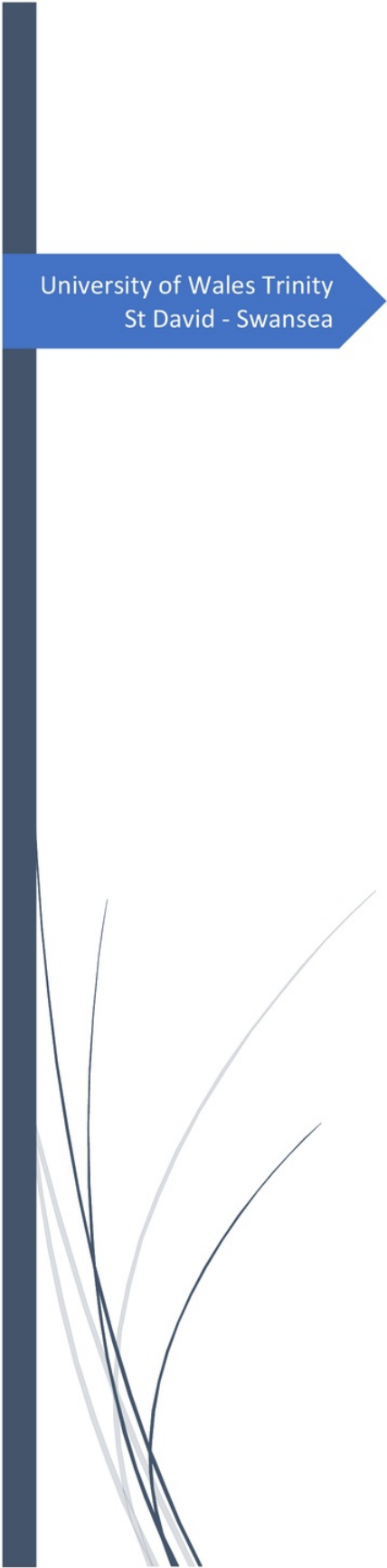


CO2 Assignment

by Liam Thomas

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The logo consists of a dark blue vertical bar on the left. A blue arrow points to the right from the bar, containing the text 'University of Wales Trinity St David - Swansea'.

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Controlling the pH of Water with Carbonic Acid

Instrumentation and Control

Liam Thomas
P143797

Abstract

The pH of water must be between 6.5 and 8.5 to be suitable for human consumption. Using carbonic acid, basic water can be treated to consumable levels. To design a control system for the process suitable pH sensor and gas valve must be chosen. Most gas valves have the option to fitted with a control module, so they were excluded for the design process. The system was then designed within Simulink, after the transfer functions had been derived for the sensor and the relationship of dissolving carbonic acid in water (this was approximated due to the logarithmic relationship of the equation). The system was able to successfully maintain a pH of 7 even after an alkaline disturbance was added to the simulation. The stability of the system was then tested using bode, Nyquist and pole zero plots, the large gain and phase margins proved the system to be incredibly stable.



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Introduction

The pH of water must be between 6.5 and 8.5 to be suitable for human consumption. This report will cover the design of a control system that will control the pH of water by using carbonic acid. It will cover the different forms of control systems (P, PI and PID). The sensors for the system will be selected with justification of the choice. The specification of the chosen parts will allow the derivation of the required transfer functions to design the control system within Simulink. The system will then be analysed using bode, Nyquist and pole-zero plots, this will ensure that the system is stable.

Literature Review

This chapter will cover the different forms of control and what effect each of the terms have on the system.

Proportional Control

Using the example of a heating element with a fixed set point. On and off controllers cycle around the set point, a proportional controller removes this, as well as decreasing the average power consumption. This is achieved by reducing the temperature as it approaches the set point, this also means it reduces/eliminates overshoot. Proportional control is achieved by cycling the heating element on and off for determined periods of time.

The ratio of time on and time off can be adjusted to control temperature. The proportioning occurs within a band either side of the set point. Outside of this band a proportional controller functions identically to an on/off controller, where the output is fully on when the temperature is below the band and fully off when it is above. While it is within the band the output the ratio between the output being on and the output being off is in accordance to the distance from the set point.[1]

The following algorithm is for the proportional control process:

$$CO = CO_{bias} + K_c \cdot e(t)$$

Where:

CO = Controller output

CO_{bias} = controller bias or null value

K_c = controller gain, a tuning parameter

$e(t)$ = controller error = $SP - PV$

SP = set point

PV = measured process variable

[2]

One of the fundamental issues with proportional control is that the output will never reach the set point. This is known as the offset and it will remain until the controller is switched to manual mode and adjusted until the offset is zero.[3] This is because if PV is equal to SP then $e(t)$ is equal to 0, if $e(t)$ is equal to 0 then CO is equal to CO_{bias} and the only way these two values can differ is if a value is added or subtracted from CO_{bias} .

Proportional-Integral Control

Integral control is used in addition to proportional control, integrating the controller error continuously for the duration of the system.

As previously mentioned the proportional term calculates the error within the system for a specific time, whereas the integral term considers the history of the error which is calculated from the moment the controller was activated. The third term of the below equation is the integral term.

$$CO = CO_{bias} + K_c \cdot e(t) + \frac{K_c}{T_i} \int e(t) dt$$

Figure 1 – PI Term

Where:

CO = controller output signal

CO_{bias} = controller bias or null value

e(t) = current controller error, defined as *SP* – *PV*

SP = set point

PV = measured process variable

K_c = controller gain, a tuning parameter

T_i = reset time, a tuning parameter[4]

When the integral term is added, the integral term can still have a value after the response has completed. This means that even if *e(t)* is equal to zero, the integral term will still have a value to combine with *CO_{bias}* to form the final output.

As long as there is an error present then the integral term will continue to change, *CO* will only cease to change when *e(t)*=0 for a sustained period.[4]

Proportional-Integral-Derivative Control

Derivative control is the final term in a PID controller and it considers the rate of change of the error as it varies over time.

$$CO = CO_{\text{bias}} + K_c \cdot e(t) + \frac{K_c}{T_i} \int e(t) dt + K_c \cdot T_d \frac{de(t)}{dt}$$

Figure 2 - PID term

Where:

CO = controller output signal

CO_{bias} = controller bias;

e(t) = current controller error, defined as SP – PV

SP = set point

PV = measured process variable

K_c = controller gain

T_i = reset time

T_d = derivative time[5]

The derivative term of the error is identical to the negative derivative of the process variable, except for where the set point changes. This is shown in the figure below.[5]

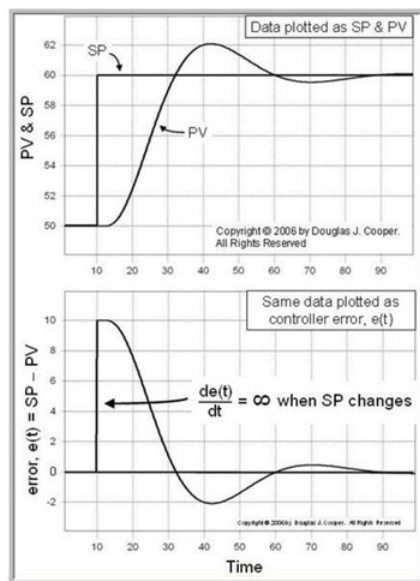


Figure 3 - Process Variable and Error Comparison[5]

When the set point changes on the lower graph there is a spike in the error, theoretically this tends to infinity which causes a large sudden manipulation of the output. This is referred to as the derivative kick.

Due to the derivative of the error providing the sudden response that is not desired the derivative of the error is swapped for the derivative of the process variable.

$$CO = CO_{bias} + K_C \cdot e(t) + \frac{K_C}{T_I} \int e(t) dt - K_C \cdot T_D \frac{dPV}{dt}$$

Figure 4 - PID Term with Derivative Changed[5]

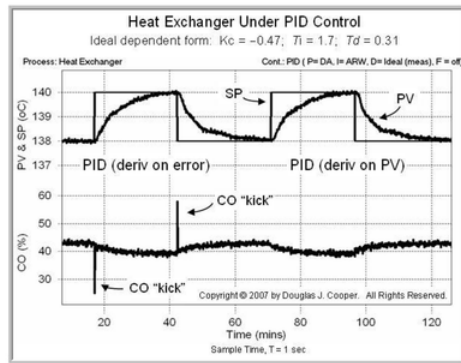


Figure 5 - Derivative on Error and Process Variable[5]

The above figure shows that when the derivative of the process variable is used instead of the derivative of the error, the momentous changes in the output are removed. The negative sign now in front of the derivative term means that when the term is negative it aims to increase the output and when it is positive it aims to decrease the output. At this point the derivative term does not consider if the process variable is moving towards or away from the set point, it only inhibits rapid movements on the process variable in the direction it was already headed towards.

pH

PH is measure of the concentration of hydrogen ions within a solution. pH of a solution ranges from 1-14 with 7 being neutral, >7 being basic (low concentration of ions) and <7 being acidic (high concentration of ions).[6]

$$pH = -\log[H^+ \text{ concentration in Moles}]$$

Method

Transducer Selection

PH Sensor

Table 1 - pH Sensor

Specification	Vernier pH Sensor[7] 	Atlus PH Probe[8] 	Oakton General-Purpose pH Probe[9] 	CSIM11-L[10] 
Sensitivity (V/pH)	0.25	0.25	0.25	0.059
Electrode Type	Ag/AgCl	Ag/AgCl	Ag/AgCl	KCl/AgCl
Response Time	90% in 1 second	95% in 1 Second	Not Stated	95% in 10 seconds
Range (pH)	0-14	0-14	0-12	0-13
Accuracy (pH)	+/- 0.2	Not Stated	Not Stated	+/-0.1%

The pH sensor that will be used for this system is the Vernier pH sensor, due to it providing the specification details required (sensitivity & response time), providing its good accuracy and for the response time being the fastest out of all the sensors that were compiled in the previous statements.

CO2 Valve

Table 2 - CO2 Valve

Specification	Cole-Parmer Proportioning Solenoid Valve[11] 	Buschjost Solenoid Valve[12] 	Electrical Ball Valve BW2[13] 	Asco Solenoid Valve[14] 
Power (VDC)	30	24	24	24
Maximum Pressure	35 Bar	16 Bar	10 Bar	4 Bar
Flow Rate	1.5m ³ /h	1.9 m ³ /h	8.6m ³ /h	0.3m ³ /h

Based on the above table, the most suitable gas valve for this system is the Cole-Parmer Proportioning Valve. This is because it has the highest maximum pressure and doesn't require a transfer function to be developed when paired with the following control module.



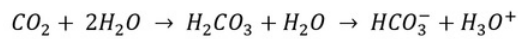
Figure 6 - Cole-Parmer Control module for 98650-series proportioning solenoid valves[15]

Before the plant can be developed within MATLAB using Simulink, the transfer functions for the plant and the pH sensor must first be derived.

Transfer Function Derivation

Carbonic Acid in Water

When carbon dioxide is added to water the following reaction occurs.



Acid Dissociation constant of Carbonic Acid

$$pK_A = 6.367$$

$$K_A = -\log 6.367 = 10^{-6.367}$$

CO₂ is 44.01g/mol and the solubility of CO₂ in water is 1.45g/L

$$1.45g(CO_2) \frac{1mol}{44.01g} = 0.03297 \text{ Mol } CO_2$$

$$K_A = \frac{[H^+][HCO_3^-]}{[CO_2]}$$

$$10^{-6.367} = \frac{x \cdot x}{0.03297 + x}$$

$$10^{-6.367} = \frac{x^2}{0.03297}$$

$$x^2 = 10^{-6.367} \times 0.03297 = 1.41317 \times 10^{-8}$$

$$x = \sqrt{1.41317 \times 10^{-8}} = 1.18877 \times 10^{-4}$$

$$pH = -\log(1.18877 \times 10^{-4}) = 3.9249 \text{ (Minimum pH for the water using Carbonic acid)}$$

$$pH = -\log\left(\sqrt{10^{-6.307} \times \frac{sol}{44.01}}\right)$$

The above equation needs to be arranged so that the result is pH/P.

$$pH = -\log \sqrt{10^{-6.367} \times \frac{392 \times 10^{-4} \times P}{Q}}$$

$$pH = -\log \sqrt{10^{-6.367} \times \frac{392 \times 10^{-4} \times P}{Q}}$$

$$pH = -\log \sqrt{10^{-6.367}} + \log \sqrt{\frac{392 \times 10^{-4} \times P}{Q}}$$

$$pH = -\log \sqrt{10^{-6.367}} + \log \sqrt{\frac{392 \times 10^{-4}}{Q}} + \log \sqrt{P}$$

$$-10^{pH} = \sqrt{10^{-6.367} \times \frac{392 \times 10^{-4}}{Q}} \times P$$

$$10^{2pH} = 10^{-6.367} \times \frac{392 \times 10^{-4}}{Q} \times P$$

$$\frac{10^{2pH}}{P} = 10^{-6.367} \times \frac{392 \times 10^{-4}}{Q}$$

Due to the logarithmic relationship between PH and pressure, the equation cannot be arranged to equal pH/p. We can there approximate the output using the following equation.

$$\frac{-K}{1 + \tau s}$$

$$\frac{-1}{1 + 0.5s}$$

PH Sensor

The transfer function for the pH sensor is as follows:

$$\frac{\text{Sensitivity}}{1 + \tau s}$$

Due to the chosen sensors response time being 90% in 1 second, the time constant must be calculated.

$$0.9 = 1 - e^{-\frac{1}{\tau}}$$

$$0.9 - 1 = -e^{\frac{-1}{\tau}}$$

$$-0.1 = -e^{\frac{-1}{\tau}}$$

$$0.1 = e^{\frac{-1}{\tau}}$$

$$\ln 0.1 = \frac{-1}{\tau}$$

$$-2.30 = \frac{-1}{\tau}$$

$$\frac{-1}{-2.30} = \tau = 0.43$$

The sensitivity is 0.25V/pH so the transfer function is as follows:

$$\frac{0.25}{1 + 0.43s}$$

Disturbances

The following disturbances are ranked in order of importance and should be considered.

- Change in plant pH
- Operational flow
- Change in CO2 temperature
- Change in Plant operating temperature

Operational flow, CO2 and plant temperatures are assumed to be constant. Operational flow at 10M³/s and temperatures at 25°C. Change in plant pH will be tested by adding a disturbance in the system design.

System Design

With the transfer functions derived the system was designed within Simulink.

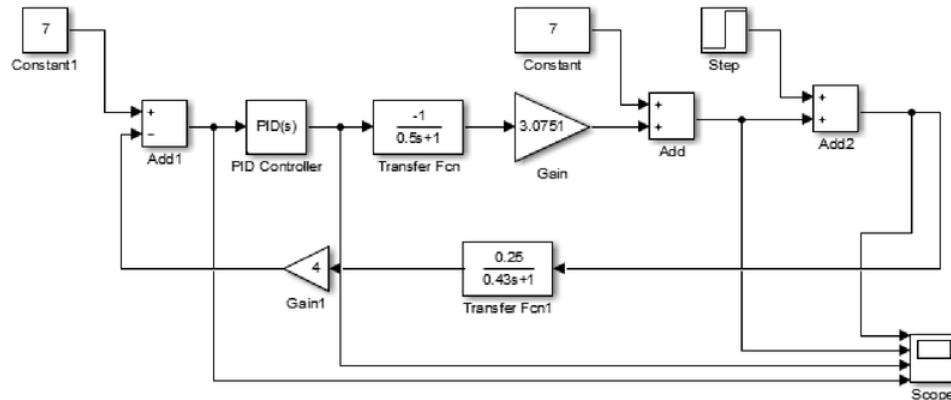


Figure 7 - System Design in Simulink

- Constant1 and Add1 – Set the system back to its neutral point 7
- PID Controller
- Transfer Fcn, Gain, Add, Constant – Make up the plant with the transfer function as the transfer function of the plant, gain is the minimum pH achievable using carbonic acid and the constant is to set the scale back to its neutral point of 7
- Add2 and Step – Are to add a disturbance to the system e.g. a strong alkaline solution being added to the system
- Transfer Fcn1 – Transfer Function for the pH sensor
- Gain1 – To amplify the output of the transfer function so that the system is reading 1V/pH

Controller Output

Once the system had been designed the PID controller required tuning, this was achieved using the auto tuner and then adjusting the response time and transient behaviour. With the goal of achieving suitable overshoot and settling time values of less than 5% overshoot and less than 10 seconds settling time.

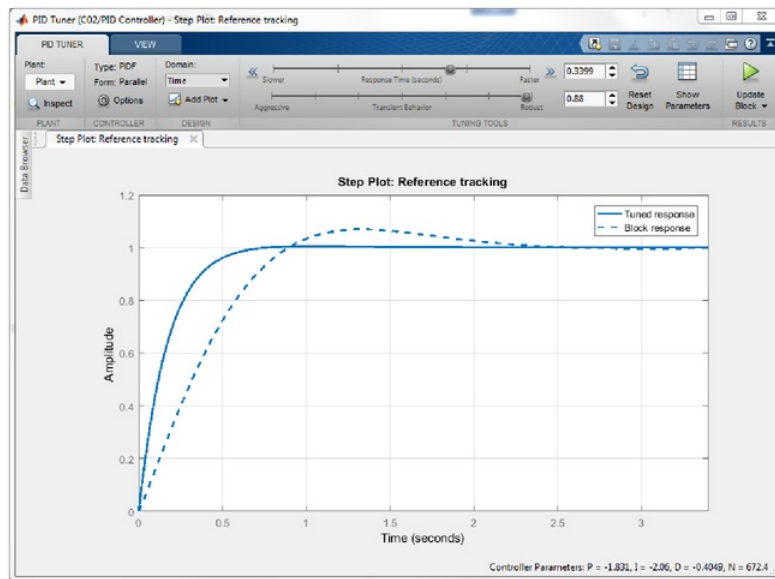


Figure 8 - Controller Output

Figure 3 shows the output for the controller, the dotted trace is the result of the auto tuner and the solid trace is the result of using the auto tuner, and then tweaking the response time and transient behaviour. This reduced both the overshoot and the settling time, their values are shown below in figure 4.

Controller Parameters		
	Tuned	Block
P	-1.8306	-0.72429
I	-2.06	-1.1021
D	-0.40486	-0.11112
N	672.3936	280.3003
Performance and Robustness		
	Tuned	Block
Rise time	0.352 seconds	0.639 seconds
Settling time	0.578 seconds	2.09 seconds
Overshoot	0.48 %	6.9 %
Peak	1	1.07
Gain margin	Inf dB @ Inf rad/s	Inf dB @ Inf rad/s
Phase margin	88 deg @ 5.88 rad/s	69 deg @ 2.45 rad/s
Closed-loop stability	Stable	Stable

Figure 9 - Controller Output Parameters

Figure 4 shows the controllers output parameters. The block column is the results from the auto tuner and the tuned column is the results of the auto tuner followed by manual tweaking. The auto

tuner produced suitable overshoot and settling time of 6.9% and 2.09 seconds. After tweaking with the manual tuner, the overshoot was reduced to 0.48% a 6.42% reduction and the settling time was reduced to 0.578 seconds, a reduction of 1.512 seconds which is a 72.34% reduction.

$$K_p + K_i * \frac{1}{s} + K_d * \frac{s}{T_f s + 1}$$

with $K_p = -1.83$, $K_i = -2.06$, $K_d = -0.405$, $T_f = 0.00149$

Figure 10 - Transfer Function of Controller

P =

From input "PID Controller" to output "u":
-14.3

$$\frac{-14.3}{s^2 + 4.326 s + 4.651}$$

Figure 11 - Transfer Function for Plant

Figure 6 shows the transfer function for the plant which is the combination of the transfer function of carbonic acid in water, an amplifier and an adder.

System Transfer Function

Now that the transfer functions for the plant, controller and sensor have been derived, below is the transfer function for the entire system, which can be calculated using the following equation.

$$System = \frac{G}{1 + GH}$$

Where:

G = Plant multiplied by the controller

H = Transfer function for the sensor

$$System = \frac{1.685 s^7 + 1.152e06 s^6 + 1.272e07 s^5 + 5.65e07 s^4 + 1.256e08 s^3 + 1.395e08 s^2 + 6.196e07 s}{0.43 s^9 + 583 s^8 + 2.008e05 s^7 + 2.163e06 s^6 + 1.009e07 s^5 + 2.64e07 s^4 + 4.169e07 s^3 + 3.8e07 s^2 + 1.549e07 s}$$

Figure 12 - Transfer Function for the Entire System

Results

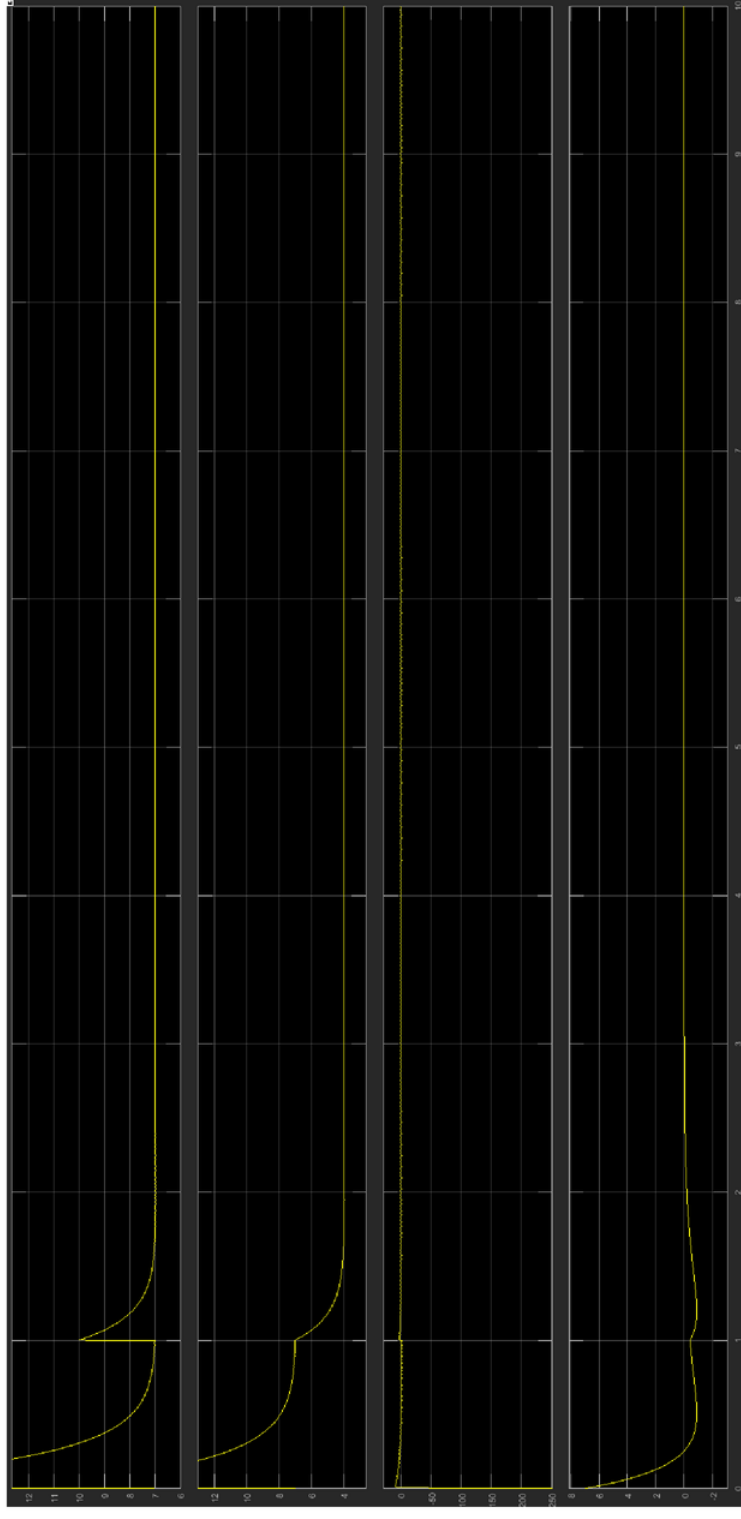


Figure 13 - Signals from System

The previous figure shows all the different signals from the system. The bottom signal is before the PID Controller, the third is after the PID Controller, the second is after the plant and the first one is after the disturbance.

As shown in the first signal reading, after 1 second the pH increases due to the disturbance being added, then over time the pH decreases until plateauing at 7. This means that the system is working as intended and the water is being treated to a consumable level.

Analysis

The stability of the system will be analysed within this chapter. Using bode, Nyquist and pole zero plots.

Bode Plot

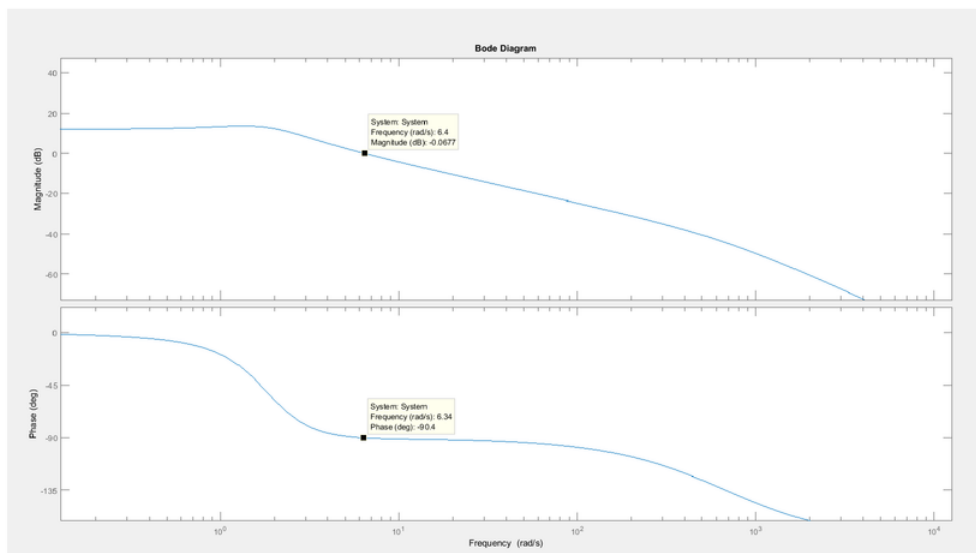


Figure 14 - Bode Plot Phase Margin

After locating the 0dB point and locating the same frequency point on the phase plot, the phase at this point is -90.4. Therefore, the phase margin is 89.6, meaning that the system has 89.6 degrees of phase before it reaches the limit of stability.

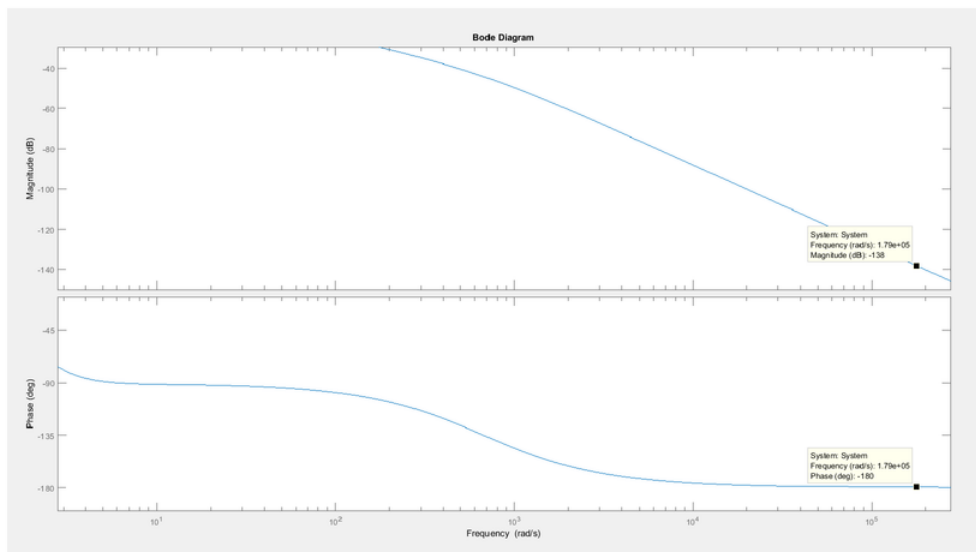


Figure 15 - Bode Plot Gain Margin

After locating the -180-degree point and locating the same frequency point on the gain plot, the gain at this point is -138dB. Therefore, the gain margin is 138dB, meaning that the system has 138dB of gain before it reaches the limit of stability. This means that the system is incredibly stable.

Nyquist Plot

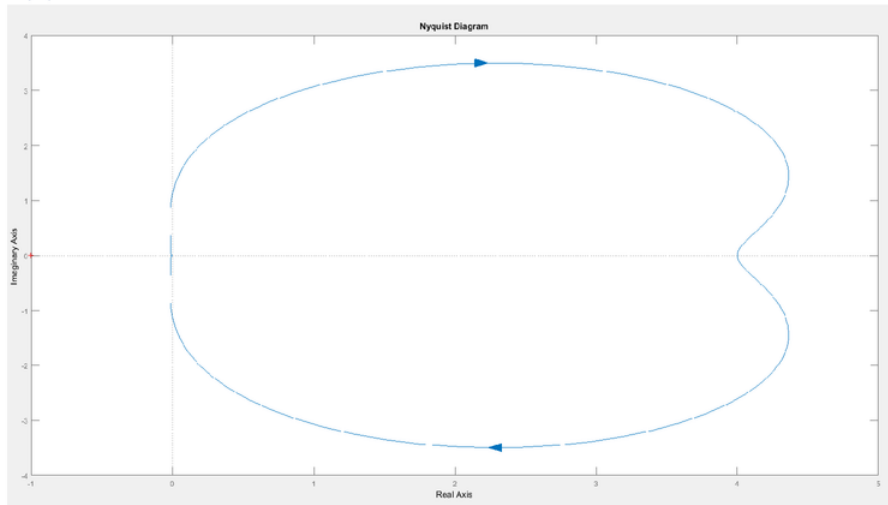


Figure 16 - Nyquist Plot

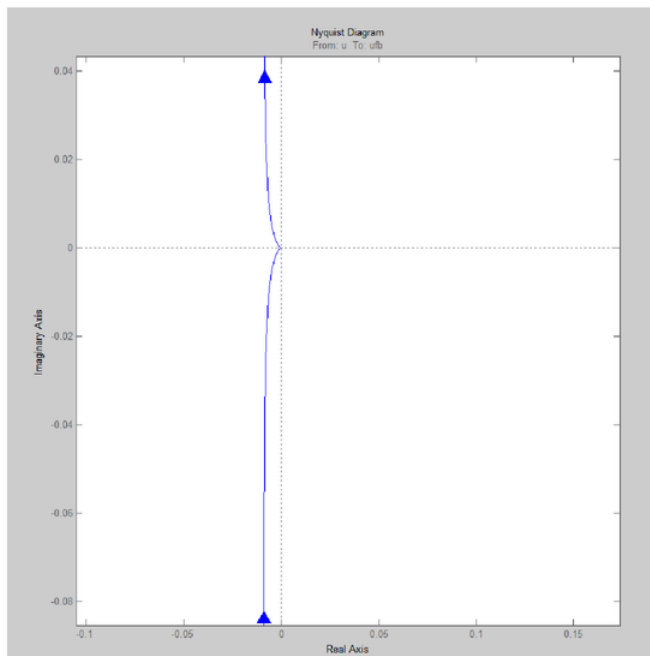


Figure 17 - Nyquist Plot Origin

Looking at the Nyquist plot above the origin comes from zero and the plot doesn't cross the real axis on the left-hand side, meaning that the gain margin for the system is very large, which was proved by the bode plot as it showed the gain margin to be 138dB. This also shows that the phase margin for the system is near 90 degrees which was also proved by the bode plot.

Pole-Zero Plot

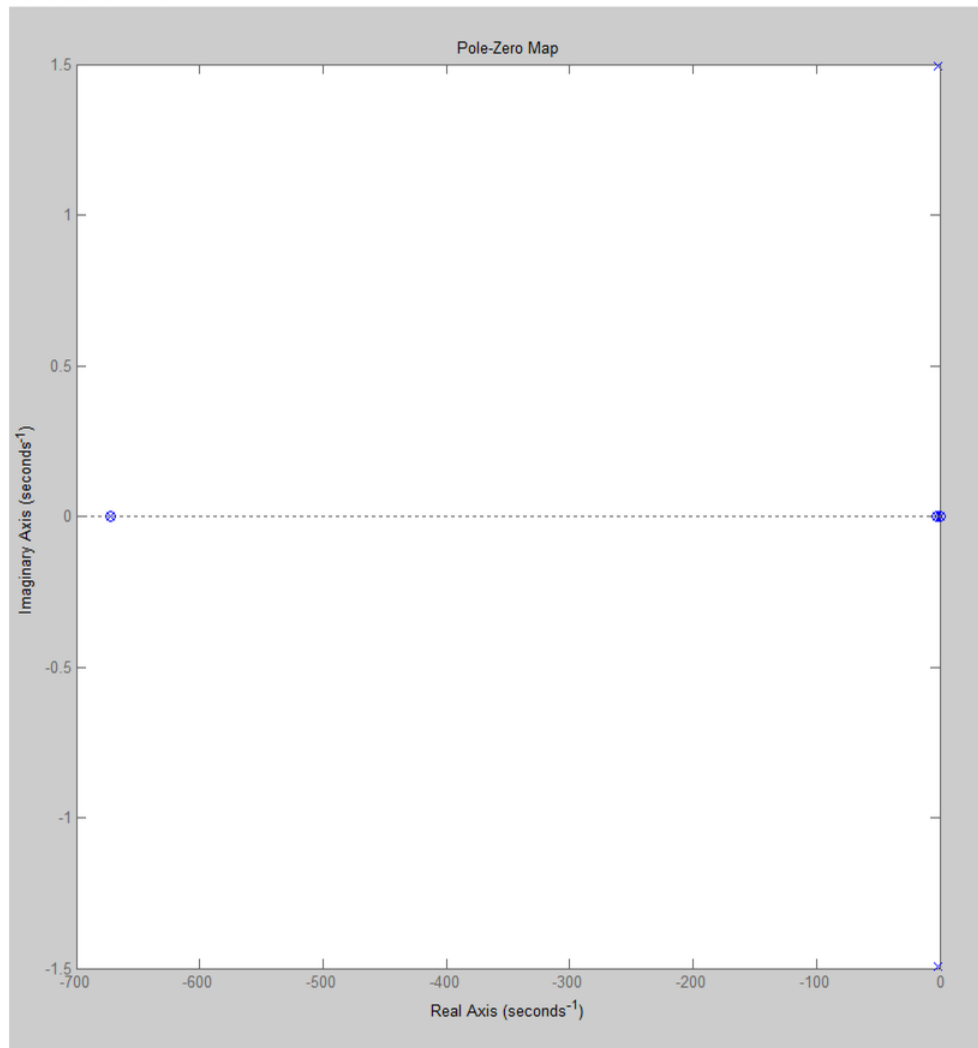


Figure 18 – Pole-Zero Plot

The pole and zero on the far left of the plot would cancel each other out since poles tend to infinity and zeros tend to zero.

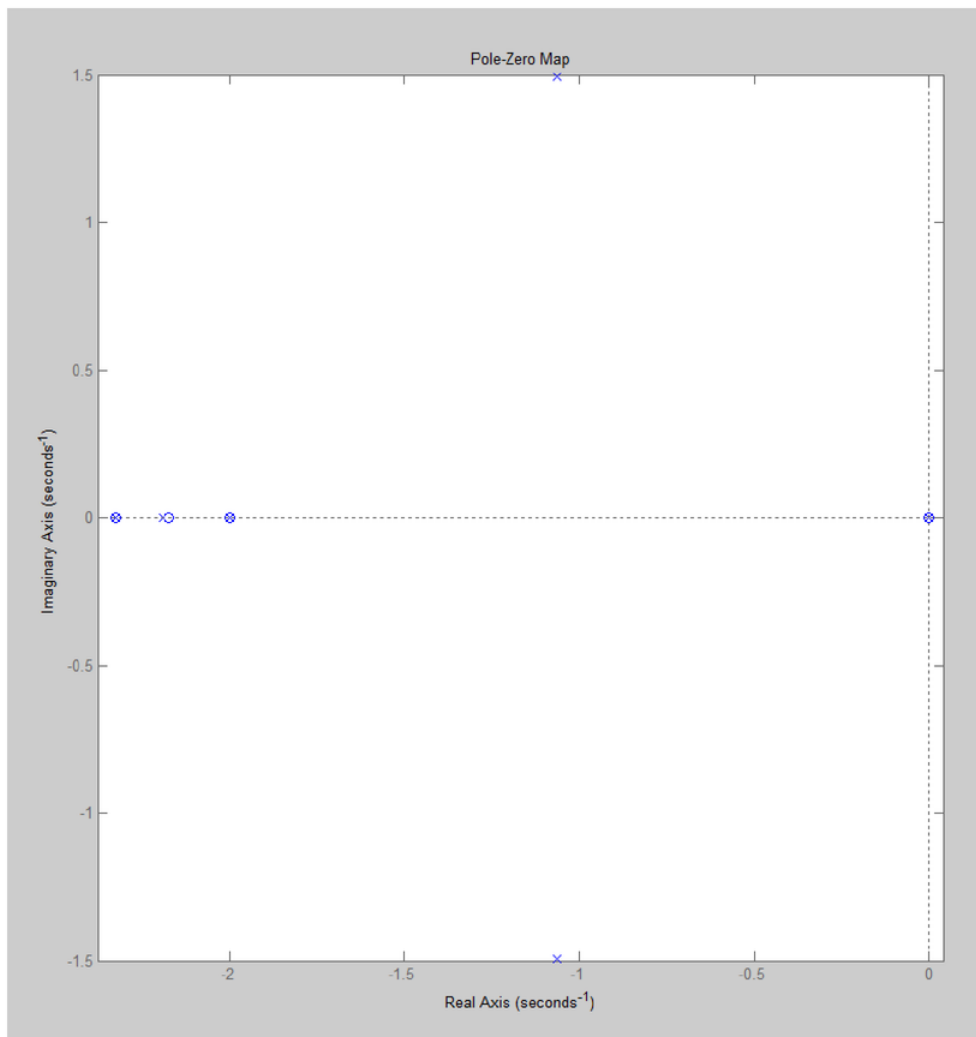


Figure 19 – Pole-Zero Plot around Origin

The complex conjugate pair at the points $-1 \pm j1.5$ would produce a decaying sinusoid. Where -1 signifies the rate of decay and $\pm j1.5$ would signify the frequency of the wave.

The pole and zero at the origin $(0, 0)$, $(-2, 0)$ and $(-2.30, 0)$ would also cancel each other out.

The pole at $(-2.19, 0)$ would decay exponentially, the rate of decay is determined by the position of the pole. The further away from the origin, the quicker it decays.

Due to all points being on the left-hand side of the graph, the system is considered stable since all responses decay over time.

Conclusion

To conclude, the system was successfully maintaining a pH of 7 using carbonic acid and responds quickly to disturbances. The system was able to achieve a settling time of 0.578 seconds with 0.48% overshoot. The system was also stable with a gain margin of 138 and a phase margin of 89.4 degrees, requiring the system to have a significant increase in gain and/or phase to reach the limit of stability.

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CO2 Assignment

GRADEMARK REPORT

FINAL GRADE

GENERAL COMMENTS

70/100

Instructor

PAGE 1

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Comment 1

Good abstract. Clearly states the problem and what you have done about it

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Comment 2

This only approximates the shape of the output against time, on its own it does not describe the pH levels themselves.

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Comment 3

Which part of the system does this relate to?

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GRADING FORM: SMU GENERIC_GJ

LIAM THOMAS

69.65

RESEARCH-INFORMED LITERATURE



Some research informed literature used, although I would have liked to see less websites and more journals and textbooks. Good introduction and background information.

9.15

KNOWLEDGE AND UNDERSTANDING



Knowledge is accurate with a good understanding of the field.

17

ANALYSIS



good strong analysis but I would have liked to see more direct links drawn between your pole zero plot and your time domain simulations.

18

PRACTICAL APPLICATION AND DEP.



A very good application of a range of methods, tools and techniques.

18.5

SKILLS FOR PROFESSIONAL PRAC.



Can communicate well. Minor spelling and grammar mistakes have let you down. But on the whole a very good piece of work.

7