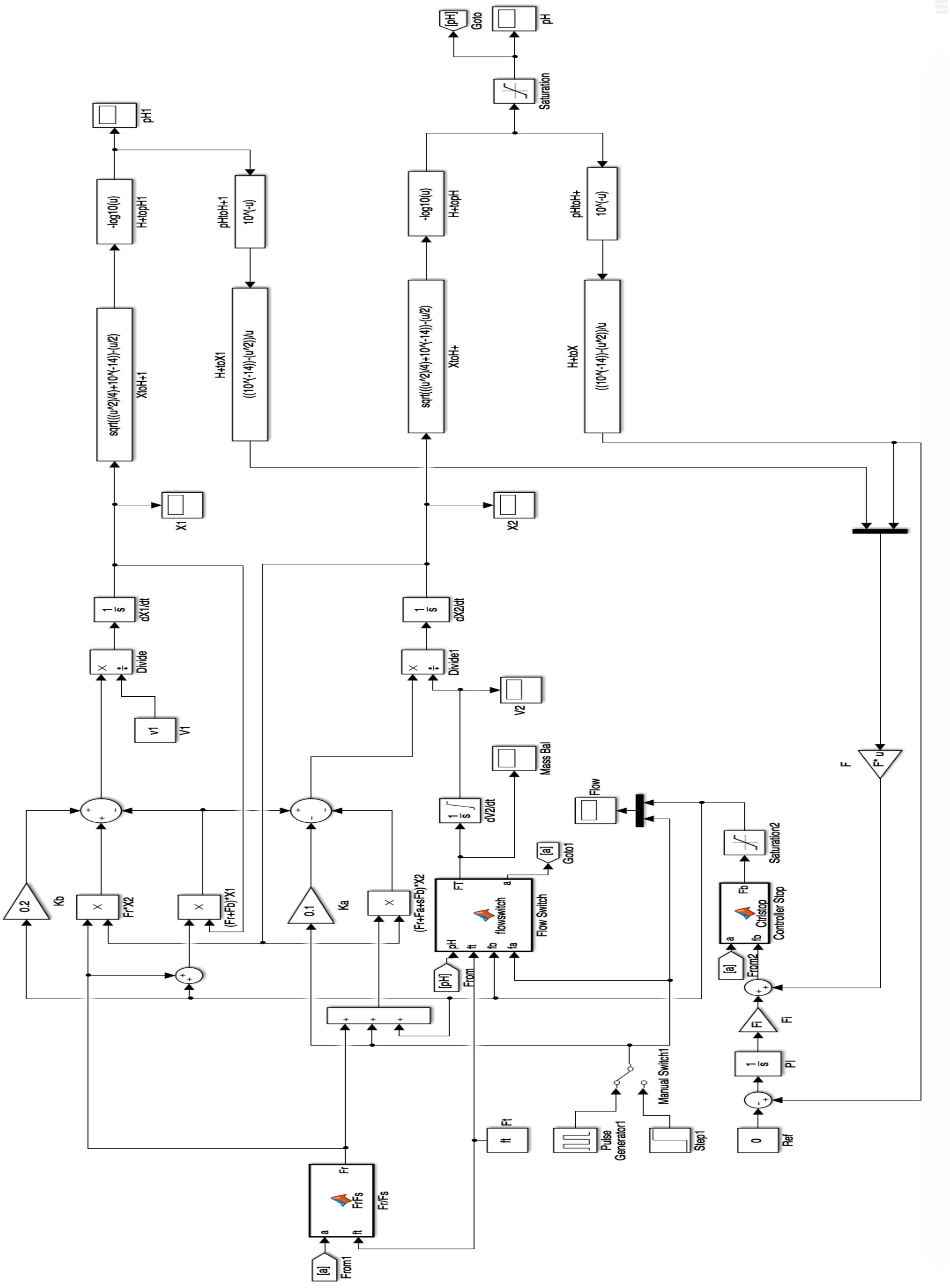

Figure A.5: PI controller without Observer Full Simulink Model

Appendix B

B.1 Model Parameters and Controller Computation with Matlab

1 tank Model

```
clear all
clc
close all


%Set Parameters
Fa=20;
Fb=10.189;
V=5.7;
ka=0.1;
kb=0.2;
x=0;
%Constract Matricies
A=-(Fa+Fb)/V;
Bc=(kb+x)/V;
Bd=-(ka-x)/V;
C=1;

olpr=poly(A);
dlpr=poly(-30);%Observer pole
L=olpr(1,2)-dlpr(1,2);
%Extended Matrices
Ae=[A 0;C 0];
Be=[Bc;0];
fe=-place(Ae,Be,-[10 20]);%Controller poles
Fi=fe(1,2);
F=fe(1,1);
```

2 tank Model

```
clear all
clc
close all

%Set Parameters
x1=0.03;
x2=0;
ka=0.1;
kb=0.2;
v1=50;
v2=2000;
ft=300;
```

```
fb=366.66;
fa=200;

%Constract Matricies
A=[-(fb+ft)/v1 (ft+fb+fa)/v1;(ft+fb)/v2 -ft/v2];
Bc=[(kb-x1)/v1;(x1+x2)/v2];
Bd=[0;-(x2+ka)/v2];
C=[0 1];

%Observability matrix
o=[C;C*A];
if det(o)~=0%must be full rank in order to be observable
    t2=inv(o)*[0;1];
    t1=A*t2;
    T=[t1 t2];
    Ao=inv(T)*A*T;
    Co=C*T;
    olpr=eig(A);
    olp=poly(olpr);
    dlpr=-[80 50];%Observer poles
    dlp=poly(dlpr);% close loop polynomial
    Lo=[olp(1,2)-dlp(1,2);olp(1,3)-dlp(1,3)];
    L=T*Lo;%Observer Gain
end

%Check the Observer poles
po = eig(A-L*C)
a=A;
b=Bc;
c=C;

%Extended Matrices
Aq=[a zeros(length(a),1);c 0];
Bq=[b;0];
Cq=[c 0];
fe=-place(Aq,Bq,-[1 15 30]);%Controller poles

for i=1:length (fe)-1
Fi=fe(1,length (fe));
    F(1,i)=fe(1,i);
end

%Check Controller Poles
pc = eig(Aq+Bq*fe)
%Check Close loop Poles
pcl = eig([Aq+Bq*[0 0 Fi] Bq*F;Bc*[0 0 Fi]-L*Cq A+Bc*F+L*C])
%Close loop Matricies
Acl = [Aq+Bq*[0 0 Fi] Bq*F;Bc*[0 0 Fi]-L*Cq A+Bc*F+L*C];
Bdcl = [Bd;0;0;0];
Ccl = [0 1 0 0 0];
%Close loop transfer function from Fa to X2
s = tf('s');
Gdcl = Ccl*(s*eye(5)-Acl)^(-1)*Bdcl
```

```
pzplot(Gdcl)
figure;
opt = stepDataOptions('StepAmplitude',200);
step(Gdcl,opt)
```

C

Nomenclature

K_a	Inlet concentration of acid
K_b	Inlet concentration of base
F_a	Flow rate of acid
F_b	Flow rate of base
V	Volume of the solution
K_w	ionic product of the water
H^+	Hydrogen ions
OH^-	Hydroxide ions
X	Difference between molar concentration of H^+ and OH^-
X_1,X_2	Difference between molar concentration of H^+,OH^- at tank 1 and tank 2 respectively.
V_1,V_2	Volume of the solution at tank 1 and tank 2 respectively
AT-1	pH meter at tank 1
AT-2	pH meter at tank 2
F_S	Flow to the sea
F_R	Recirculation flow
F_T	$F_R + F_S$
$\bar{X}$ $\bar{F_b}$ $\bar{F_a}$	steady state values
X^Δ F_b^Δ F_a^Δ	Difference from Operating point

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List of Figures