ESTIMATION ON GAS DENSITY INTERNAL MODEL CONTROL (IMC) CONTROLLER USING PARTIAL LEAST SQUARES

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ESTIMATION ON GAS DENSITY INTERNAL MODEL CONTROL (IMC) CONTROLLER USING PARTIAL LEAST SQUARES

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A thesis submitted to the Faculty of Chemical and Natural Resources Engineering in partial fulfillment of the requirements for the Degree of Bachelor of Engineering

in

Chemical Engineering

Faculty of Chemical and Natural Resources Engineering
University Malaysia Pahang

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I declare that this thesis entitled "*Estimation on Gas Density Internal Model Control (IMC) Controller using Partial Least Squares*" is the result of my own research except as cited in the references. The thesis has not been accepted for any degree and is not concurrently submitted in candidature of any other degree.

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DEDICATION

Special dedication to my beloved mother and father, Wan Rokiah Bte Hj Wan Abd Raof and Abd Rahim B Mokhtar, my two sisters and brother, my grandmothers, all my family members and to the memory of my grandfathers that always inspire, love and stand besides me.

Also to my supervisors, my lecturers, my beloved friends, my fellow colleagues, and all faculty members

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ABSTRACT

This research was carried out to develop a gas density control model using Aspen Plus with Internal Model Control (IMC) method application for data generation purpose and to analyze on the process estimation using Partial Least Squares (PLS) regression. In making this process, the Air Flow Pressure Temperature (AFPT) pilot plant is use as the case study. The AFPT pilot plant is a process control training system (PCTS) that uses only air to simulate gas, vapor or steam. This AFPT pilot plant is a scale-down Real Industrial Process Plant built on 5ft X 10ft steel platform, complete with its own dedicated control panel. The AFPT pilot plant can be use to control the gas density by manipulating the pressure, flow, and temperature of the plant. This AFPT pilot plant then will be simulating using Aspen Plus to develop a gas density control model. The model will be run in steady-state and dynamic mode. In dynamic mode, the controller for all the parameters to control the gas density is putted. This entire controller then will be tune using the Internal Model Control (IMC) method in order to get its best performance. After the simulation is done, the gas density data generated from the simulation will be compared with the actual (experiment) data for validation of the data. The data shows that the error between the two data is less than 5%, meaning that the data generated from the simulation is valid. Then, this data will be use to develop a process estimator model using Partial Least Squares (PLS) method. After the estimation model is done, the mean squares error (MSE) between the estimated data and actual data is 0.001584743. This shows that the Partial Least Squares can be use as the estimator model for gas density control purpose and the estimation model developed is reliable.

ABSTRAK

Kajian ini dijalankan adalah untuk membangunkan alat kawalan ketumpatan udara menggunakan Aspen Plus dengan applikasi Internal Model Control (IMC) bagi tujuan pengumpulan data dan untuk menganalisis proses penganggaran menggunakan cara Partial Least Squares (PLS). Dalam kajian ini mesin Air Flow Pressure Temperature (AFPT) digunakan sebagai kajian kes. Mesin AFPT adalah alat latihan proses kawalan bagi simulasi udara, steam atau wap air. Mesin AFPT ini adalah diambil daripada applikasi berdasarkan industri yang sebenar dilengkapi dengan kesemua alat kawalan yang terkini. Mesin AFPT ini kemudian akan disimulasikan menggunakan applikasi Aspen Plus bagi tujuan untuk membangunkan alat kawalan ketumpatan udara. Simulasi ini dilakukan dalam dua keadaan, iaitu dalam keadaan statik dan dinamik. Dalam simulasi dinamik, alat kawalan diletakkan di setiap alat di dalam simulasi AFPT bagi tujuan memanipulasikan proses. Setiap alat kawalan ini akan dikemaskini menggunakan Internal Model Control (IMC). Ini bertujuan bagi mendapatkan prestasi kawalan yang lebih baik daripada alat kawalan terbabit. Selepas simulasi ini dijalankan, data yang terhasil akan dibandingkan dengan data daripada eksperimen. Hasil daripada perbandingan kedua-dua data ini, mendapati, perbezaan data simulasi dengan eksperimen adalah kesemuanya kurang daripada 5%. Dengan itu, ini telah menjelaskan akan kesahihan data simulasi tersebut. Data-data daripada simulasi ini seterusnya digunakan dalam membina atau membangunkan model penganggaran menggunakan cara Partial Least Squares (PLS). Selepas pembangunan model penganggaran ini dilakukan, perbezaan data daripada proses penganggaran dan data simulasi adalah 0.001584743. Perbezaan yang sangat kecil ini menunjukkan bahawa data daripada model penganggaran menggunakan cara PLS ini boleh dipercayai dan pembangunan model penganggaran telah berjaya dibangunkan bagi tujuan pengawalan ketumpatan udara.

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LIST OF ABBREVIATIONS

IMC	Internal Model Control
PLS	Partial Least Squares
AFPT	Air Flow Pressure Temperature
EOS	Equation of State
PID	proportional-integral-derivative
PI	proportional-integral
P-controller	Proportional Controller
PV	process variable
RHP	Right half-plane
AR	amplitude ratio
ISE	Integral Square Error
PCA	Principal Component Analysis
NIPALS	Non-linear Iterative Partial Least Squares
MLR	Multiple Linear Regression
SSE	sum square error
RMSE	root mean square error
MAPE	mean absolute percentage error
MSE	mean square error

EPV	explained prediction variance
PCTS	process control training system
FCV	Flow control valve
FT	flow transmitter
TIC	temperature controller
PT	pressure transmitter
DT	density indicator
K_p	steady state gain
t_D	dead time
τ_C	time constant
lv	latent variable

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CHAPTER I

INTRODUCTION

1.1 Introduction

Stringent product specification, stiff competition among manufacturers and increasingly strict regulation from local authority in the face of full capacity operation with zero accidents and emission have forced many existing plants to revamp their existing control system. More advanced control schemes have been implemented. Despite these successful implementations, many issues remained as hindrances to efficient process control. For example, the success in the implementation of any optimization scheme requires adequate performance of all control loops. This is however, sometimes hampered by two issues. The first is related to inadequacy of conventional controller used since chemical process dynamics are typically non-linear whilst the controllers are based on linear theory. The second issue is associated with process measurement, the accuracy of which is a prerequisite to successful process control.

Since measurement devices are not one of the main factors in achieving effective process control, selection of appropriate sensors and their location should be properly consider. However, not all variables in a process plant are readily to be measured on-line. Product quality variables such as chemical concentration and their composition are rarely available on-line, and are usually obtained by laboratory sample analysis. This is usually performed at long intervals and is therefore not practical to be used for process control. Over the years, various on-line measurement devices have been developed. However, many of these on-line devices are still suffering from problems due to the availability, reliability, complexity and large delays. For some quality variables, existing analytical tools used are simply unavailable for on-line applications. Hence, the development of inferential estimation and control has been advocated as one of the alternative solution to deal with measurement difficulties.

1.1.1 Background Of The Study

Gas density represents one of the gas properties which need to be set precisely in a few processes such as combustion (i.e. furnace and motor engine), polymerizations process as well as chemical industries. Research on the effect of gas density in chemical processes has been conducted in the recent decades, for examples, gas density effect on mass transfer in bubble and slurry bubble column and the effect of gas density in frequency response of gas-filled pressure transducers. Therefore gas density requires to be controlled.

In feed back control, controlled variable compared to set point and then calculated in the controller. Output of controller then adjusts the manipulated variable in order the controlled variable is equal to setting point. Control strategy can be conducted either indirect or direct. Direct control is chosen if measurement controlled variable is available, and vice versa. For example, control gas density can be conducted by controlling pressure or temperature, because based on PVT gas correlation, gas density is a function of pressure,P and tempertature,T. However, indirect strategy usually gives unfavorable performance.

Another strategy which is commonly used by inferential model instead of unavailable sensor of controlled variable. This model is developed from available measurements i.e. temperature, rate flow and pressure. The model can be developed first principal, semi-empirical or empirical model.

In this study gas density model will be developed base on Internal Model Control (IMC) method. IMC is one of the techniques that are used to determine a controller setting. The objective of IMC method is to provide a good initial controller setting that can subsequently be fine tuned on-line. The model is then implemented to PID controller of gas density with equipment based on AFTP control system (Air Flow Temperature and Pressure control system).

1.2 Identification Of Problem

In recent years, changing industrial needs and advances in computer technology had gives some impact in education, research, and practice of process control. From industrial perspective, improved in productivity, efficiency, and product quality goals generated a demand for more effective operational strategies to be applied in the production line, while the developments in digital computers and communications have revolutionized the practice of process control and allowed more advanced tools to be implemented. As a consequences, a vast broadening of the domain of what is technologically and economically achievable in the application of computers to control industrial process. This domain now includes process information and data gathering, control, and online optimization, and even production scheduling and maintenance planning function.

In chemical industries, process control gives many contributions in assuring a smooth process. In industries, many of the process involve liquid, solid and gas. All the parameter involved should always be in the rightful manner. A slight miscalculation might bring to accident, loss in productivity, increase the operating cost or loss of operational time. This is where process control gives a contribution role in preventing that all the risk mention before might not happen.

There are many factors that can give an effect in a chemical process. One of the factors is the gas density. Gas density has its own effect in some chemical process, for example the gas density effect on mass transfer in bubble and slurry bubble column. Base on its importance in chemical process, research on gas density measurement is performed to measure and control the gas density in some chemical process. To control the gas density in a chemical process means to control the effect of it in the process itself. Gas density is strongly influenced by temperature and pressure; therefore there are ideas that maybe by controlling this two variables, the gas density in a process can be controlled too.

In order to control a variable in a pilot plant, a controller is needed. By introducing a controller such as cascade control or PID in a pilot plant, the gas density that is required in some process can be measured and control accurately. But, the controller design that was proposed to be use in any chemical process needs to be proven its effectiveness first. With the advance of computer technology in industry, a simulation model can help in testing the effectiveness of the proposed controller design. Therefore, in this research, a pilot plant equipment will be simulated using software to test the effectiveness of a controller design then, the gas density resulted from this controller will be estimated using Partial Least Squares (PLS) Method.

1.3 Objectives:

In this research, there are two (2) main objectives. The two objectives of this research are:

i. To develop a gas density control model using ASPEN PLUS with Internal Model Control (IMC) method application for data generation purpose
ii. To analyze on the process estimation using Partial Least Squares (PLS) method.

1.4 Scope Of The Study:

To achieve the objectives of the research, this scope of study are to be apply:

i. Develop an AFPT simulation model using ASPEN PLUS with the introduction of a controller set using Internal Model Control (IMC).
ii. Generate data from the ASPEN PLUS simulation.

iii. Validating the data from ASPEN PLUS model by comparing it with the data from the actual model (experiment)
iv. Analyze dynamic response of AFPT simulation model.
v. Analyze the process estimation using Partial Least Squares (PLS) method.

1.5 Significances Of Study

For decades, research on effect of gas density towards chemical process has been performed. Gas density has its own effect on some chemical process, such as gas density effect on mass transfer in bubble and slurry bubble column and effect of gas density in frequency response of gas-filled pressure transducers. Because of the importance of the gas density towards some chemical process, research has been done in order to control the gas density. But, gas density is hard to be controlled, therefore, it is important to develop a model that is equipped with the density control strategy. With a good control system strategy, robustness or fault in a process can be eliminated, and a more effective process can be achieved. Also, a good control system can assured in maintaining some level of desired performance. Moreover, a control strategy aims to keep the operating condition variations at a minimum, and allow the operating target to stay as close as possible to the true (optimal) maximum profit. The control system is expected to minimize the variations around the operating target (performance objective) while, in turn, shrinking the tolerable operating limits. The more advanced the control system is, the better the chances are that the plant will operate even closer to the optimum target. This gain, quantified by the move toward a more profitable regime, helps establishing the financial benefits of the control system.

CHAPTER II

LITERATURE REVIEW

2.1 Gas Density

Gas density represents one of the gas properties which need to be set precisely in a few processes such as combustion, polymerizations, as well as chemical industries. Also, density is heavily affected by temperature and pressure in many cases. By knowing the temperature, pressure, and composition, an accurate density can be calculated by using the proper Equation of State (EOS).

However, the accuracy of such an equation of state (EOS) in turn depends on the accuracy of the experimental data use to establish it. Therefore, because of this factor, to develop a references quality EOS, reliable thermodynamic property measurements of the fluids must be available. Gas density has its own effect in chemical processes. For example, the effect of gas density on mass transfer in bubble and slurry bubble column, and gas density effect on frequency response of gas-filled pressure transducers For this reason, many research has been done in order to control the gas density whether by developing a measurement device to measure the density accurately or by developing a controller to control the gas density in a desired value.

2.2 Control Law

A control signal c(t) is calculated, given the value of the error e(t) through a predefined equation:

$$c(t) = C\,[e(t)] \qquad \textbf{(2.1)}$$

The function C[.] constitutes the control law. By specifying C[.] , we are, in effect, establishing the manner which the error information is utilized by the controller. The most common functional form is the three mode proportional-integral-derivative (PID) control law.

2.2.1 Proportional Mode

This mode produces a control signal that is proportional to the error.

$$c(t) = k_c e(t) + c_b \qquad \textbf{(2.2)}$$

k_c represents the proportional gain of the controller, and defines how sensitive the controller is to errors present in the system. c_b is bias signal that corresponds to the value of control signal when error is zero. The bias signal can also be interpreted as the steady-state value of the control signal. Thus, defining the deviation variable c(t) = c(t) - c_b, and recognizing that by definition e(t) = e(t), Eq (2.2) results in the following transfer function:

$$\frac{\bar{c}(s)}{\bar{e}(s)} = g_c(s) = k_c \qquad \textbf{(2.3)}$$

2.2.2 Integral Mode

The control signal for this mode is produced by integral equation:

$$c(t) = \frac{K_C}{\tau_I} \int e(t)dt + C_b \tag{2.4}$$

The new parameter τ_I is introduced as the integral time constant or the reset time. With this mode, the controller responds effectively to errors that build up over time. This is a very important feature because even if the error is small, as long as it persists, a large control signal may be calculated, thus helping to eliminate the error quickly. The transfer function of a controller with integral mode only is:

$$\frac{\bar{c}(s)}{\bar{e}(s)} = g_c(s) = k_c\left(\frac{1}{S\tau_I}\right) \tag{2.5}$$

2.2.3 Derivative Mode

In this mode, the control signal responds to the rate of change of the error signal.

$$c(t) = k_c\tau_D \frac{de(t)}{dt} + c_b \tag{2.6}$$

A new parameter τ_D is introduced as the derivative time constant. The role of this mode is to judge the change in the error. For instance, if the error is still present but not increasing as fast, the controller may use this information ti decrease the control signal, thus possibly avoiding overly aggressive control actions. In other words, the derivatives mode introduces an anticipatory control action as it extrapolates the future status of the error. The transfer function if a controller in derivative mode is as follows:

$$\frac{\bar{c}(s)}{\bar{e}(s)} = g_c(s) = k_c(\tau_D s) \quad \textbf{(2.7)}$$

2.2.4 Three Mode Controller (PID)

The PID control law yields a three term expression where the behavior of the controller can be affected by judicious choice of three parameters. The transfer function of the PID control law can be expressed as follows:

$$\frac{\bar{c}(s)}{\bar{e}(s)} = g_c(s) = k_c\left(1 + \frac{1}{\tau_I s} + \tau_D s\right) \quad \textbf{(2.8)}$$

Common forms of the PID controller such as the Proportional Controller (P-controller) and the proportional-integral controller (PI controller) can be easily obtained by setting $\tau_I = \infty$, and $\tau_D = 0$, respectively. The PI controller is sometimes referred to as the proportional-plus-reset-time-controller.

2.2.5 Limitation Of The PID Control

PID controllers, when used alone, can give poor performance when the PID loop gains must be reduced so that the control system does not overshoot, oscillate or "hunt" about the control setpoint value. The control system performance can be improved by combining the feedback (or closed-loop) control of a PID controller with feed-forward (or open-loop) control. Knowledge about the system (such as the desired acceleration and inertia) can be "fed forward" and combined with the PID output to improve the overall system performance. The feed-forward value alone can often provide the major portion of the controller output. The PID controller can then be used primarily to respond to whatever difference or "error" remains between the setpoint (SP) and the actual value of the process variable (PV). Since the feed-forward output is not affected by the process feedback, it can never cause the control system to oscillate, thus improving the system response and stability. For example, in most motion control systems, in order to accelerate a mechanical load under control, more force or torque is required from the prime mover, motor, or actuator. If a velocity loop PID controller is being used to control the speed of the load and command the force or torque being applied by the prime mover, then it is beneficial to take the instantaneous acceleration desired for the load, scale that value appropriately and add it to the output of the PID velocity loop controller. This means that whenever the load is being accelerated or decelerated, a proportional amount of force is commanded from the prime mover regardless of the feedback value. The PID loop in this situation uses the feedback information to effect any increase or decrease of the combined output in order to reduce the remaining difference between the process setpoint and the feedback value. Working together, the combined open-loop feed-forward controller and closed-loop PID controller can provide a more responsive, stable and reliable control system.

Another problem faced with PID controllers is that they are linear. Thus, performance of PID controllers in non-linear systems (such as HVAC systems) is variable. Often PID controllers are enhanced through methods such as PID gain scheduling or fuzzy logic. Further practical application issues can arise from instrumentation connected to the controller. A high enough sampling rate, measurement precision, and measurement accuracy are required to achieve adequate control performance.

A problem with the Derivative term is that small amounts of measurement or process noise can cause large amounts of change in the output. It is often helpful to filter the measurements with a low-pass filter in order to remove higher-frequency noise components. However, low-pass filtering and derivative control can cancel each other out, so reducing noise by instrumentation means is a much better choice. Alternatively, the differential band can be turned off in many systems with little loss of control. This is equivalent to using the PID controller as a PI controller.

2.3 Model Base Design Method

If a reasonably accurate, dynamic model of the process is available, it is advantageous to base the controller design on the process model. A wide variety of model base design strategies are available for designing PID controller (Åström and Hägglund, 1995; Tan et al., 1999). This concept leads to the paradigm of model base control that advocates the use of the process model explicitly in the formulation of the control law. This naturally allows the designer to take advantage of any information provided by the model, thus creating a more intelligent control system.

2.3.1 Internal Model Control (IMC)

Most practical system are inherently non-linear to some extent in their behavior and for their cost effective, smooth, and safe operation, optimized control system based on the non-linear models are required. New artificial intelligence based techniques such as fuzzy logic, neural networks and probabilistic reasoning, are becoming more and more popular. Among these techniques, neural networks have an edge over the others, mainly because of their ability to process large amount of available data, subsequent to the development of some interpretable models for solving engineering problems. The problem becomes more computationally worse and uncontrollable when inverse of the system does not exist. The problem resolved when Neural Network based techniques such as Internal Model Control (IMC) is applied to the real system.

Internal Model Control is more comprehensive model-based design method that was developed by Morari and coworkers (Garcia and Morari, 1982; Rivera et al., 1986). The IMC approach is based on an assumed process model and relates the controller settings to model parameters in a straightforward manner. Owing to the equivalence of the two configurations, there is a direct link between the classical control structure and the IMC structure. This link can be illustrated by defining the controller $g_c(s)$ in the classical control structure and the controller c(s) in the IMC structure as follows:

$$g_c = \frac{c}{1 - c\tilde{g}}, \quad c = \frac{g_c}{1 + g_c\tilde{g}} \tag{2.9}$$

The close-loop transfer functions with the IMC configuration can be derived as:

$$y(s) = \frac{c\tilde{g}}{1 + c(g - \tilde{g})} y_{sp}(s) + \frac{1 - c\tilde{g}}{1 + c(g - \tilde{g})} d(s) \tag{2.10}$$

2.3.2 IMC Design Procedure

The design procedure in IMC designing is first establishes if the model has any time delays or Right half-plane(RHP) zeros and decomposes the model in such a way as to create a minimum-phase part, $\breve{g}_M(s)$, and a nonminimum-phase part, $\breve{g}_A(s)$:

$$\tilde{g}(s) = \tilde{g}_A(s)\tilde{g}_M(s) \tag{2.11}$$

The nonminimum-phase part is also known as the all pass element since, by choice, the amplitude ratio (AR) of its Bode plots remain at 1 for all frequencies. Naturally, the minimum-phase element represents the invertable part of the transfer function as far as the limitations to inverting a process model is concerned. The decomposition in Equation (2.11) yields an optimal closed-loop response based on the Integral Square Error (ISE) criterion with respect to an input interest of interest. In other words, if we assume the model is a perfect representation o the process, g(s) = $\breve{g}(s)$, the close-loop error is minimized if the nominal IMC controller is chosen as

$$c(s) = \frac{1}{\tilde{g}_M(s)} \tag{2.12}$$

Therefore, this is the closest that we can get to the ideal performance of the perfect control. Although perfect control cannot be achieved, it is of great theoretical and practical interest to determine how closely this ideal can be approached. Thus, this is just an idealization of our performance expectation and not practically possible.

2.3.3 PID Tuning Using IMC Rules

The equivalence between the classical controller and the IMC controller is showed by the equation stated below:

$$g_c = \frac{c}{1 - c\tilde{g}} \tag{2.13}$$

This equation points to a rather intuitive fact, asserting that the complexity of the classical controller is determined by the complexity of the model. This is a valuable observation that underscores the point out designing controllers whose complexity commensurate with the process that they are being implemented on. This equivalence can be exploited to derive the parameters of PID controllers for a number of specific models.

2.4 Process Simulation

Simulation plays an increasingly important role in the process of designing various production facilities. It can be applied in many different fields ranging from strategic market prediction and business process simulation at the highest management level of the control hierarchy, to the production sell and process control loop simulation at the lowest control level. Generally, simulation helps in predicting future behavior of the observed system and can be used a tester for system that are being designed. Process simulation also allows engineer to predict the behavior of the process by using basic engineering relationships such as mass and energy balance, and phase and chemical equilibrium. Given reliable thermodynamic data, realistic operating conditions, and variety of equipment models, an engineer can simulate actual plant behavior. Process simulation also enables engineer to run many cases, conduct “what if” analyses, and perform sensitivity studies and optimization runs. With a simulation process, engineer can design a better plants and increase profitability in existing plants. Process simulation is useful throughout the entire lifecycle of a process, from research and development through process design and production.

2.4.1 Aspen Plus

Aspen Plus system is one of the standard software for flowsheet simulation in the processing industries. It is supported by strong databases, complete sets of modules, and flexible simulation tools. The system provides many built-in modules for simulating various processes. Aspen Plus makes it easy to build and run a process simulation model by providing a comprehensive system of online prompts, hypertext help, and expert system guidance at every step.

2.5 Process Estimation

The purpose of process estimation is to arrive at an estimator, and preferably an implementable one that could actually be used. An estimator takes the measured data as input and produces an estimate of the parameters. Engineers are usually concerned with eventual implementation, and so the material presented is geared towards discrete time systems. However, continuous time systems are also discussed in order to get the actual completeness, and because there is still the possibility for the implementations of continuous time filters. For many engineers, state estimation is interesting for at least two reasons:

i. Often an engineer needs to estimate system states in order to implement a state feedback controller. For example, the electrical engineer needs to estimate the winding currents of a motor in order to control its position. The aerospace engineer needs to estimate the attitude of a satellite in order to control its velocity. The economist needs to estimate economic growth in order to control unemployment. The medical doctor needs to estimate blood sugar levels in order to control heart and respiration rates.
ii. Often an engineer needs to estimate the system states because those states are interesting in their own right. For example, if an engineer wants to measure the health of an engineering system, it may be necessary to estimate the internal condition of the system using a state estimation algorithm. An engineer might want to estimate satellite position in order to more intelligently schedule future satellite activities. An economist might want to estimate economic growth in order to make a political point. A medical doctor might want to estimate blood sugar levels in order to evaluate the health of a patient.

It is also preferable to derive an estimator that exhibits optimality. An optimal estimator would indicate that all available information in the measured data has been extracted, for if there was unused information in the data then the estimator would not be optimal

2.5.1 Partial Least Square (PLS)

Chemical processes are monitored at frequent time intervals producing data sets consisting of many variables. Estimation method like Principal Component Analysis(PCA) and Partial Least Squares (PLS) have been shown to be one of the efficient approach in monitoring such a complex process. Process drift are not always observed directly by looking at one variable at a time. Often these drifts take place simultaneously in many variables and even though the variation may be very small it still can give a significant influence on product quality. If the process drifting towards out-of-control state can be detected early, also corrective measures can be made early enough to avoid serious out-of-control states, like bulking in an activated sludge process, and thus the efficiency of the process is maintained.

Partial Least Squares regression is one of the multivariate analysis methods. According to Wold (Wold, 1985), it is a linear system identification method that projects the input-output data down into latent space, extract a number of principal factors with an orthogonal structure, while capturing most of the variance in the original data. Reffering to this definition, it is also named as Projection to Latent Squares. PLS is built using the Non-linear Iterative Partial Least Squares (NIPALS) algorithm introduced by Wold. Details description of the PLS algorithm can be found in Geladi and Kowalski (1986).

Table 2.1: Algorithm of PLS model by Geladi and Kowalski (1986).

Step	Summary of Steps	
0	Mean center and scale X and Y	
1	Set the output scores u equal to Y	
2	Compute input weights w by regressing X	$w^T = \frac{u^T \cdot X}{u^T \cdot u}$
3	Normalize w to unit length	w = w/‖w‖
4	Calculate the input scores t	$t = \frac{X \cdot w}{w^T \cdot w}$
5	Compute output loadings q	$q^T = \frac{t^T \cdot Y}{t^T \cdot t}$
6	Normalize q to unit length	q = q/‖q‖
7	Calculate new output scores u	$u = \frac{Y \cdot q}{q^T \cdot q}$
8	Check convergence on u If yes, go to step 9, else go to step 2	

9	Calculate the input loadings p by regressing X on t	$p^T = \frac{t^T \cdot X}{t^T \cdot t}$
10	Compute inner model regression coefficient b	$b = \frac{t^T \cdot u}{t^T \cdot t}$
11	Calculate input residual matrix	$E = X - t \cdot p^T$ and $F = Y - b \cdot t \times q^T$
12	If additional PLS dimensions are necessary, replace X and Y by E and F, respectively and repeat steps 1 to 12	

2.5.2 Structure Of PLS Model

The selection input variables play a pivotal role in ensuring high accuracy of the model estimation. One important criterion is to have variables that give direct impact on the intended product quality. The inputs must also be available at high frequency. So, the first stage in the development of the estimation system is to generate data necessary from the dynamic simulation of the Air Flow Pressure Temperature (AFPT) pilot plant.

In PLS one is concerned with two blocks of data, X and Y. The objective in PLS modeling is to model X in such a way that information in Y can be predicted as well as possible. PLS maximize the covariance between matrices X and Y. It can be described with the following equations:

$$X = TP' + E, \qquad \textbf{(2.14)}$$

$$Y = UQ' + F, \qquad \textbf{(2.15)}$$

The matrix X is decomposed into a score matrix T and a loading matrix P as described in equation (2.14) above. Similarly, matrix Y is decomposed into a score matrix U and a loading matrix Q as in equation (2.15). In a n inner relation score vector ***t*** into a corresponding score vector ***u***. The first latent variable is extracted from the matrices X and Y and explains as much as possible of the variance of the matrix Y. In a similar manner second latent variable is extracted from the variance of the residual matrices which has not been described by the first latent variable, and so forth. The idea behind calculating the latent variables iteratively can be seen as a way of extracting informative features one by one. When optimal number of latent variable has been determined, what remains is considered to be contributed by noise.

In PLS, one can also calculate similar kind of regression coefficient as one does in Multiple Linear Regression (MLR). These MLR-type regression coefficients relate matrices X directly into Y.

$$Y = XB + H \tag{2.16}$$

$$B = W(P'W)^{-1} (\mathrm{diag}\ (d)\ Q')' \tag{2.17}$$

Symbol H represents the residuals. Size of matrix B for MLR-type regression coefficients equals to number of X-variables times the number of Y-variables. In equation (2.17), diag (d) stands for the matrix with cross term equal to zero and diagonal elements equal to element of vector d. This mean that vector q is multiplied by the corresponding regression coefficient d for every latent variable.

MLR-type regression coefficients, B and loading weights W can be used to study the model. In PLS, loading weights are orthogonal while the loadings are not. Orthogonally of the loading weights is a very important feature of PLS. Thus a highly redundant set of variables can be represented by a much smaller set of latent variables. Weight are use because the decomposition in PLS is rotated in order to maximize covariance between X and Y. By studying loading weights one can see how important the variables in each of latent variable. Large positive or negative weight value indicates that the corresponding X-variable is highly correlated with values in score matrix U and hence with matrix Y.

Correlation between two or more variables can be verified by looking at the loading weights. Often there mat be a set of variable groupings. Similarly, one can look for the object groupings. Objects are projected into the plane (hyper plane) defined by the latent variable scores T (or U). Score value gives a new coordinate along the latent variable axis. Object with resembling features are close to one another.

The notation of the inner relation is written in Equation (2.18).

$$\text{Inner relation:} \qquad U = TB \qquad \textbf{(2.18)}$$

The procedure of determining the scores and loadings vector is carried out sequentially from the first factor to the *f*th factor. Scores and loading vectors for each factor is calculated from the previous residual matrices as shown in Equation (2.19) and (2.20), where initially $E_0 = X$ and $F_0 = Y$.

$$\text{For X,} \qquad E_f = E_{f-1} - T_f\, P_f^T \qquad \textbf{(2.19)}$$

$$\text{For Y,} \qquad F_f = F_{f-1} - U_f\, Q_f^T \qquad \textbf{(2.20)}$$

Calculation of the inner and outer relations is performed until the last factor, f or when residual matrices are below certain threshold. The algorithm of the PLS model is attached in Table 2.1, while Figure 2.1 illustrated the PLS model schematically.

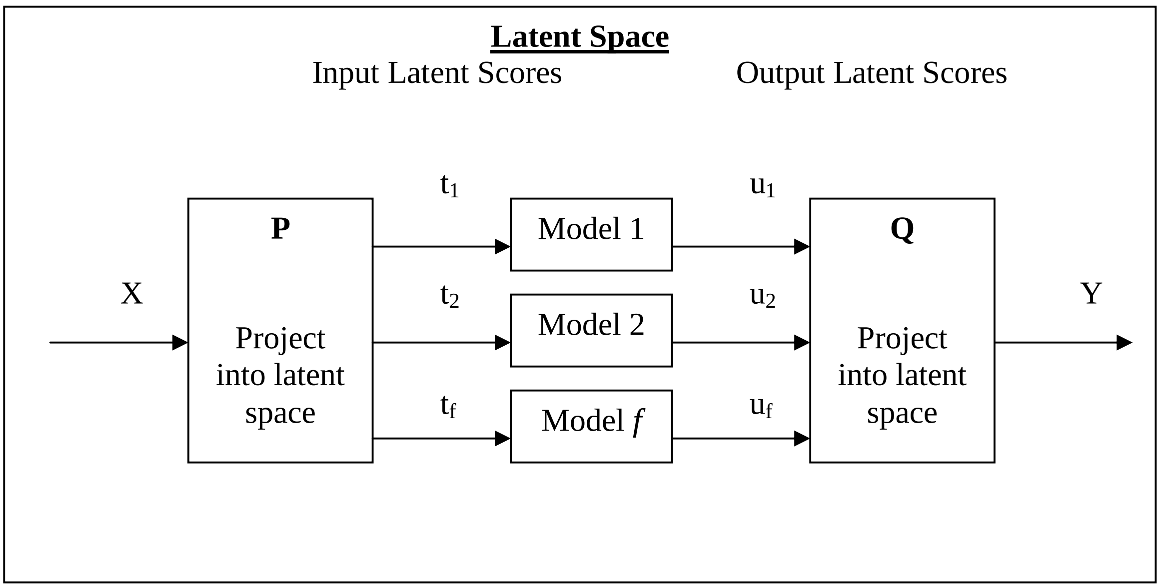


Figure 2.1 Schematic of the PLS model (Adebiyi and Corripio, 2003)

2.5.3 Model Development

In this section, development of the inferential estimator based on PLS model is described. The procedure of the PLS model development is as follows:

i. Measurable secondary measurements were selected as input variables of the model
ii. Several sets of data were prepared for training and validation
iii. Data sets were pre-processed using appropriate method
iv. The model was trained using sets of data generated.
v. Performance of the model was investigated. When the performance was not satisfactory, the dimension used in the model was adjusted until the lowest MSE was achieved.
vi. The final model was finally formulated using adjusted dimension and applied for off-line estimation

The procedure shown above can be illustrated in Figure 2.2

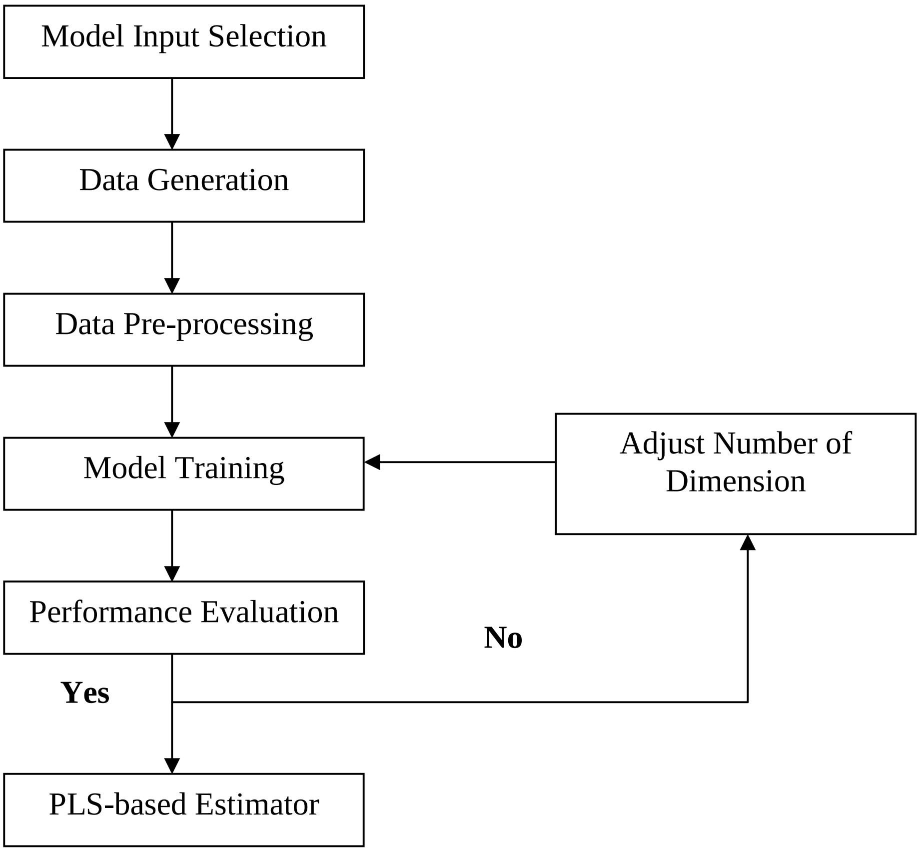


Figure 2.2 Procedure of formulating PLS-based estimator

2.5.4 Data Pre-processing

In order to ensure the model consistency, data pre-processing was implemented in this estimator model. The implementation of data pre-processing also prevents the latent variable from being biased towards variables with larger magnitude. In this work, data pre-processing step can be divided into two parts, i.e., mean-centering and scaling of variables. The data was tailored in mean-centered form prior to scaling. Generally, there are three ways to treat the variables (Geladi and Kowalski, 1986):

i. No scaling is needed when all variables in a block are measured in the same units
ii. Variance scaling is utilized as the variables are measured in different units

iii. Assigning smaller weights to variables with less importance as well as influence on the model

For convenience and simplification, variance scaling was selected among the above method. Mean and variance scaling can be carried out using the following equation:

$$x_m = (x - \bar{x}) / \sigma_x \tag{2.21}$$

Where

x represents the original data;

x_m represents the mean-scaled data;

$\bar{x}$ represents the mean value;

σ_x represents the standard deviation.

2.5.5 Model Training and Validation

In general, the most important and easiest way to evaluate the performance of a model is to measure the estimation accuracy. The estimation accuracy can be defined as the different between the actual and estimated values. Some of the approaches of measuring the accuracy is sum square error (SSE), root mean square error (RMSE) and mean absolute percentage error (MAPE). But the most frequently used is the mean square error of prediction (MSE) (Zhang and Lennox, 2004). The calculation of MSE is shown in Equation (2.22).

$$MSE = \frac{1}{N} \sum_{i=1}^{N} (x_i - \hat{x}_i))^2 \tag{2.22}$$

Where

x is the measurement of the product composition;

$\hat{x}$ is its estimation value;

N is the number of measurement.

In addition, explained prediction variance (EPV) as shown in Equation (2.23) which describes the statistical properties of the estimation model was also computed. EPV of X indicates how much of the X block is used in the estimation model and EPV of Y indicates how far the Y block has been estimated.

$$EPV = \left\{ 1 - \frac{\sum_{n=1}^{N} (x(n) - \hat{x}(n))^2}{\sum_{n=1}^{N} (x(n) - \bar{x})^2} \right\} \times 100\% \qquad \textbf{(2.23)}$$

Where

x is the measurement of the product composition;

$\bar{x}$ is the mean value of measurement;

$\hat{x}$ is its estimation value;

N is the number of measurement.

CHAPTER III

METHODOLOGY

3.1 Introduction

This chapter will focus on the achievement of the conceptual study, simulation work, analyzing, and completion of the project. The detailed research procedure will be discussed throughout this chapter. There are several main stages in achieving the estimation of gas density IMC controller.

3.2 Research Stages

The objectives of this research are to develop an IMC gas density controller and estimated its data using Partial Least Squares (PLS) method. In achieving these objectives the methodologies were divided into several stages.

Firstly, the Air Pressure Flow Temperature Pilot Plant (AFPT) is developed using the Aspen Plus software. All the equipment that is equipped in an AFPT pilot plant is putted in the flow sheet of the Aspen Plus. Then, all the controller needed in an AFPT pilot plant also is applied in the simulation. Test run the simulation whether it can be simulated or not.

Secondly, all the parameter needed to run the experiment like temperature, flow, and pressure is measured using thermodynamic properties and material and energy balances. After all the input that is needed is confirmed, the simulation is run in nominal state (without the application of the Internal Model Control (IMC) method). The simulation is run in its steady-state. Then, after all the data in steady-state is generated and recorded, the entire controller in the AFPT simulation is implemented with the Internal Model Control (IMC) method. After the controller is set, the simulation is run again, this time with the application of the Internal Model Control (IMC). The simulation is run in two conditions, first in steady-state then in dynamic mode. All the data generated in both steady-state and dynamic mode is recorded.

Thirdly, the data generated from the simulation is compared with the data from the actual AFPT pilot plant (experiment). The data is validated by the mean square error (MSE) between the two sets of data. If the error is too large, let say in more than 30%, then the data from the simulation is not valid. But, if the percentage error is small, then the data from the simulation is valid.

After the validation of the data, the dynamic response from the simulation is analyzed using Partial Least Squares Method (PLS). Using the PLS method, it can estimate the gas density data from the IMC controller for control propose.

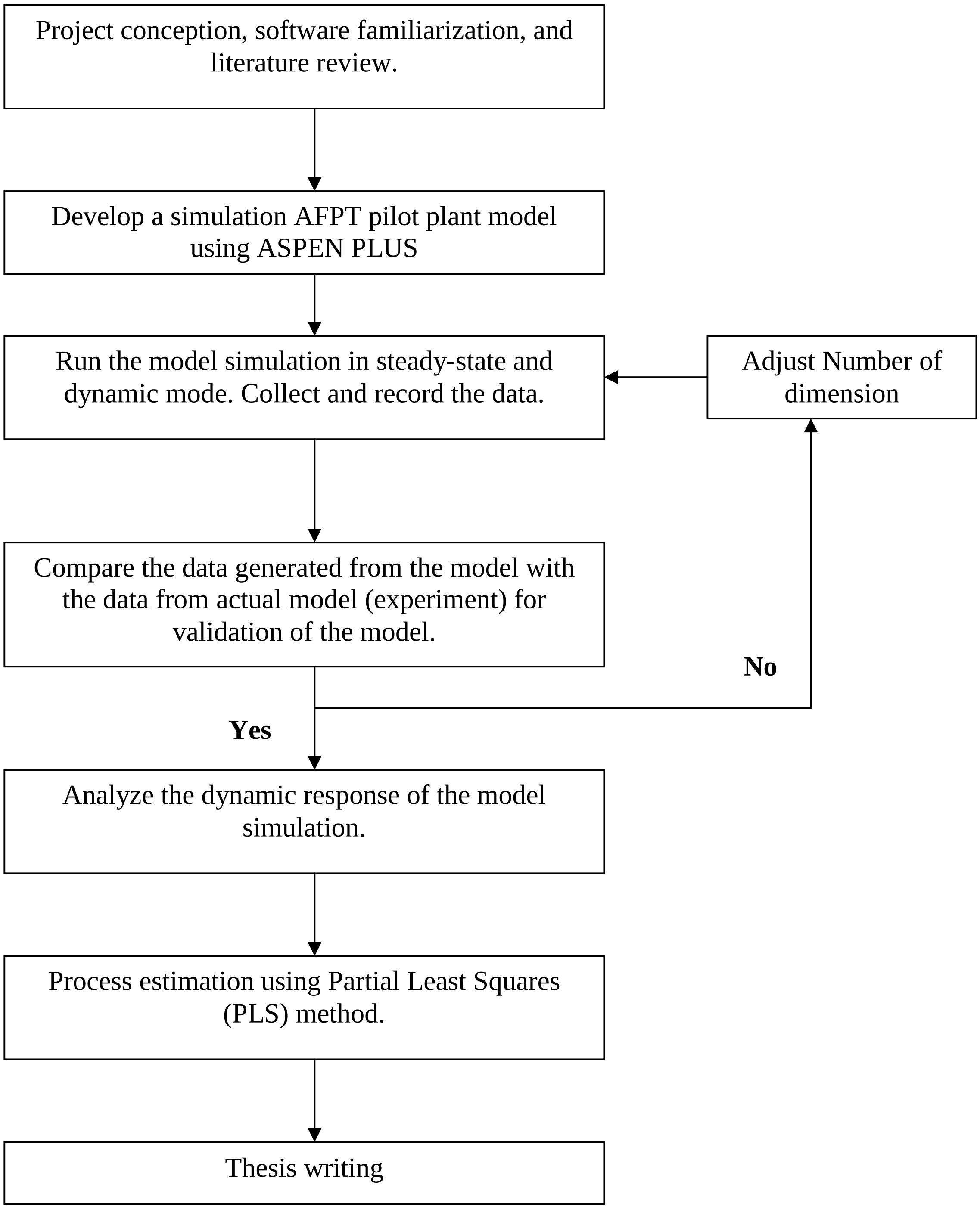


Figure 3.1: Methodology flowchart

3.3 Overall Methodology

3.3.1 Project Conception, Software Familiarization, and Literature Review.

i. Preliminary discussions – general briefing by supervisor undergraduate research project. This involved discussion on company background, process description, structure, and general operating system.
ii. Software familiarization – a general reading of the software to be studied with
appropriate method that are using for the system in the plant.
iii. Detailed process description has been providing.

3.3.2 Develop a Simulation AFPT Pilot Plant Model using ASPEN PLUS

i. By using ASPEN PLUS software, the simulation of Air Flow Pressure Temperature (AFPT) pilot plant with the application of Internal Model Control (IMC) is developed.
ii. All the control system that was needed in the AFPT pilot plant must be place in the simulation diagram.

3.3.3 Run The Model Simulation in Steady-State and Dynamic Mode. Collect and Record The Data.

i. After all the input is confirm, the simulation is run in steady-state and dynamic mode.
ii. All the data generated from this simulation process is recorded.

3.3.4 Compare The Data Generated From The Model With The Data From Actual Model (experiment) For Validation of the Model.

i. All the data that has been recorded is compared with the data recorded from the actual model (experiment) by calculating the percentage error between the two data.
ii. Both sets of data are compared. If, the percentage error is larger than 5%, then data recorded from the simulation model is unreliable and the simulation model that was developed is not valid. If the data is not valid, then the simulation has to be done again.
iii. If the data is valid (which is the percentage error is less than 5%), then the data is reliable and can be used for the next procedure.

3.3.5 Analyze the Dynamic Response of the Model Simulation.

The data from the simulation will be used to analyze the dynamic response from the simulation model.

3.3.6 Process Estimation using Partial Least Squares (PLS) Method.

Estimation of gas density IMC controller from the data generated from the process is made using the Partial Least Squares (PLS) method for control propose.

3.3.7 Thesis Writing

All the results, findings, conclusions and recommendation from the research are documented in the thesis writing.

3.4 Research Tools

Several tools have been used throughout this research. There are two main tools that were used, and that was the ASPEN PLUS software and MATLAB software.

3.4.1 ASPEN PLUS

Aspen Plus system is one of the standard software for flow sheet simulation in the processing industries produced by Aspentech. It is supported by strong databases, complete sets of modules, and flexible simulation tools. The system provides many built-in modules for simulating various processes. Aspen Plus makes it easy to build and run a process simulation model by providing a comprehensive system of online prompts, hypertext help, and expert system guidance at every step. In this research, Aspen Plus software was use to develop the simulation model for AFPT pilot plant. For steady-state simulation, ASPEN PLUS version 12.1 is used, while for dynamic state simulation, ASPEN PLUS DYNAMIC version 12.1 is applied.

3.4.2 MATLAB

MATLAB is a mathematic analysis package produced by Mathworks. This program enables immediate access to high numerical computing and extended with interactive graphical capability. The entire estimation task was performed using MATLAB Version R2007A. In this research, MATLAB software is used for estimation process using Partial Least Squares (PLS) method.

CHAPTER IV

SIMULATION MODEL DEVELOPMENT

4.1 Gas Densitometer / Gas Density Measurement

Gas density measurement devices (densitometer) have been developed using some methods. Generally, densitometer is made based on tuning fork technology (resonance frequency) and calculated from temperature and pressure measurement with different strategies. A sensor technology for measuring and monitoring gas density based on tuning fork technology was developed by Zeizel et al (2000). It comprises a pair of tuning forks oscillating at their resonance frequency. One oscillator is exposed to the gas to be monitored, the other one is used for comparison and temperature compensation. Exposure to gas leads to a shift in the resonance frequency proportional to the gas density.

Thuries and Dupraz (1997) developed method and a system for determining the density of an insulating gas in an electrical apparatus based on temperature and pressure measurement. The method is conducted in the following steps; the temperature is computed by adding reference temperature (outside apparatus) and temperature rise of the apparatus, the gas pressure inside apparatus is measured, the density of gas then computed based on equation of state the gas, $\rho = F(T,P)$.

Beehler and Medin (2003) invented method for determining air density. The method consists of three actions, first action is action determining and storing nominal air density (calculated based on ideal gas correlation) and nominal fan parameter. Second action is increasing fan input until the known pressure has been reached. The present air density is then calculates from fan parameter and nominal density. Sprague (2005) proposed process density meter based on differential pressure and temperature through the pipeline.

4.2 Gas Virial Equation of State

In general, density is one of gas physical properties in which it is very much dependant on the pressure and temperature of the given process under consideration, as illustrated in the PVT correlation (in Poling, et.al, 2001; Smith, et.al, (2001):

$$PV = Z \frac{m}{M} RT \tag{4.1}$$

therefore, density $\rho = \frac{m}{V} = \frac{1}{Z}\frac{MP}{RT}$ (4.2)

where Z = 1 for ideal gas and for real gas $Z \neq 1$, and were expressed in many forms (see polling et al (2001)), an example, the Z is described by virial equation of state as in equation (4.3) below.

$$Z = 1 + B\left(\frac{P}{RT}\right) + \left(C - B^2\right)\left(\frac{P}{RT}\right)^2 + ... \tag{4.3}$$

$$Z = 1 + \frac{B}{V} + \frac{C}{V^2} + ... \tag{4.4}$$

Where the coefficient B, C, … are the second, third, … virial coefficients.

Based on equation (4.3) the simplest form of the virial equation is illustrated by equation (4.5)

$$Z = 1 + \frac{BP}{RT} = 1 + \left(\frac{BP_C}{RT_C}\right)\left(\frac{\Pr}{Tr}\right) \tag{4.5}$$

Pitzer et al proposed a second correlation, which yields values for BPc/RTc

$$\frac{BPc}{RTc} = B^0 + \omega B^1 \tag{4.6}$$

So, equation (4.5) become:

$$Z = 1 + B^0 \frac{\Pr}{Tr} + \omega B^1 \frac{\Pr}{Tr} \tag{4.7}$$

where $B^0 = 0.083 - \frac{0.422}{Tr^{1.6}}$ and $B^1 = 0.139 - \frac{0.172}{Tr^{4.2}}$ (4.7a)

$$\Pr = \frac{P}{Pc} \text{ and } Tr = \frac{T}{Tc} \tag{4.7b}$$

Where Tc and Pc are critical temperature and pressure, respectively.

Equation (4.7) can as described as:

$$Z = 1 + \frac{0.083Tc}{Pc}\frac{P}{T} - \frac{0.422Tc^{2.6}}{Pc}\frac{P}{T^{2.6}} + \omega\frac{0.139Tc}{Pc}\frac{P}{T} - \omega\frac{0.172Tc^{5.2}}{Pc}\frac{P}{T^{5.2}} \tag{4.8}$$

Or $$Z = 1 + a\frac{p}{T} + b\frac{P}{T^{2.6}} + c\frac{P}{T^{5.2}} \tag{4.8a}$$

Where $a = \frac{Tc}{Pc}(0.083 + \omega 0.139)$, $b = -\frac{0.422Tc^{2.6}}{Pc}$, and $c = -\omega\frac{0.172Tc^{5.2}}{Pc}$ (4.8b)

4.3 Air Flow Pressure Temperature (AFPT) Pilot Plant.

In this research, Air Flow Pressure Temperature (AFPT) pilot plant is used as a case study. Air Flow Pressure Temperature (AFPT) pilot plant is a process control training system (PCTS) that uses only air to simulate gas, vapor or steam. This AFPT pilot plant is a scale-down Real Industrial Process Plant built on 5ft X 10ft steel platform, complete with its own dedicated control panel. The process equipment and process instrumentation are real Industrial Process type. The plant is constructed in accordance to industrial process plant standard and practices, with fail-safe features. For example, the air heater cannot be turned ON unless there is enough air flow in the pipeline. The process flowrates are at commercial production flowrates, using pipes and not tubings. Air is readily available from a compressor. It provides the simple gas physical processes where the measurement and control of their important variables of flow, temperature and pressure can be studied. This pilot plant consists of an electric heater, a flow meter and 3 vessels.

4.3.1 AFPT Air Temperature Control

The inlet air is heated at the electric heater and the heated air flows into pipeline PLI (or automatically into pipeline PLII if the air flow rate through PLI is too low). Heated air from the heater can flow into pipeline PLI (or pipeline PLII) via two flow paths:-

1. Via the Flow control valve (FCV91), cooling vessel C90, vessel T91 and vessel T92A.
2. Via a parallel pipeline (pipeline PLII) from the heater directly into pipeline PLI, by-passing flow control valve (FCV91), cooling vessel C90, vessel T91 and vessel T92A.

There are three basic process control systems found in this plant for air temperature control:

1. Single Loop PID Temperature Control: TE91/TT91 - TIC91 - TCY90/Heater
2. Single Loop PID Temperature Control: TE92/TT92 - TIC92 - TCY90/Heater
3. ON/OFF Temperature Control: TE92/TT92 - TIC910 – Power Supply to Heater
4. Temperature Auto-Selector Control:TE91/TT91 - TIC91 - TCY90/Heater
   TE92/TT92 - TIC92 - TCY90/Heater

4.3.2 AFPT Air Flow Control

The flowrates of the air in this pilot plant is control using the flow controller. All this controller is located at the many pipelines that the air might passes through. The error in flowrates is detected from the orifices that will detect the pressure differences in the pipeline, and then the controller will calculate the error in the flowrates and corrected it according to its setpoint. There is various flow controls in the AFPT pilot plant.

At the process pipeline PL1 are:

a. FT91 : multivariable air mass flow transmitter, with

  i. Integral orifice plate FE91
  ii. Differential Pressure transmitter DPT911
  iii. Absolute pressure transmitter PT911
  iv. RTD/Temperature Transmitter (TE911/TT911)

b. FI911 : Variable Area Flowmeter (or Rotameter)
The calibration Temperature and Pressure is tagged at the Flowmeter.

The PID mass flow control system consists of the following in feedback:

FIC91-FCY91/PP/FCV91

Where:

FIC91 : Flow PID Controller

FCY91: Current-to-Air Converter

PP : Pneumatic Positioner, with By-passs

FCV91: Flow Control Valve, Air-to-Close (ATC)

4.3.3 AFPT Air Pressure Control

There are 3 pressure vessels in this AFPT pilot plant, there are cooling vessel C90, vessel T91 and vessel T92A. This 3 vessels act as a pressure control final elements. The gauge pressures at vessels T91 and T92 or its discharge Pipeline are measured by their respective gauge pressure transmitters PT91 and PT92. Note that PT92 can be connected to either one of the following tapping points viz at T92 or at the discharge pipeline of T92. The vessel T92 and T92A are interconnected with a large interconnecting pipe so that their pressure and pressure response are usually the same. Hence T92 + T92A behave like a 1-Capacity process of double tank volume.

There are five basic process control loops found in this plant for Air Pressure Control system.

1. ON/OFF Air Pressure Control: PT92-PIC90-PSV90/PCV90
2. PID Air Pressure Control, Single Loop: PT911-PIC911-FCY91/PP-FCV91
3. PID Air Pressure Control, Single Loop, Single Capacity or Pipeline: PT92-PIC92-PCY91/PP-PCV91
4. PID Air Pressure Control, Single Loop, Multi-capacities: PT91-PIC91-PCY91/PP-PCV91
5. PID Air Pressure Control, Cascade: PT91-PIC91-PIC92-PCY91/PP-PCV91 (PT92)

4.4 AFPT Model Development

In this research one of the scopes of study is to simulate AFPT pilot plant model using Aspen Plus. To build a model of an AFPT pilot plant, it is important to simulate the AFPT pilot plant as precise as possible. All the control system, instrument, and equipment in the AFPT pilot plant has to be known. As mention before, an AFPT pilot plant consist of an electric heater, a flowmeter, vessels, temperature controller, flow controller, and pressure controller. This can be simplified as figure 4.1 below:

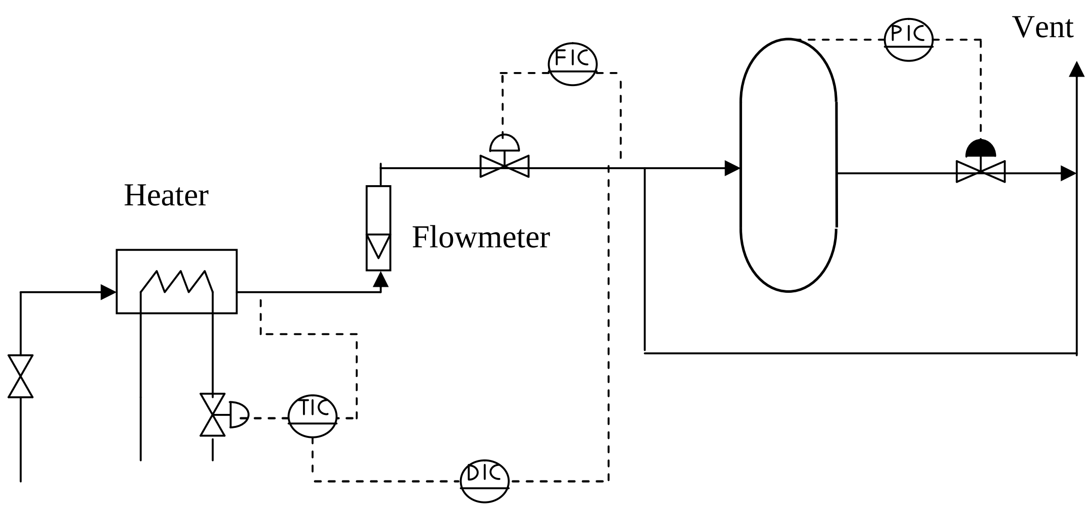


Figure 4.1: Block diagram of an AFPT pilot plant

Now that the structure of the AFPT pilot plant is known, the development of the AFPT pilot plant can be developed accordingly using Aspen Plus version 12.1.

4.4.1 Aspen Plus AFPT Simulation (steady-state)

In this section, the simulation of the AFPT pilot plant in steady state is described. First of all, the only chemical component that is use in this simulation is air. Air that is flowed into the AFPT pilot plant comes from the compressor. Its pressure is 40 psia and the temperature is 25 ^{0}C. Air from the compressor then is brought into the electric heater, and then it flows through the flowmeter before it gets into the pressure vessels. In this research, the pressure vessel used is vessel T91. The temperature controller that will be referring to as reference is TIC91A, while for pressure controller is PT911, and for flow controller FT91. The air gas density for the process is calculated and indicated by the density indicator DT91.

The simulation is run in nominal state of condition. For the nominal condition the following condition is taken for air in the heater, flowmeter, and vessels:

Heater setpoint : 100 ^{0}C
Flow setpoint : 35 kg/hr
Pressure setpoint : 46 psia

However, there was some modification which is needed in making this simulation from the real plant. From PVT correlation, with pressure 40 psia the air temperature is 154 ^{0}C, and then in the simulation a cooler is installed before heater. Another modification, liquid stream from bottom vessel is set up to zero by a controller to avoid negative mass flow rate (in real plant, there is no liquid product).

The process is then run in steady state where there will be no changes at any time. In this simulation, no controller will be put in the model because of its steady state condition where there will be no changes in setpoint or any disturbances occur. The flow diagram for the steady-state simulation using Aspen Plus is illustrated in Appendix A1.

4.4.2 Aspen Plus AFPT Simulation (dynamic mode)

After the simulation in steady-state mode is done, the simulation will be continued with the dynamic mode simulation. In dynamic mode, the steady-state simulation from Aspen Plus is converted to dynamic mode using Aspen Plus Dynamic. In Aspen Plus Dynamic, the controller for the equipment like electric heater, flowmeter, and pressure vessels is putted in its place. The position of the equipment in dynamic mode is the same as in the steady-state mode. The difference is just the presence of controller. The controller is needed because in dynamic mode, there will be disturbance that can occur, and the controller will react against this disturbance to achieve the process setpoint. The flow diagram for the dynamic mode simulation using Aspen Plus is illustrated in Appendix A2.

4.4.2.1 Determination of Steady State Gain, Dead Time, and Time Constant

Before the simulation on the dynamic condition can be run, the steady state gain(K_p), dead time(t_D), and time constant(τ_C) of the controller has to be determined. The steady state gain (K_p), dead time(t_D), and time constant(τ_C)for all the controller is determined first using the data from the steady state process. Using this data and doing some calculation, the steady state gain(K_p), dead time(t_D), and time constant(τ_C) is calculated. This is done by using the equation in table 4.1:

Table 4.1: Equation for calculating the controller steady state gain(K_p), dead time(t_D), and time constant(τ_C).

Process Parameter	Equations
1. Steady State Gain, K_p	$K_p = \dfrac{\Delta\text{Output\%(at steady state)}}{\Delta\text{Input\%(at steady state)}} = \dfrac{\left(\dfrac{B_2 - B_1}{B_\infty - B_o}\right)}{\left(\dfrac{M_2 - M_1}{M_\infty - M_o}\right)}$
3. Dead time, t_D	$t_D = t_1 - t_0$
4. Time constant, τ_C	It is the time $(t_2 - t_1)$. When the measure variable, $B_3 = (63.2\% \times (B_2 - B_1)) + B_1$

4.4.2.2 Tuning Using the Internal Model Control (IMC) Method.

The Air Flow Pressure Temperature (AFPT) pilot plant uses the PID controller in their control system. Usually, a controller performance can be influence by their controller settings. With difference controller settings, difference controller performance is achieved. A controller setting can be adjusted to achieve the desired performance, a procedure referred to as controller tuning. For the simulation in dynamic mode, after all the steady state gain(K_p), dead time(t_D), and time constant(τ_C) for all the controller is determined, the controller needs to be tuned in order to achieve its desired performance. In this research, the Internal Model Control (IMC) controller is used as the tuning method.

By tuning the controller settings, the steady state gain(K_p), dead time(t_D), and time constant(τ_C) determined before will changed into a new value. This is done by using the Internal Model Control (IMC) tuning relation as showed in table 4.2.

Table 4.2: Internal Model Control (IMC) tuning relation

Controller Type	**Gain (K_c)**	**Reset (τ_I)**	**Rate (τ_D)**
PID when $\frac{\lambda}{t_D} > 0.8$ $\lambda > \frac{\tau_c}{10}$	$\frac{1}{K_p}\frac{2\left(\frac{\tau_c}{t_D}\right)+1}{2\left(\frac{\lambda}{t_D}\right)+1}$	$\frac{t_D}{2}+\tau_c$	$\frac{\tau_c}{2\left(\frac{\tau_c}{t_D}\right)+1}$

.

After all the calculation has done, the new gain (Kc), reset (τ_I), and rate (τ_D) is in table 4.3:

Table 4.3: Gain, reset, rate for flow, temperature, and pressure controller

Controller	**Gain, K_c**	**Reset, τ_I (seconds)**	**Rate, τ_D (seconds)**
Flow	0.90	11	0.1
Temperature	0.53	10	0.1
Pressure	1.70	30	0.1

4.5 Load Disturbance and Setpoint Change.

In the steady-state simulation, the simulation is done in nominal condition where the temperature is set at100^{0}C, the flow is 35 kg/hr, and the pressure is 46 psia. Now, to test the performance of the gas density controller which has been tuned using Internal Model Control (IMC) method in the dynamic mode, this temperature, flow, and pressure needs to be changed. The change in this parameter is called load disturbance and setpoint change. This load disturbance and setpoint change is need to be done in order to test the controller weather it can act towards the disturbance to achieve the actual setpoint or not. It is to test the effectiveness of the controller itself. The change of the parameter will not be too drastically like 50% or 100% change. The parameter will be increase and decrease to 5% from its nominal condition. When these parameters are changed, the simulation in the dynamic mode can be run. The change in temperature, pressure, and flow from its nominal condition for this research is as follows:

Table 4.4: Process Variables for the research

Pressure (psia)	**Temperature(^{o} C)**	**Flow (kg/hr)**
46	90	15
46	90	25
46	90	35
46	90	45
46	100	15
46	100	25
46	100	35
46	100	45
46	110	15
46	110	25
46	110	35
46	110	45
40	90	35
42	90	35
46	90	35
48	90	35
50	90	35
40	100	35
42	100	35
46	100	35
48	100	35
50	100	35
40	110	35
42	110	35
46	110	35
48	110	35
50	110	35

4.6 Analyze the Dynamic Response

After the simulation had been done, the dynamic response of the process by the controller has to be done. This is to assured and checked whether the controller can react towards the disturbance that had occurred. This is also to see the performance of the controller that had been tuned by the Internal Model Control (IMC). A good controller is a controller that can react towards the disturbance in a short interval time. The dynamic response need to be analyzed first is whether the controller can react towards the disturbance and lead the process variables to its setpoint. If a controller cannot bring the controller to achieve its setpoint, then controller is considered as failed to achieve its objective. A controller is introduced in a process to control the process as it should be. Therefore, the controller must be effective and reliable in assuring that the process in its rightful condition. Another dynamic response need to be analyzed is the time interval for the controller to react towards disturbance rejection and set point tracking. If the time taken by the controller is long, then it shows that the controller performance was not at its best. This is because of the long time it needed in the process. In industrial practices, time consuming is critical. The less time the controller need to react towards the disturbance the better the controller is. Figure 4.2-4.7 below show all the dynamic response produced by the IMC controller from the simulation of the Air Flow Pressure Temperature (AFPT) pilot plant.

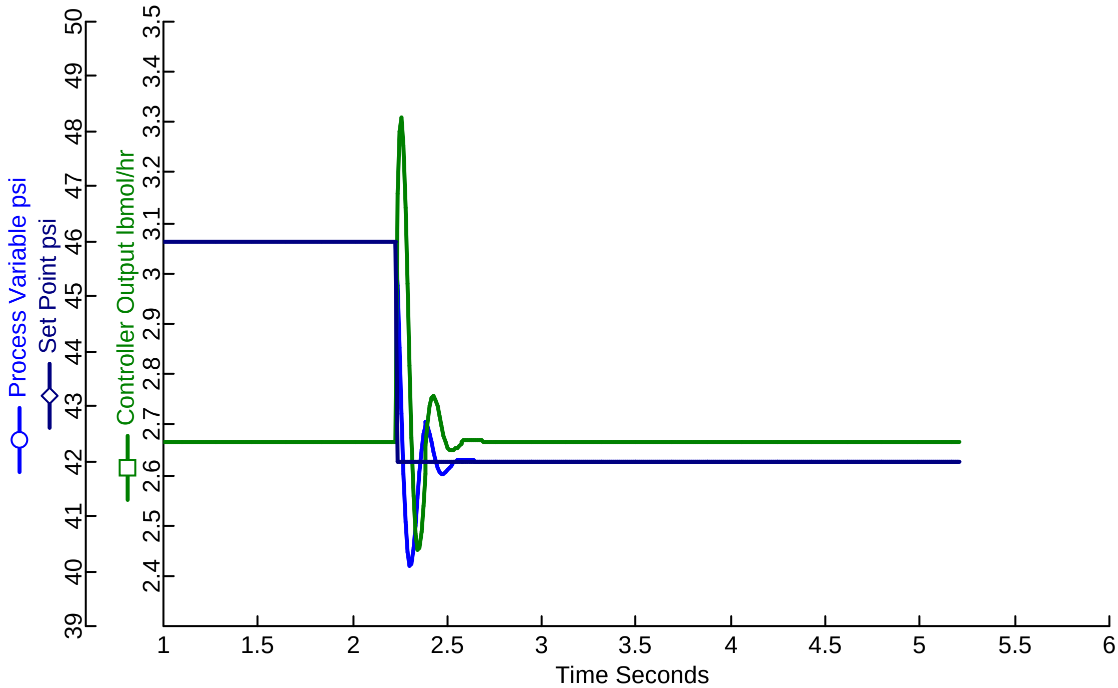


Figure 4.2 : Dynamic response when setpoint change to 42 psia

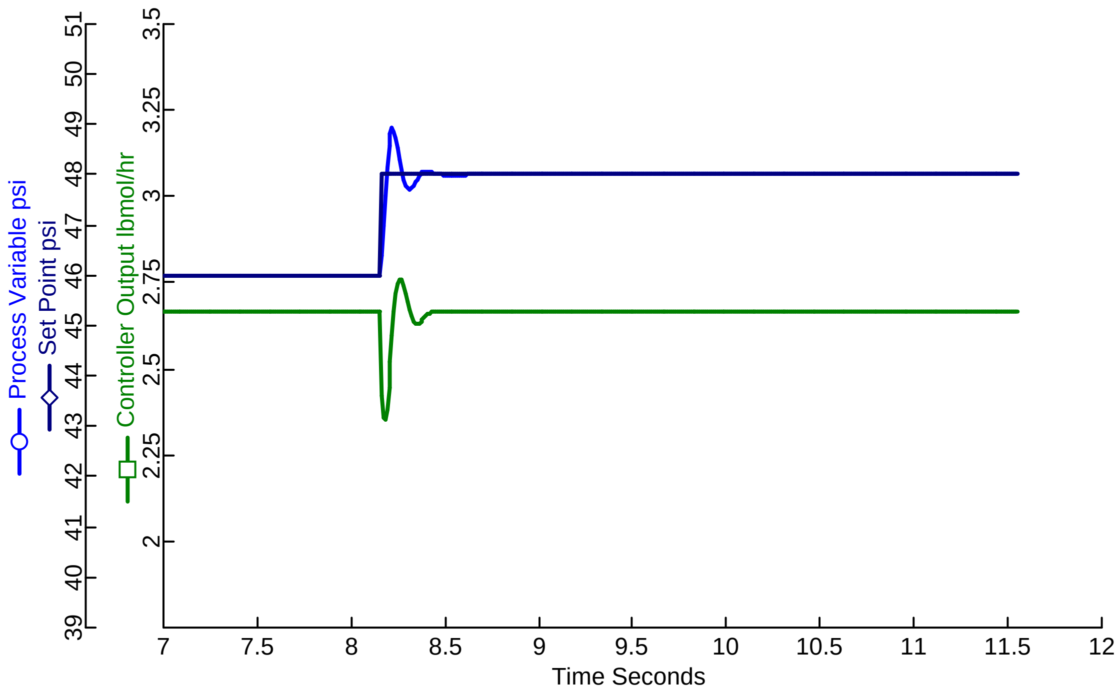


Figure 4.3: Dynamic response when setpoint change to 48 psia

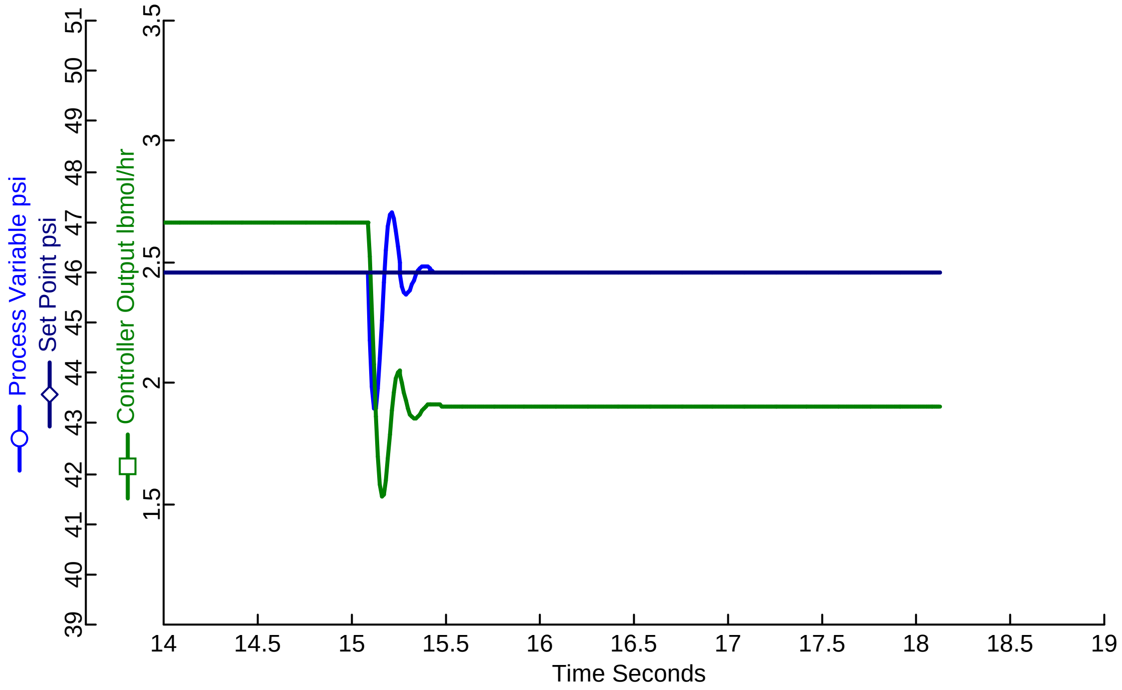


Figure 4.4: Dynamic response when load change to 25 kg/hr

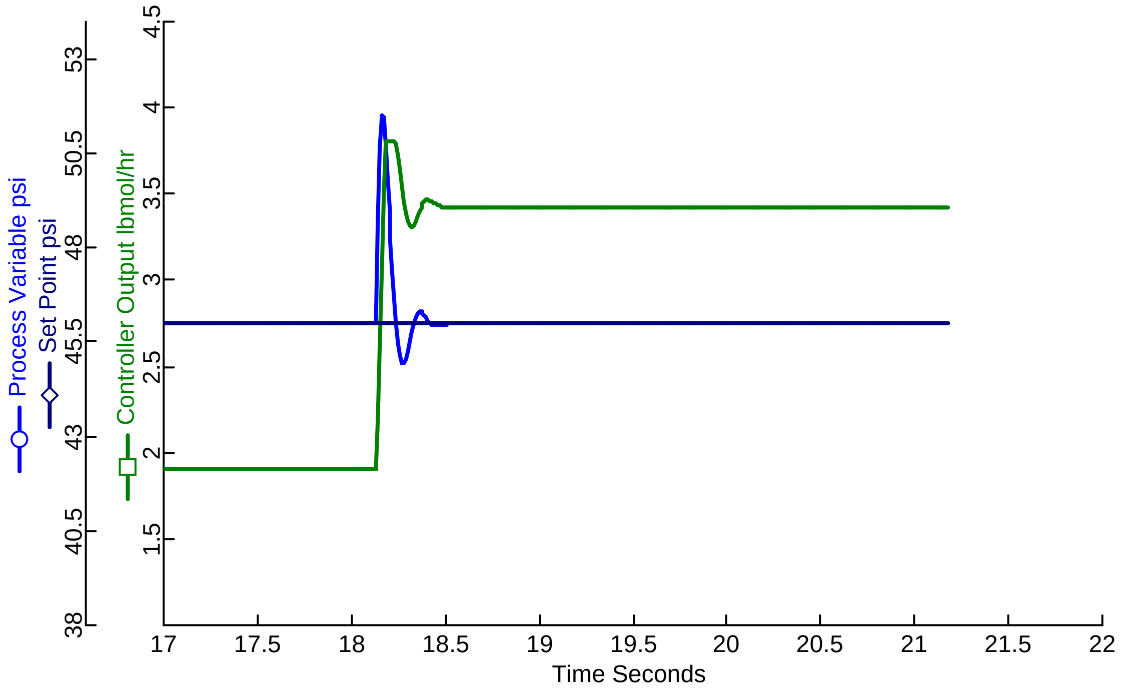


Figure 4.5: Dynamic response when load change to 45 kg/hr

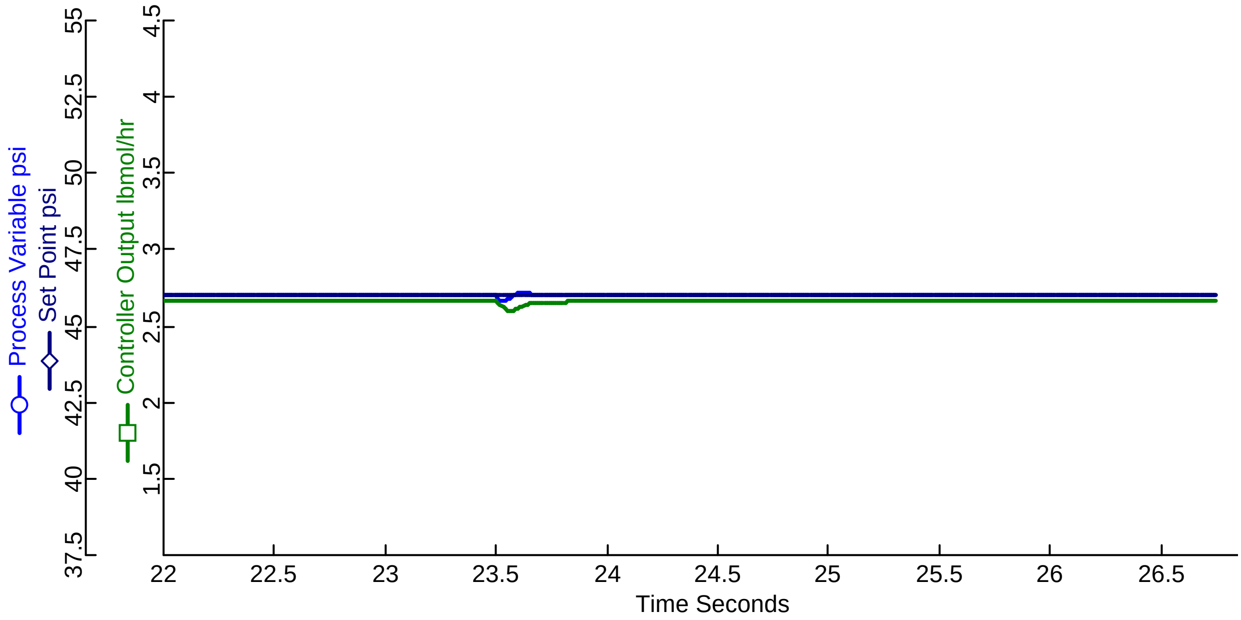


Figure 4.6: Dynamic response when load change to 90^0C

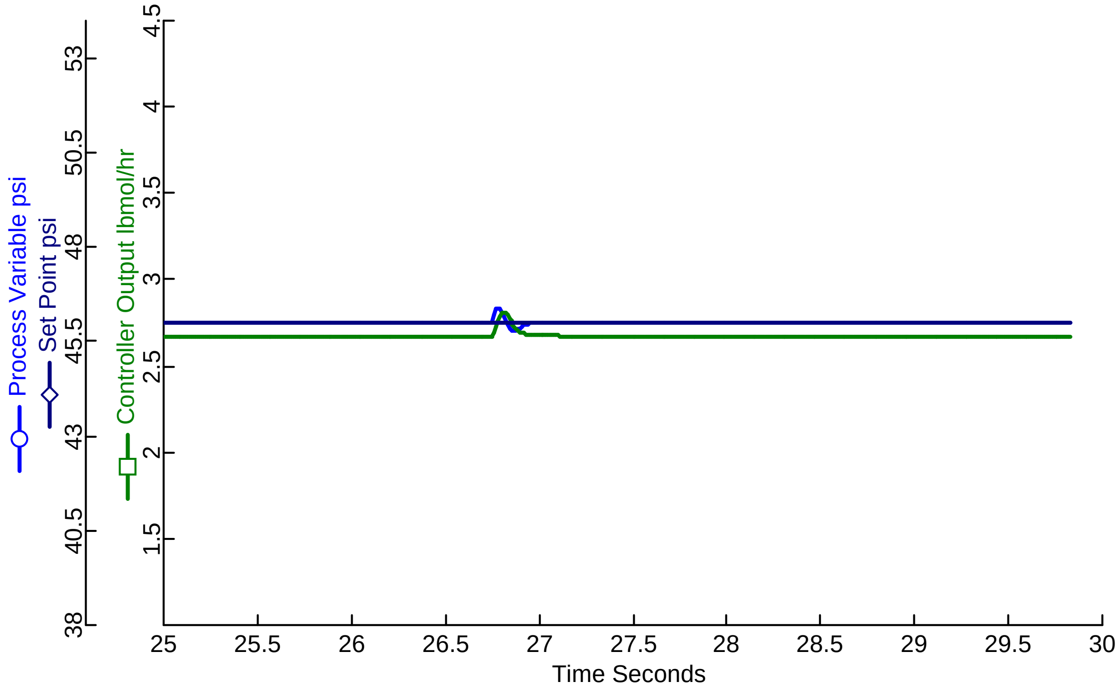


Figure 4.7: Dynamic response when load change to 110^0C

The setpoint changes come in the form of pressure changes, while for the disturbances changes comes in the form of temperature and flow rates changes. From the entire graph showed, the controller can react towards the disturbances and setpoint changes. The controller can react toward the disturbance by guiding the process variable toward its setpoints and also react in a very short period of time. This proved that the controller that had been tuned using the Internal Model Control (IMC) before can be use in order to control the process variable in the process. The small time interval taken by the controller to react towards the disturbances to achieve its setpoint showed the good performances of the controller itself. The controller just consumes a small amount of time to reacts towards disturbances rejection. This had proved that the Internal Model Control method can be used to tune the controller in order get a better performances from the controller. From all the response recorded here, it showed that the controller that was developed can reacts towards the disturbance and therefore can be use for control purpose in this study.

4.7 Simulation Data Validation

All the data as in table 4.4 will be used in the simulation and in actual plant for data generation purpose. The data generated here is the air gas density. After all the data has been generated, all the data generated from the simulation will be compared with the actual plant data to ensure the simulation reliability, exactness, and relevant. This is done by calculating the error between the two data. In this research, if the error is less than 5%, then the data is reliable and meaning that the simulation model is valid for data generation purpose and its process is almost precise as in the actual plant. The results for the validation between the simulation data and actual plant data are described in table 4.5.

Table 4.5: Validation data for simulation and actual plant

Density (exp)	Density (model)	% error
2.748574	2.647	3.7
3.826432	3.63521	4.99
3.41472	3.37034	1.3
3.450879	3.36996	2.34
2.658324	2.63986	0.69
3.716044	3.53735	4.81
3.307714	3.2797	0.85
3.422952	3.27937	4.19
2.600651	2.50786	3.57
3.517666	3.44464	2.08
3.318231	3.25636	1.86
3.212396	3.13099	2.53
2.692866	2.64414	1.81
2.754454	2.64659	3.92
3.147939	3.10632	1.32
3.206146	3.17233	1.05
3.254064	3.23834	0.48
2.598246	2.57303	0.97
2.722264	2.63729	3.12
3.068713	3.02277	1.5
3.142794	3.08701	1.77
3.186596	3.21547	0.91
2.534475	2.50566	1.14
2.735779	2.63081	3.84
2.966926	2.88107	2.89
3.135446	3.00618	4.12
3.142647	3.13128	0.36
Mean percentage error (%)		2.30

As was shown in table 4.5, the percentage error for all the data between simulation and actual plant is less than 5%. This proved that the simulation model that was developed can generate a data that was almost the same and accurate as data generated in the actual plant with the same parameters used. Therefore, this can be concluding that the data generated from the simulation is valid, and the simulation model developed is reliable, precise, and relevant as in the actual plant and can be used for data generation proposes.

CHAPTER V

DEVELOPMENT OF PROCESS ESTIMATOR USING PARTIAL LEAST SQUARE REGRESSION

5.1 Introduction

The lack of method in determining the gas air density has been a significant obstacle in obtaining good control and optimization solutions. Available on-line techniques densitometer such as the one based on tuning fork technology (resonance frequency), and determining the density of an insulating gas in an electrical apparatus are unfortunately both expensive and have been shown to be unreliable when applied to large scale systems. This is one of the reasons for the lack of density measurements or instruments in the plant. Processes are operated by fixing measurable variables at some known optimum conditions while inferring that the desired outcome on the product qualities follow suit. This is verified by off-line laboratory analyses of selected variables. Adjustments are made when needed. Despite its widespread use, such practices suffer from many weaknesses. Delay in analyses, varying input conditions and the nonlinear nature of the process often lead to something unintended and frequent manual adjustments by plant personnel may be needed, hence putting the plant to high human dependence.

Another way of dealing with this issue is to make use of inferential model to estimate the desired properties based on easy to measure variables. In this case, process variables such as temperature, flowrates and pressure are used to infer the non-measurable or difficult to measure primary process outputs such as gas density. Some forms of models are used to represent the relationships between these secondary variables with the primary variables of interest. A convenient way is to formulate input-output configuration such that when given the inputs, i.e., in this case the secondary measurements, the corresponding expected output can be reproduced. The estimated values are then fed into the controller for control purposes. For practical implementation, the estimator should provide reliable prediction of the unmeasured.

A particularly promising approach is the application of multivariate statistical process control techniques such as Principal Component Analysis (PCA) and Partial Least Squares (PLS). In this research, Partial Least Squares (PLS) analysis will be use as the process estimator to estimate the gas density IMC controller.

5.2 Partial Least Squares Regression (PLS)

Partial least squares regression is one of the multivariate analysis methods. It is a linear system identification method that projects the input-output data down into a latent space, extracts a number of principal factors with an orthogonal structure, while capturing most of the variance in the original data (Wold, 1985). Referring to this definition, it is also named as Projection to Latent Structures. PLS model is built using the Non-linear Iterative Partial Least Squares (NIPALS) algorithm introduced by Wold (1985). Details description of the PLS structure can be found in Geladi and Kowalski(1986).

The structure of PLS model has been elaborated in Chapter 2. The procedure of developing PLS-based inferential model takes the following stages which are:

i. Generate quality input-output for PLS model training.
ii. Pre-process the data by scaling the data around zero average and unit variance. Split the data into training and validation set.
iii. Train the model using “least-squares method”
iv. Evaluate the performance of the model using validation data. If unsatisfactory, back to Step (iii) and repeat the procedure.

v. Save the optimum model parameters for implementation.

Data having sufficient excitation was used for model training and validation. Before the training and validation procedure, the data were scaled around zero average and unit variance. Following the scaling stage, the input and output data were ready to be used for model training and validation. The NIPALS algorithm of PLS and the validation steps shown in previous chapter, was coded in MATLAB programming language for the purpose of model development. The model was first trained using a training data in order to obtain associate score factors and followed by model validation.

The number of dimension referred to how much iteration that is required for the residual matrices to reach certain threshold. It was determined using cross validation technique, where the training was stopped when the prediction error of the testing set reached a minimum and started to increase. It is noted the prediction error reached the early stopping criteria of cross-validation before the 20th dimension but it did not give the optimum performance. This was due to the problem of local minima. In order to avoid convergence at local minima, the iteration was allowed to continue until the optimum model was obtained where it gave the lowest MSE for the validation data. Hence, the optimum number of dimension was 20 and the relevant parameters were summarized in list of table below:

Table 5.1: Mean square error (MSE) for partial least squares at latent variable = 1

lv	**z**	**traning mse**	**validation mse**
1	11	4.74E-02	4.74E-02
1	12	4.89E-02	4.89E-02
1	13	3.79E-02	3.79E-02
1	14	3.68E-02	3.68E-02
1	15	3.79E-02	3.79E-02
1	16	3.71E-02	3.71E-02
1	17	3.59E-02	3.59E-02
1	18	2.56E-02	2.56E-02
1	19	2.40E-02	2.40E-02
1	**20**	**1.21E-02**	**1.21E-02**

Table 5.2: Mean square error (MSE) for partial least squares at latent variable = 2

lv	**z**	**traning mse**	**validation mse**
2	11	3.21E-02	3.21E-02
2	12	3.42E-02	3.42E-02
2	13	2.33E-02	2.33E-02
2	14	2.37E-02	2.37E-02
2	15	2.37E-02	2.37E-02
2	16	2.10E-02	2.10E-02
2	17	1.71E-02	1.71E-02
2	18	9.00E-03	9.00E-03
2	19	8.17E-03	8.17E-03
2	**20**	**2.60E-03**	**2.60E-03**

Table 5.3: Mean square error (MSE) for partial least squares at latent variable = 3

lv	z	traning mse	validation mse
3	11	2.46E-02	2.46E-02
3	12	2.68E-02	2.68E-02
3	13	1.64E-02	1.64E-02
3	14	1.81E-02	1.81E-02
3	15	1.83E-02	1.83E-02
3	16	1.42E-02	1.42E-02
3	17	1.26E-02	1.26E-02
3	18	7.25E-03	7.25E-03
3	19	6.74E-03	6.74E-03
3	**20**	**1.86E-03**	**1.86E-03**

Table 5.4: Mean square error (MSE) for partial least squares at latent variable = 4

lv	z	traning mse	validation mse
4	11	2.06E-02	2.06E-02
4	12	2.29E-02	2.29E-02
4	13	1.33E-02	1.33E-02
4	14	1.49E-02	1.49E-02
4	15	1.55E-02	1.55E-02
4	16	1.17E-02	1.17E-02
4	17	1.13E-02	1.13E-02
4	18	6.74E-03	6.74E-03
4	19	6.44E-03	6.44E-03
4	**20**	**1.70E-03**	**1.70E-03**

Table 5.5: Mean square error (MSE) for partial least squares at latent variable = 5

lv	z	traning mse	validation mse
5	11	1.81E-02	1.81E-02
5	12	2.02E-02	2.02E-02
5	13	1.16E-02	1.16E-02
5	14	1.32E-02	1.32E-02
5	15	1.37E-02	1.37E-02
5	16	1.10E-02	1.10E-02
5	17	1.08E-02	1.08E-02
5	18	6.58E-03	6.58E-03
5	19	6.01E-03	6.01E-03
5	**20**	**1.66E-03**	**1.66E-03**

Table 5.6: Mean square error (MSE) for partial least squares at latent variable = 6

lv	z	traning mse	validation mse
6	11	1.61E-02	1.61E-02
6	12	1.87E-02	1.87E-02
6	13	1.05E-02	1.05E-02
6	14	1.23E-02	1.23E-02
6	15	1.29E-02	1.29E-02
6	16	1.04E-02	1.04E-02
6	17	1.04E-02	1.04E-02
6	18	6.40E-03	6.40E-03
6	19	5.80E-03	5.80E-03
6	**20**	**1.61E-03**	**1.61E-03**

Table 5.7: Mean square error (MSE) for partial least squares at latent variable = 7

lv	z	traning mse	validation mse
7	11	1.41E-02	1.41E-02
7	12	1.72E-02	1.72E-02
7	13	8.60E-03	8.60E-03
7	14	1.14E-02	1.14E-02
7	15	1.23E-02	1.23E-02
7	16	9.92E-03	9.92E-03
7	17	1.00E-02	1.00E-02
7	18	6.22E-03	6.22E-03
7	19	5.65E-03	5.65E-03
7	**20**	**1.58E-03**	**1.58E-03**

Table 5.8: Mean square error (MSE) for partial least squares at latent variable = 8

lv	z	traning mse	validation mse
8	11	1.33E-02	1.33E-02
8	12	1.64E-02	1.64E-02
8	13	7.21E-03	7.21E-03
8	14	1.10E-02	1.10E-02
8	15	1.21E-02	1.21E-02
8	16	9.74E-03	9.74E-03
8	17	9.86E-03	9.86E-03
8	18	6.13E-03	6.13E-03
8	19	5.50E-03	5.50E-03
8	**20**	**1.61E-03**	**1.61E-03**

Table 5.9: Mean square error (MSE) for partial least squares at latent variable = 9

lv	z	traning mse	validation mse
9	11	1.27E-02	1.27E-02
9	12	1.81E-02	1.81E-02
9	13	6.21E-03	6.21E-03
9	14	1.08E-02	1.08E-02
9	15	1.19E-02	1.19E-02
9	16	9.61E-03	9.61E-03
9	17	9.71E-03	9.71E-03
9	18	6.04E-03	6.04E-03
9	19	6.12E-03	6.12E-03
9	**20**	**1.61E-03**	**1.61E-03**

Table 5.10: Mean square error (MSE) for partial least squares at latent variable = 10

lv	z	traning mse	validation mse
10	11	1.24E-02	1.24E-02
10	12	2.02E-02	2.02E-02
10	13	5.96E-03	5.96E-03
10	14	1.06E-02	1.06E-02
10	15	1.17E-02	1.17E-02
10	16	9.37E-03	9.37E-03
10	17	9.54E-03	9.54E-03
10	18	6.46E-03	6.46E-03
10	19	6.08E-03	6.08E-03
10	**20**	**1.61E-03**	**1.61E-03**

Table 5.11: Mean square error (MSE) for partial least squares at latent variable = 11

lv	z	traning mse	validation mse
11	11	1.19E-02	1.19E-02
11	12	2.10E-02	2.10E-02
11	13	5.63E-03	5.63E-03
11	14	1.05E-02	1.05E-02
11	15	1.16E-02	1.16E-02
11	16	9.26E-03	9.26E-03
11	17	1.01E-02	1.01E-02
11	18	6.44E-03	6.44E-03
11	19	6.08E-03	6.08E-03
11	**20**	**1.61E-03**	**1.61E-03**

Table 5.12: Mean square error (MSE) for partial least squares at latent variable = 12

lv	z	traning mse	validation mse
12	11	1.11E-02	1.11E-02
12	12	2.01E-02	2.01E-02
12	13	5.48E-03	5.48E-03
12	14	1.02E-02	1.02E-02
12	15	1.14E-02	1.14E-02
12	16	1.01E-02	1.01E-02
12	17	1.01E-02	1.01E-02
12	18	6.44E-03	6.44E-03
12	19	6.08E-03	6.08E-03
12	**20**	**1.61E-03**	**1.61E-03**

Table 5.13: Mean square error (MSE) for partial least squares at latent variable = 13

lv	z	traning mse	validation mse
13	11	1.05E-02	1.05E-02
13	12	1.90E-02	1.90E-02
13	13	5.33E-03	5.33E-03
13	14	9.92E-03	9.92E-03
13	15	1.33E-02	1.33E-02
13	16	9.98E-03	9.98E-03
13	17	1.01E-02	1.01E-02
13	18	6.44E-03	6.44E-03
13	19	6.08E-03	6.08E-03
13	**20**	**1.61E-03**	**1.61E-03**

Table 5.14: Mean square error (MSE) for partial least squares at latent variable = 14

lv	z	traning mse	validation mse
14	11	9.61E-03	9.61E-03
14	12	1.79E-02	1.79E-02
14	13	5.08E-03	5.08E-03
14	14	1.18E-02	1.18E-02
14	15	1.29E-02	1.29E-02
14	16	9.98E-03	9.98E-03
14	17	1.01E-02	1.01E-02
14	18	6.44E-03	6.44E-03
14	19	6.08E-03	6.08E-03
14	**20**	**1.61E-03**	**1.61E-03**

Table 5.15: Mean square error (MSE) for partial least squares at latent variable = 15

lv	z	traning mse	validation mse
15	11	8.87E-03	8.87E-03
15	12	1.66E-02	1.66E-02
15	13	6.16E-03	6.16E-03
15	14	1.12E-02	1.12E-02
15	15	1.29E-02	1.29E-02
15	16	9.98E-03	9.98E-03
15	17	1.01E-02	1.01E-02
15	18	6.44E-03	6.44E-03
15	19	6.08E-03	6.08E-03
15	**20**	**1.61E-03**	**1.61E-03**

Table 5.16: Mean square error (MSE) for partial least squares at latent variable = 16

lv	z	traning mse	validation mse
16	11	8.54E-03	8.54E-03
16	12	2.13E-02	2.13E-02
16	13	6.08E-03	6.08E-03
16	14	1.13E-02	1.13E-02
16	15	1.13E-02	1.13E-02
16	16	9.98E-03	9.98E-03
16	17	1.01E-02	1.01E-02
16	18	6.44E-03	6.44E-03
16	19	6.08E-03	6.08E-03
16	**20**	**1.61E-03**	**1.61E-03**

Table 5.17: Mean square error (MSE) for partial least squares at latent variable = 17

lv	z	traning mse	validation mse
17	11	8.92E-03	8.92E-03
17	12	2.08E-02	2.08E-02
17	13	6.08E-03	6.08E-03
17	14	1.13E-02	1.13E-02
17	15	1.29E-02	1.29E-02
17	16	9.98E-03	9.98E-03
17	17	1.01E-02	1.01E-02
17	18	6.44E-03	6.44E-03
17	19	6.08E-03	6.08E-03
17	**20**	**1.61E-03**	**1.61E-03**

Table 5.18: Mean square error (MSE) for partial least squares at latent variable = 18

lv	z	traning mse	validation mse
18	11	8.92E-03	8.92E-03
18	12	2.08E-02	2.08E-02
18	13	6.08E-03	6.08E-03
18	14	1.13E-02	1.13E-02
18	15	1.29E-02	1.29E-02
18	16	9.98E-03	9.98E-03
18	17	1.01E-02	1.01E-02
18	18	6.44E-03	6.44E-03
18	19	6.08E-03	6.08E-03
18	**20**	**1.61E-03**	**1.61E-03**

Table 5.19: Mean square (MSE) error for partial least squares at latent variable = 19

lv	z	traning mse	validation mse
19	11	8.92E-03	8.92E-03
19	12	2.08E-02	2.08E-02
19	13	6.08E-03	6.08E-03
19	14	1.13E-02	1.13E-02
19	15	1.29E-02	1.29E-02
19	16	9.98E-03	9.98E-03
19	17	1.01E-02	1.01E-02
19	18	6.44E-03	6.44E-03
19	19	6.08E-03	6.08E-03
19	**20**	**1.61E-03**	**1.61E-03**

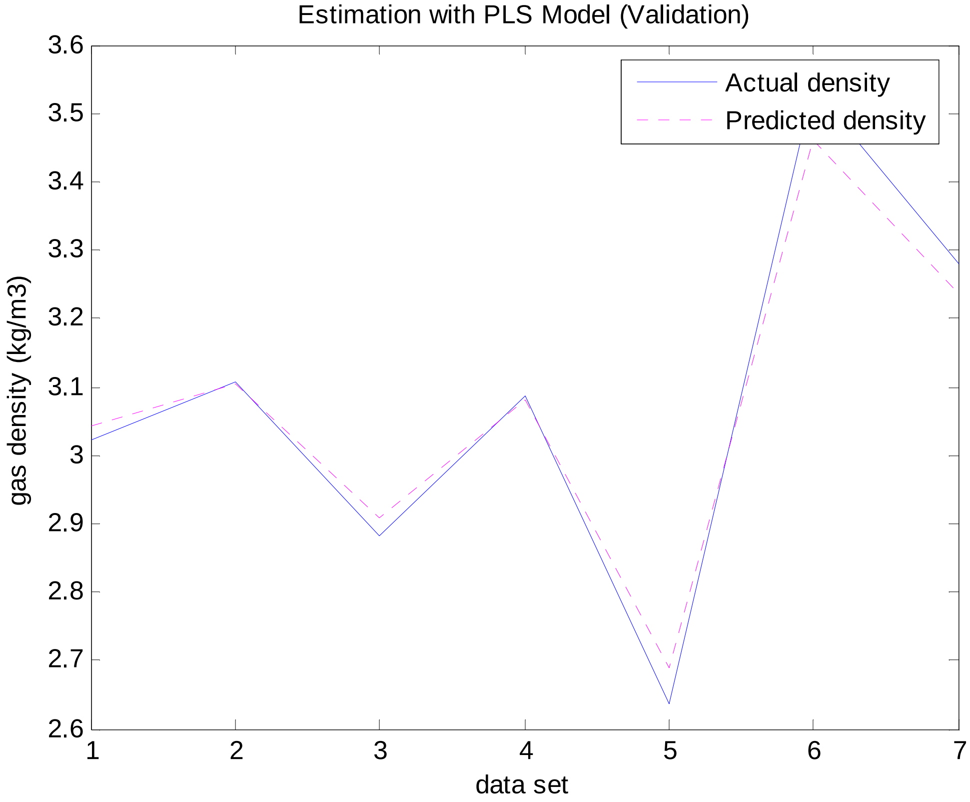
Table 5.20: Mean square error (MSE) for partial least squares at latent variable = 20

lv	z	traning mse	validation mse
20	11	8.92E-03	8.92E-03
20	12	2.08E-02	2.08E-02
20	13	6.08E-03	6.08E-03
20	14	1.13E-02	1.13E-02
20	15	1.29E-02	1.29E-02
20	16	9.98E-03	9.98E-03
20	17	1.01E-02	1.01E-02
20	18	6.44E-03	6.44E-03
20	19	6.08E-03	6.08E-03
20	**20**	**1.61E-03**	**1.61E-03**

The calculated MSE for training and validation data was same for each other for each data respectively. Based on these results, the PLS-based estimation model was considered successfully constructed. The trend of the model predictions compared to the actual output is displayed below. Here, the graph indicates the actual output and the predicted output are represented by dotted line. It is noted that the estimated output reasonably matched the actual composition in both training and validation set.

The best data is taken when the mean square error (MSE) between the actual and predicted data is lowest as was listed in table 5.1-5.20. Figure 5.1 and 5.2 showed the graph which has the lowest mean square errors (MSE) that was produces in Partial Least Squares (PLS) model estimation. After the Partial Least Squares (PLS) estimation is done, the lowest mean squares error (MSE) recorded is when latent variable, lv = 7 and dimensions, z = 20 where the mean square error (MSE) is 0.001584743.

The small error between the estimated data and actual data showed that there is not so much different between the simulation data and the data generated from PLS estimation. Therefore, this proved that the simulation model is reliable for data generation and control purposed. This also proved that the PLS model developed is a reliable model for estimation. This is base from the data that showed that the PLS model can predict the gas density with the small mean square error (MSE) when compared to the simulation data. With this very small MSE, the objective to develop a process estimator using Partial Least Squares (PLS) is well constructed.



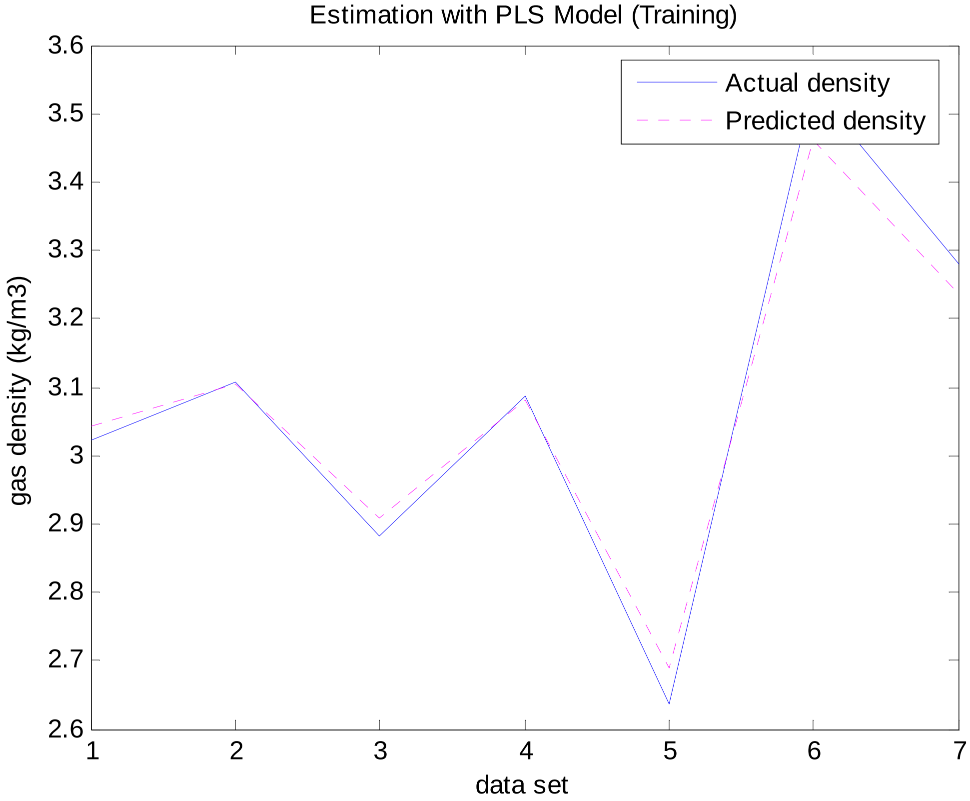


Figure 5.1: Estimation of PLS model with MSE = 0.001605057

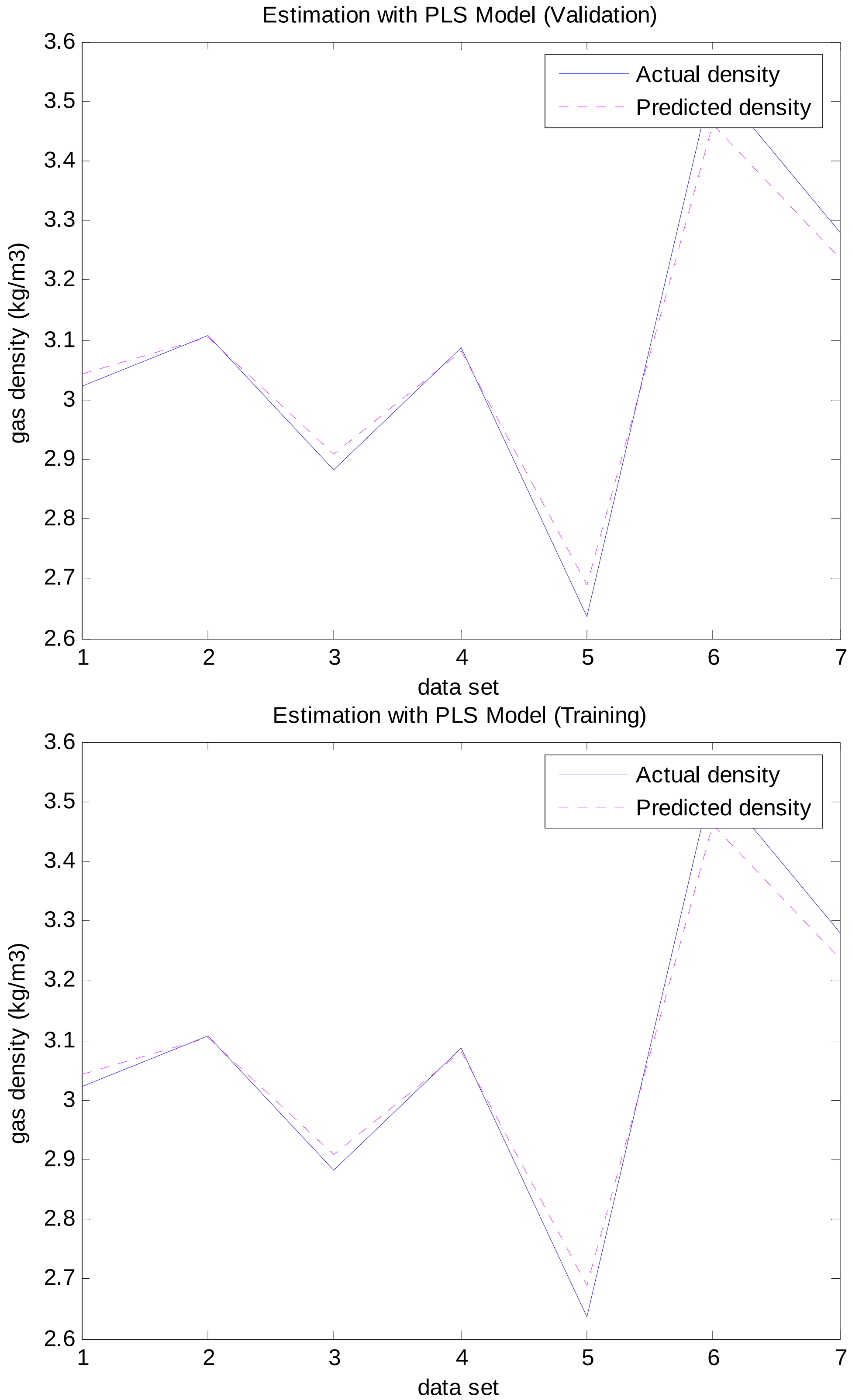


Figure 5.2: Estimation of PLS model with MSE = 0.001584743

5.3 Concluding Remark

In this chapter, the inferential estimator for the gas density IMC controller was built using a PLS model. This estimator had been performing well in the nominal condition. The robustness and accuracy of the PLS estimator were also tested in by doing the load disturbances and setpoint changes as mentioned in chapter 4. In all cases, reasonably accurate estimations were obtained. As a conclusion, the PLS proposed model is considered adequate to be used as process estimators for the estimation of gas density IMC controller.

CHAPTER VI

CONCLUSION AND RECOMMENDATION

6.1 Conclusion

Based on the results provided in this research, the conclusion that can be drawn out are as follows:

i. The AFPT pilot plant model simulation can be develop using Aspen Plus.
ii. The data from the simulation is reliable for data generation purposed.
iii. The controller can be tuned in order to get its better performances.
iv. The Internal Model Control (IMC) method is reliable method to tune the gas density controller.
v. Partial Least Squares (PLS) provide a reliable prediction as estimation.
vi. The implementation of Partial Least Squares (PLS) as estimation method on gas density IMC controller was successfully developed for control purposed.

This research has provided a development of simulation model for gas density control purpose. The tuning of the controller can be achieved with a better controller tuning. Also, the development of inferential estimation model using Partial Least Squares (PLS) based model and its application toward the gas density control.

6.2 Recommendation

Numerous additional works can be done to further improve the reliability of the inferential model. Some of the recommendations are as follows:

i. More tuning method used for tuning purpose in order to get a better understanding in the controller performances.
ii. Better understanding on the development of inferential estimator using PLS in order to measure gas density.
iii. Application to other system. The application of Internal Model Control (IMC) method is widen to other control system such as concentration or composition control system.
iv. Further research is done to get the controller towards a perfect or ideal set point tracking and disturbance rejection controller.

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APPENDIX A1

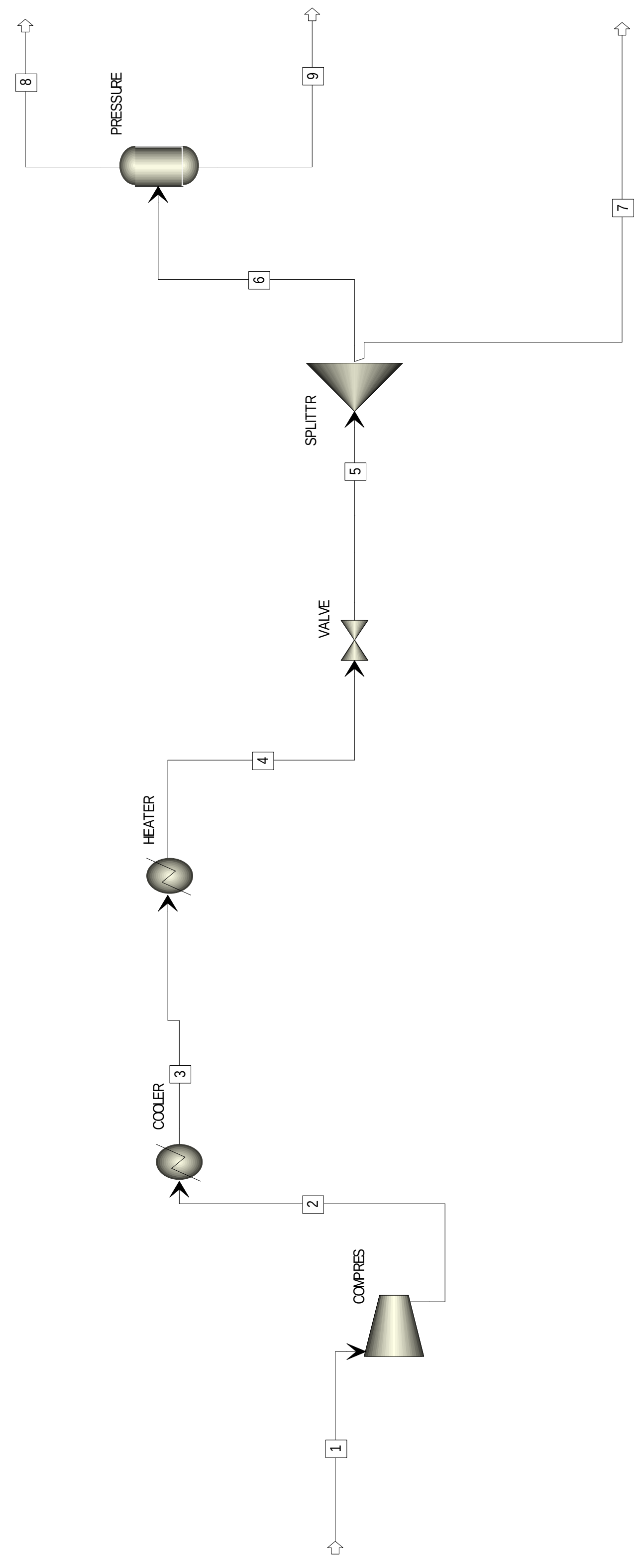

Figure A1: Simulation model for steady-state

APPENDIX A2

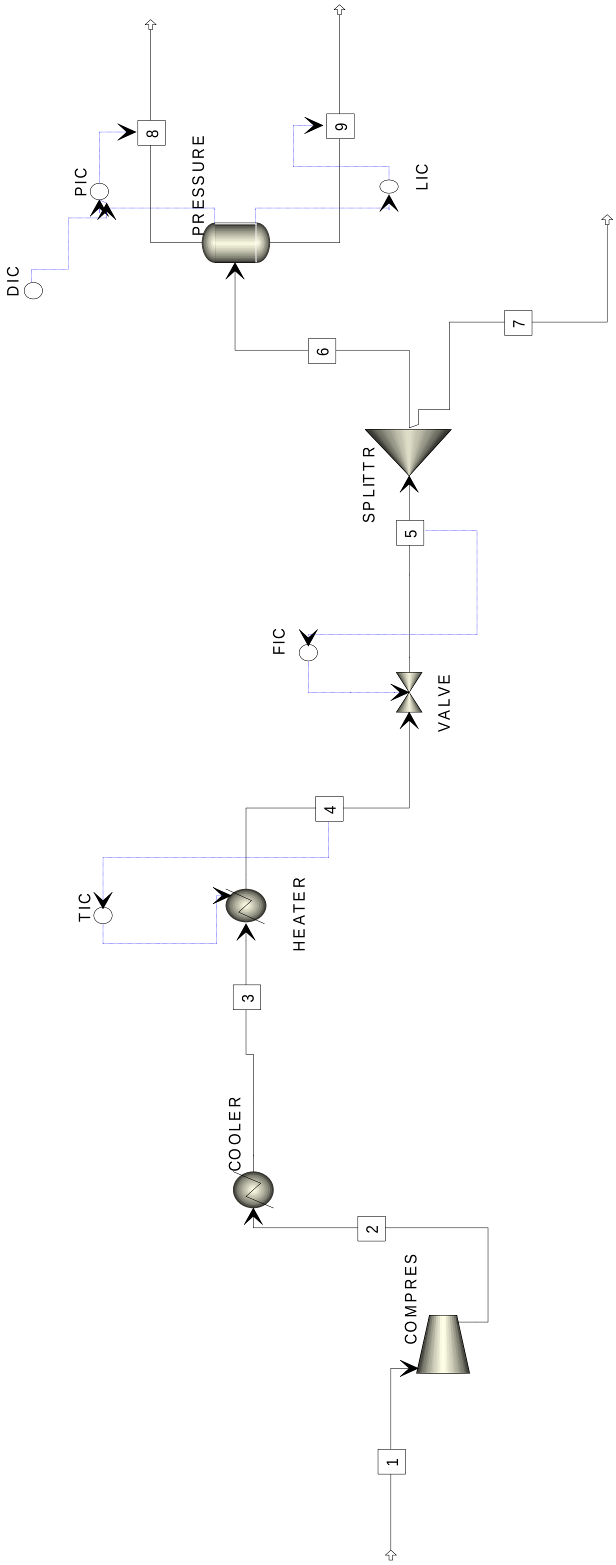

Figure A2: Simulation model for dynamic state.

APPENDIX B1

The MATLAB code for Partial Least Squares (Preparation of data)

```
function [x,y,vx,vy,m,n,CODOX]=prepdata3

load dCODOX

%raw data
[m,n]=size(CODOX);

%mean-centering and variance-scaling data
for j=1:n
   for i=1:m
      mdatat(i,j)=CODOX(i,j)-mean(CODOX(:,j));
      msdatat(i,j)=mdatat(i,j)/std(CODOX(:,j));
   end
end


% Prepare data for training
for i=1:m
   for j=1:n-1
      x(i,j)=msdatat(i,j);
      y(i,1)=msdatat(i,n);
   end
end

% Prepare data for validation
for i=1:m
   for j=1:n-1
      vx(i,j)=msdatat(i,j);
      vy(i,1)=msdatat(i,n);
   end
end

% save data1
```

APPENDIX B2

The MATLAB code for Partial Least Squares (regression)

```
function [z,theta,trmse,vlmse,nyp,nvyp]=plstr

[x,y,vx,vy,m,n,output]=prepdata3;

z=20;
[xr,yr] = wrtreg(x,y,z);
[vxreg,vyreg] = wrtreg(vx,vy,z);

lv=7;
xreg=xr;
yreg=yr;
u=yreg;

ssqx=sum(sum(xreg.^2)');
ssqy=sum(sum(yreg.^2)');

[rx,cx]=size(xreg);
w=zeros(cx,lv);

for i=1:lv

   w(:,i)=xreg'*u;
   w(:,i)=w(:,i)/norm(w(:,i));
   t(:,i)=xreg*w(:,i);
   tnew(:,i)=t(:,i)/norm(t(:,i));
   q(:,i)=yreg'*tnew(:,i);
   q(:,i)=q(:,i)/norm(q(:,i));
   unew(:,i)=yreg*q(:,i);
   p(:,i)=xreg'*t(:,i);
   p(:,i)=p(:,i)/norm(p(:,i));
   b(:,i)=tnew(:,i)'*unew(:,i);
   E=xreg-(t(:,i)*p(:,i)');
   F=yreg-(b(:,i)*tnew(:,i));
   ssq(i,1)=sum(sum(E.^2)')*100/ssqx;
   ssq(i,2)=sum(sum(F.^2)')*100/ssqy;

   xreg=E;
   yreg=F;
```

```
  u=yreg;
end

ssqdif = zeros(lv,2);
ssqdif(1,1) = 100 - ssq(1,1);
ssqdif(1,2) = 100 - ssq(1,2);
for i = 2:lv
 for j = 1:2
  ssqdif(i,j) = -ssq(i,j) + ssq(i-1,j);
 end
end
disp('  ')
disp('       Percent Variance Captured by PLS Model')
disp('  ')
disp('           ----X-Block------   ----Y-Block------')
disp('     LV#    This LV    Total    This LV    Total ')
disp([(1:lv)' ssqdif(:,1) cumsum(ssqdif(:,1)) ssqdif(:,2) cumsum(ssqdif(:,2))])

cw = t\yr;
theta=w*cw;

%training data
yp=xr*theta;

ny=(y*std(output(:,n)))+mean(output(:,n));
nyp=(yp*std(output(:,n)))+mean(output(:,n));

[c,d]=size(nyp);
for i=1:c
  for j=1:d
    nyr(i,j)=ny(z+i,j)-nyp(i,j);
  end
end
trmse=sumsqr(nyr)/c;

for i=1:c
  for j=1:d
    newy(i,j)=ny(z+i,j);
  end
end

%validate data
vyp=vxreg*theta;

nvy=(vy*std(output(:,n)))+mean(output(:,n));
nvyp=(vyp*std(output(:,n)))+mean(output(:,n));
```

```
for i=1:c
   for j=1:d
      nvyr(i,j)=nvy(z+i,j)-nvyp(i,j);
   end
end

vlmse=sumsqr(nvyr)/c;

for i=1:c
   for j=1:d
      newvy(i,j)=nvy(z+i,j);
   end
end

% save info
%show value of error
fprintf('trmse=%e, vlmse=%e\n', trmse,vlmse);

figure(1)

plot(1:((m)-z),newy,'b',1:((m)-z),nyp,':m');
ylabel('gas density (kg/m3)'); xlabel('data set')
title('Estimation with PLS Model (Training)')
legend ('Actual density','Predicted density',1)

figure(2)

plot(1:((m)-z),newvy,'b',1:((m)-z),nvyp,':m');
ylabel('gas density (kg/m3)'); xlabel('data set')
title('Estimation with PLS Model (Validation)')
legend ('Actual density','Predicted density',1)
```