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Fault modelling and diagnosis for a phthalic anhydride reactor

by

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I, J.L. Pickard (16565088), have read and understood the meaning and consequences of plagiarism as detailed in the university's Calendar 2016 Part 1.

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Abstract

Active process monitoring plays a significant role in the stable operation of chemical process plants. In such environments, there is an ever-increasing emphasis on environmentally responsible, safe and cost-effective operation. The aim of this paper is to evaluate the principal component analysis (PCA) algorithm as the basis for statistical monitoring of the phthalic anhydride reactor (PAR) system. The purpose of this investigation is to establish a suitable monitoring strategy so that detection and diagnosis of faults can be achieved.

This paper takes a case study approach. Six simulated faults are used to test the performance of the method. A conclusion about the suitability of this approach can be based on these results.

Before designing and deploying the monitoring system, a simulation capable of generating normal and fault data needs to be developed. To keep normal operation stable, a control system needs to be designed and implemented.

The objectives are as follows: The first objective is to implement and validate the closed loop PAR model. Once validated, the second objective was to design, implement and assess an improved control strategy. The third objective was to model and simulate six selected faults. The fourth objective was to develop, deploy and evaluate a process monitoring plan, allowing for detection and identification of the simulated fault scenarios.

Models taken from the literature were implemented into simulation software, followed by qualitative validation of responses to input changes. To stabilize the system, a multivariate control strategy, using multiple single loops tuned using the direct synthesis method was employed. The interaction was accounted for with trial and error detuning and fine tuning until acceptable performance and stability were achieved. To pair controlled and manipulated variables optimally, the relative gain array approach was used. Monitoring is cast into the data-driven fault diagnosis framework in which PCA is the feature extraction algorithm. Simulated normal operating condition data was used to train the model and thresholds which were then applied to simulated fault data, to detect faults and identify cause variables.

All six faults were detected and identified with near perfect performance. This, however, was attributed to the large magnitude of the faults, making them easy to detect, rather than the suitability of the PCA method to the PAR system. Therefore, it is suggested that smaller, harder to detect faults be simulated as these are likely to bring out the unique features of this method. Using the same data additional methods can also be tested to gauge the relative performance of this method.

Contents

Chapter 1

Introduction

Active monitoring is necessary for early fault detection and correction in chemical processes to avoid the dire consequences of unmanaged faults. Proper fault management ensures a safer, more environmentally friendly and more profitable process. A variety of different monitoring strategies exist, however, they vary in their suitability to different scenarios. The purpose of this study is to investigate an appropriate monitoring plan for the phthalic anhydride reactor (PAR) system. The aim of this paper is to evaluate the performance of principal component analysis PCA, as part of data driven monitoring strategy, on the PAR system.

Statistical process control was first popularized by univariate Shewhart charts in the 1920's. However, it is only with the recent and drastic increase in computing power that such methods have gained so much attention. A data-driven approach is appealing in chemical processes as it avoids the time consuming and expensive process of developing fundamental models. Furthermore, it can handle many variables and draw from data collection already taking place. PCA is selected as it considers relationships between variables which expected in chemical systems.

The first objective is to implement and validate the PAR model. The second objective is to design, implement and assess an improved control strategy. The third objective is to model six fault scenarios presented in [Kauffman, 1990]. The fourth objective is to design, implement and assess an appropriate monitoring strategy.

Performance parameters calculated from simulated data are used to determine the suitability of the method. The investigation is limited to six major faults that may occur in the system. The monitoring strategy is tested on its ability to detect faults and identify cause variables.

Normal operating and fault data need be simulated to test the performance of a strategy. The approach taken is to develop a simulation capable generating normal operation data with enough variation to characterize its underlying structure. This step requires the addition of process noise and stabilization by automated control. Additionally, the simulation must be able to capture the dynamic responses of monitored variables during faults. The normal data set is used to train a classifier which is tested with fault data on its ability to distinguish between normal and fault samples.

The structure of this report is as follows. Chapter 2 contains a literature review which provides a theoretical foundation for the methodology. The three most important themes along which the literature divides are modeling and simulations 2.1, automated process control 2.2 and statistical process control 2.3.

The objectives are presented in Chapter 3. The methodology, detailing the technical approach is presented in 4. The results generated by the methodology are then presented in 5 which are interpreted to determine whether the aim has been achieved.

To be considered successful, this study must demonstrate the success or failure of PCA as a basis for a monitoring strategy.

Chapter 2

Literature Review

This literature reviews the important principles and terminologies encountered in three main themes: modeling and simulation 2.1 , control 2.2 and statistical process control 2.3. Figure 2.1 below shows the relationship between the literature and method used in achieving the objectives stated in chapter 3.

FIGURE 2.1: Overview of literature and relation to methodology

In 2.1.1, a process description, reaction mechanism and existing control strategy, with the P& ID presented in Appendix B are given to provide context to the simulated physical system. The methodology 4.1 contains the mathematical models that describe the system.

In 2.2 control theory is reviewed, providing the basis for selecting the multivariate control strategy (2.2.1 & 2.2.2) and controlled and manipulated variable pairing 2.2.3.

In 2.3 statistical process control is reviewed, providing the basis for detection, identification, and correction of faults. A comparison between univariate and multivariate statistical process control methods is used as motivation for the selection of the multivariate class to this particular system. A general framework for data-driven process fault diagnosis in steady state systems 2.3.1 is presented, an element of which is feature extraction. The feature extraction algorithm investigated is principal component analysis (2.3.2). Finally monitoring performance parameters presented in 2.3.5 are used to quantify the success of the strategy.

2.1 Modeling and Simulation

The following literature reviews the PAR system that is developed as a benchmark system upon which monitoring performance is evaluated. Section 2.1.1 provides a physical description of the system, the nominal operating conditions and the control structure presented in [Kauffman, 1990].

2.1.1 Process description

Naphthalene (NA) can be partially oxidized to phthalic anhydride in a fluidized bed catalytic reactor at a temperature between the ranges of 500 and 633 K and a pressure of 130kPa. In addition to the desired partial oxidation of NA given in 2.1,

$$\underset{NA}{C_{10}H_8} + 4\frac{1}{2}O_2 \;\rightarrow\; \underset{phthalicanhydride}{C_6H_4(CO)_2O} + 2CO_2 + 2H_2O \tag{2.1}$$

There are three completing reactions, all of which are also exothermic:

$$\underset{naphthalene}{C_{10}H_8} + 1\frac{1}{2}O_2 \;\rightarrow\; \underset{naphthoquinone}{C_{10}H_6O_2} + H_2O \tag{2.2}$$

$$\underset{naphthoquinone}{C_{10}H_6O_2} + 3O_2 \;\rightarrow\; \underset{phthalicanhydride}{C_6H_4(CO)_2O} + 2CO_2 + H_2O \tag{2.3}$$

$$\underset{phthalicanhydride}{C_6H_4(CO)_2O} + 4\frac{1}{2}O_2 \;\rightarrow\; \underset{maleicanhydride}{C_2H_2(CO)_2O} + 4CO_2 + H_2O \tag{2.4}$$

Regarding control, the system has multiple inputs and outputs, with the coolant flow rate controlling the reactant temperature and product gas flow rate controlling the pressure.

2.1.2 Fault tree

The portion of the fault tree developed by [Kauffman, 1990] relating to the faults simulated in this paper is given in figure 2.2. This tree provides the basis for an operator to establish appropriate corrective action after cause variable identification is successful.

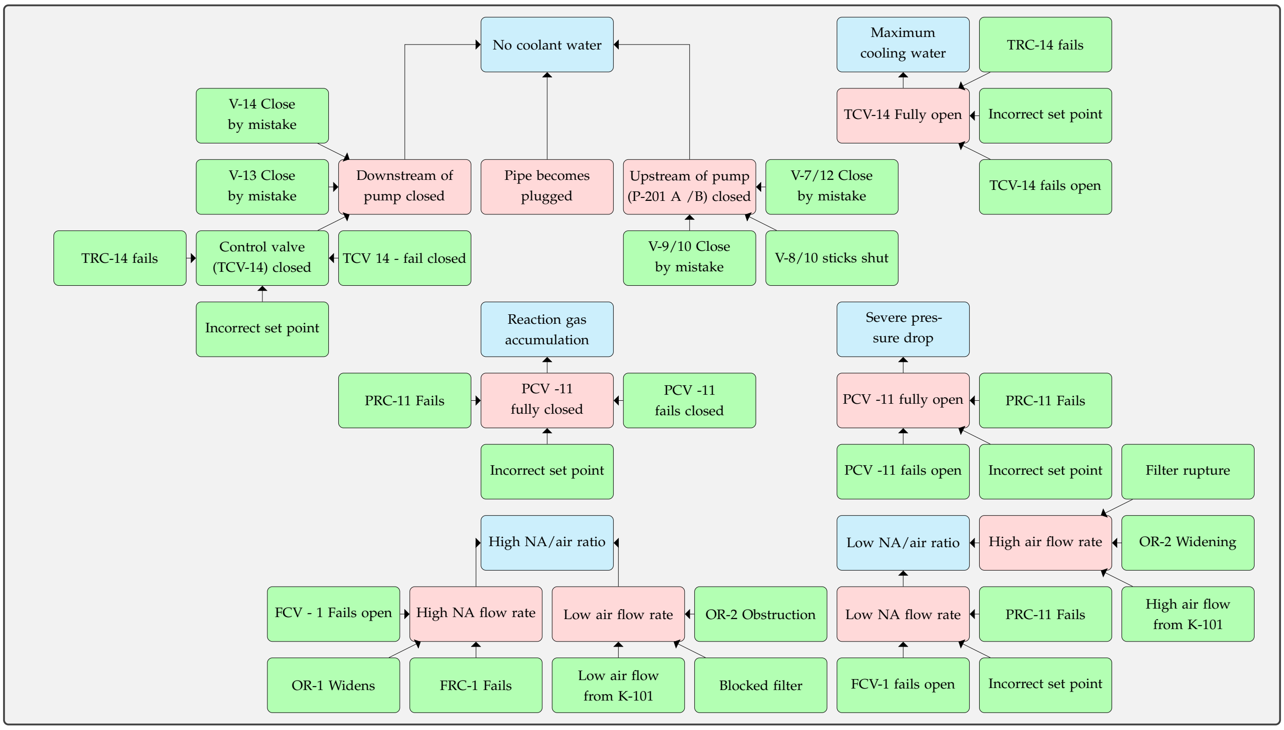


FIGURE 2.2: Fault Tree analysis of 6 faults obtained from [Kauffman, 1990]

2.2 Control

The control structure of the PAR system has multiple inputs and outputs meaning that a multivariate control approach is necessary. Multivariate control is achieved by using multiple single loops followed by accounting for interaction with an iterative detuning and fine tuning step. First, single loop negative feedback control is reviewed as the existing control loops are of this type. Control interaction and its effects on tuning are then presented. Finally, the pairing of controlled and manipulated variables is explained.

2.2.1 Feedback control

Negative feedback control can be used to automate control over an output variable by manipulating an input variable. In this type of control, the controlled variable is measured and compared to a reference set point to calculate an error. The error signal is then inputted into a control algorithm calculation to produce a control signal which controls the manipulated variable. There are many different control algorithms, the most common of which are the proportional-integral-derivative type. In the proportional mode, the control signal is proportional to the error. In the integral mode, it proportional to the accumulated error, which means it can eliminate steady state offsets. In the derivative mode, it is proportional to the derivative of the error allowing predictive capability. Various combinations of these modes and the adjustable parameter associated with each can result in many different control algorithm designs.

2.2.2 Control interaction

Feedback control algorithms apply to single loop control; however, often multiple single loops are implemented simultaneously which results in interaction between loops. This interaction is caused by relationships within the system which lead to a manipulated variable affecting more than one controlled variable. This impacts on performance and stability of the loops as well as opens the opportunity different controlled-manipulated variable combinations. Choosing which controlled and manipulated variables to pair is dealt with in section 2.2.3. The main goal of multi-loop control is to maintain multiple controlled variables at different set points simultaneously.

2.2.3 Relative gain array

The relative gain array (RGA) is a tool that allows for loop interaction to be quantified. This knowledge is then used to indicate appropriate pairing of controlled and manipulated variables. It is a matrix where each of the elements is defined as the ratio of the open to closed loop gains.

The following literature obtained from [Marlin, 2000] explains the basis for using the relative gain array (RGA) for pairing manipulated variables (MV's) and controlled variables (CV's). Suppose there are two MV's: u_1 and u_2 , both of which have an impact on two CV's: y_1 and y_2, then equations 2.5 and 2.6 would be true:

$$y_1 = g_{11}(s)u_1 + g_{12}(s)u_2 \tag{2.5}$$

$$y_2 = g_{21}(s)u_1 + g_{22}(s)u_2 \tag{2.6}$$

Two cases need to be considered and then compared to quantify interaction. First, the case where the other MV (u_2) is constant (or 0 in deviation variables) and the u_1 controls y_1 only.

$$u_2 = 0\ ,\ y_1 = g_{11}(s)u_1 \tag{2.7}$$

The second case is when both loops are closed simultaneous. Assuming this results in zero offset, equation 2.8 holds.

$$0 = g_{12}(s)u_1 + g_{22}u_2 \tag{2.8}$$

$$u_2 = -\frac{g_{12}}{g_{22}} \tag{2.9}$$

Substituting 2.9 into 2.5 gives:

$$y_2 = 0 \;\; y_1 = \underbrace{\left(g_{11} - \frac{g_{21}}{g_{22}} g_{12}\right)}_{\hat{g_{11}}} u_1 \tag{2.10}$$

Implying that when there is interaction , g_{11} changes to $\hat{g_{11}}$, where the ratio of these two cases is given by:

$$\lambda_{11} = \frac{case\ 1\ with\ (u_2 = 0)}{case\ 2\ with\ (y_2 = 0)} = \frac{g_{11}(s)}{\hat{g_{11}(s)}} = \frac{1}{1 - \frac{g_{12}(s)g_{21}(s)}{g_{11}(s)g_{22}}} \tag{2.11}$$

At steady state this simplifies to equation 2.12

$$\lambda_{11} = \frac{1}{1.0 - \frac{K_{12}K_{21}}{K_{11}K_{22}}} \tag{2.12}$$

Additionally, it can be shown that entries of the rows and columns of the RGA add to one. For the 2x2 case 2.13 holds.

$$RGA = \begin{bmatrix} \lambda_{11} & 1 - \lambda_{11} \\ 1 - \lambda_{11} & \lambda_{11} \end{bmatrix} \tag{2.13}$$

2.3 Statistical process control

Statistical process control (SPC) refers to a family of statistical procedures that are used as online monitoring tools. Systems are monitored to detect, isolate and manage faults. Faults can be defined as abnormal process behavior resulting from events such as equipment wear, failure of even large disturbances. Before corrective action can be applied, diagnosing which fault has occurred is necessary. This can be narrowed down by identification of the variable/s that are most closely related to the fault.

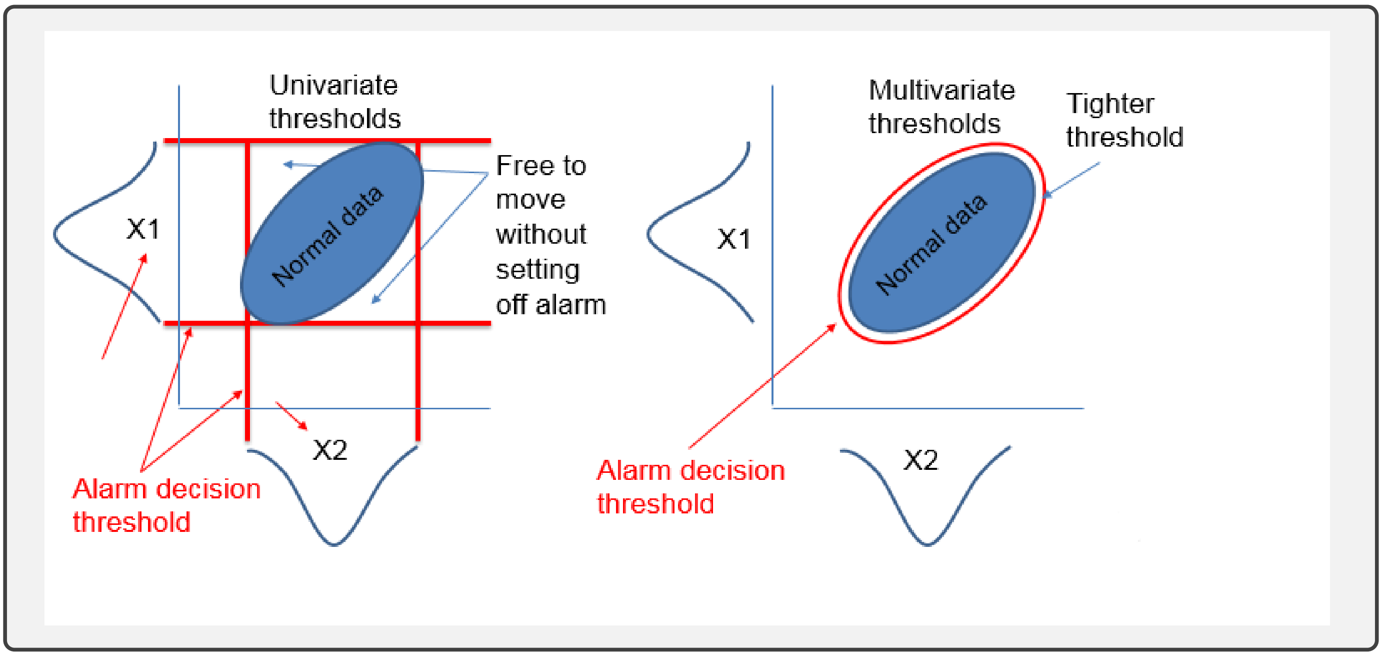


FIGURE 2.3: A comparison between univariate and multivariate thresholds

Two different classes of statistical methods are univariate and multivariate methods. Univariate methods require variables be selected and monitored by placing thresholds on each one of them. As shown in figure 2.3 this left area in which the data can move away from the data cluster but not break a threshold. This area can be eliminated by using a multivariate method which considers relationships between variables. In chemical systems, these relationships are due to conservation equations [Aldrich and Auret, 2013] and control algorithms. Better performance is expected if a method that takes these relationships into account is used.

2.3.1 Data driven process fault diagnosis in steady state systems

Figure 2.4 below is the data-driven fault diagnosis framework consisting of data spaces connected by mapping functions, both of which are represented by blocks.

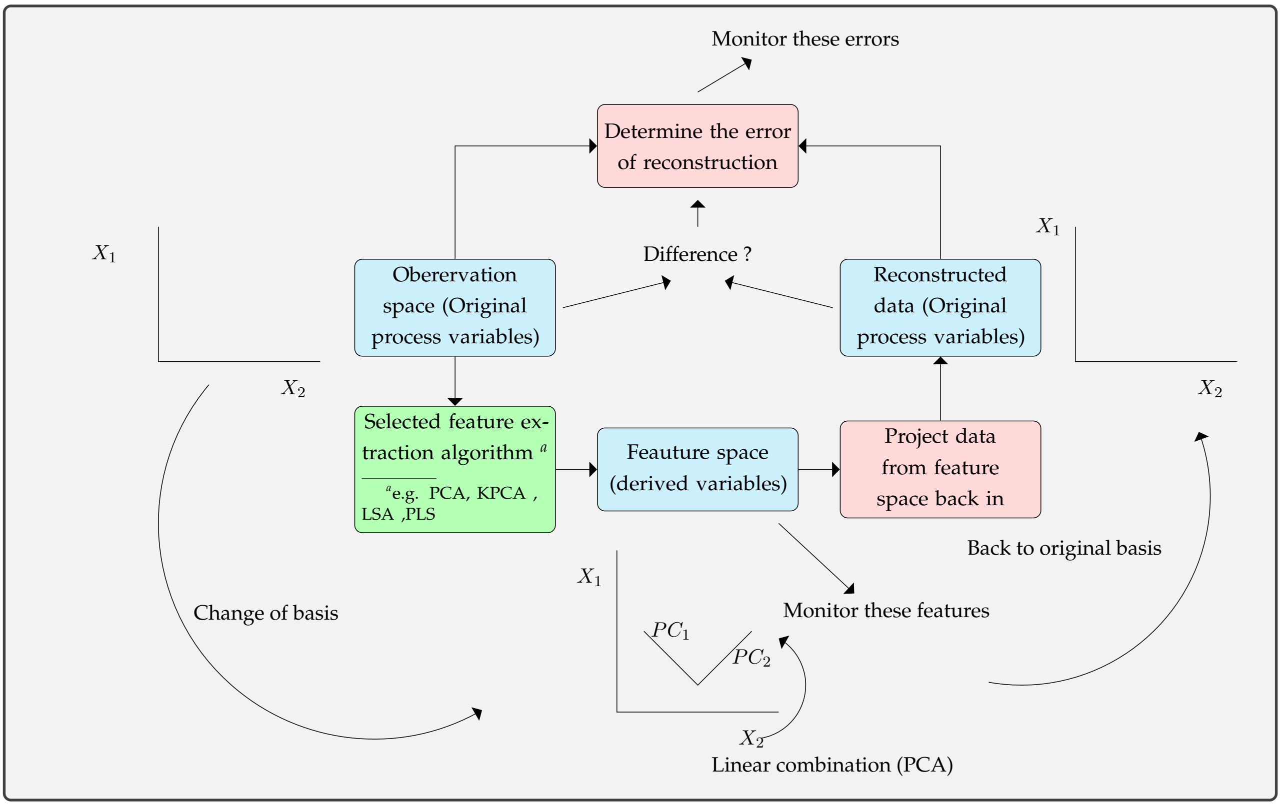


FIGURE 2.4: Fault diagnosis framework

The matrix of monitored process variables is inputted and then mapped to the feature space by a feature extraction algorithm. In this space, a derived diagnostic called Hotelling's T^2 statistic 2.3.2 can be used to monitor the process and detect faults. A model reconstruction of the matrix of monitored variables can be achieved by reversing this mapping. The difference between the reconstruction and the original observation matrix gives the matrix of residuals, which serve as an additional monitoring space. This space can be monitored with the SPE diagnostic 2.3.2.

Data-driven fault diagnosis consists of a training stage and an application stage. The training stage makes use of normal operating condition data, offline, to train an extraction model and set thresholds on the diagnostics. During application stage, online data is mapped by the model and the feature and residual spaces are monitored via diagnostics. Detection occurs when the value of a diagnostics exceeds that of its threshold value.

2.3.2 Principal Component Analysis (PCA)

In the context of the data-driven fault diagnosis framework 2.3.1, principal component analysis (PCA) can be used as a feature extraction algorithm. The algorithm is a statistical dimensional reduction procedure given in table 2.3.2, optimal in capturing variability. It is limited to considering only linear relationships between variables and is best suited to Gaussian distributions and steady state conditions. Dimensional reduction is achieved by defining a new set of variables called principal components, identified as a linear combination of the original variables. By only retaining a few of these the dimension of the data is decreased. The first principal component contains the most variance, and each subsequent component contains less. Additionally, all principal components are orthogonal to one another. This means that most of the variability can be explained by only retaining the first few components in the model.

The PCA algorithm is presented as an algorithm in table 2.3.2 which gives an overview of the method, which is then more fully explained in the text that follows.

PCA Algorithm:

- Training

1. Center and scale all original variables to have a mean of 0 and a variance of 1. (variable index $\rightarrow$ i , sample index $\rightarrow$ j)
   (a) Evaluate the mean of each original variable
   $\mu_i = \frac{1}{N}\sum_{j=1}^{N} \mathbf{X}^{(\mathbf{Unscaled,\ Uncentered})}$
   (b) Evaluate the standard deviation of each original variable
   $\sigma_i = \sqrt{\frac{1}{N-1}\sum_{j=1}^{N}(\mathbf{X}^{(\mathbf{Unscaled,\ Uncentered})})^{\mathbf{2}}}$
   (c) Center to 0 by subtracting the average mean of each variable for every sample of that variable
   $\mathbf{X}_{\mathbf{i,j}}^{(\mathbf{Unscaled})} = \mathbf{X}_{\mathbf{i,j}}^{(\mathbf{Unscaled,\ uncentered})}$
   (d) Scale each variable to unit variance by dividing each sample by standard deviation.
   $\mathbf{X}_{\mathbf{i,j}} = \frac{\mathbf{X}_{\mathbf{i,j}}^{(\mathbf{Unscaled})}}{\sigma_i}$
2. Obtain the co variance matrix $\mathbf{C}$
3. Obtain ordered eigenvector (principal component) matrix $\mathbf{P}$ and eigenvalue matrix $\mathbf{\Lambda}$ by computing the eigenvalue decomposition of the co-variance matrix such that: $\mathbf{CP} = \mathbf{\Lambda P}$
4. Choose a subset of principal components $\mathbf{P_{retained}}$ to retain based on desired variance explain.
5. Project data from original space variables onto principal components in the feature space.
   $\mathbf{T} = \mathbf{XP_{retained}}$
6. Evaluate feature space diagnostic
   $T_i^2 = \mathbf{t_i}\lambda^{-1}\mathbf{t_i^T} = x_i\mathbf{P}\lambda^{-1}\mathbf{P^T}\mathbf{t_i^T}$
7. Evaluate the Residual space diagnostic
   $Q_i = e_i e_i^T = \mathbf{x_i}(\mathbf{I} - \mathbf{P_i}\mathbf{P}_i^T)\mathbf{x_i^T}$
8. Evaluate the contributions to the residual space diagnostic
   $\{C_{r,j}\}_i = (\mathbf{X}_{i,j} - \hat{\mathbf{X}}_{i,j})^2$

Scaling and centering data

To successfully apply the principal component analysis algorithm, scaling and centering data preprocessing steps are necessary.

The purpose of scaling is to standardize the data variables since temperature, pressure composition, etc. [Aldrich and Auret, 2013] have different numerical ranges. This prevents some variables from having a higher weighting than others.

Eigendecomposition of the covariance matrix relies only on rotation and not a translation. Therefore, to correctly define the directions of most variance; the data must be centered around 0 by subtracting the means of each of the process variables.

$$\mu_i = \frac{1}{N}\sum_{n=i}^{N} \mathbf{X}_{i,j}^{(NOC:unscaled)} \tag{2.14}$$

$$\sigma_i = \sqrt{\frac{1}{N-1}\sum_{n=i}^{N}(\mathbf{X}_{i,j}^{(NOC:Unscaled)} - \mu_i)^2} \tag{2.15}$$

$$\mathbf{X}_{i,j} = \frac{X_{i,j}^{(NOC:Unscaled)} - \mu_i}{\sigma_i} \tag{2.16}$$

Equation 2.15 is used to evaluate the standard deviation of process variables i (σ_i) of the centered data matrix ($\mathbf{X}_{i,j}^{(NOC:Unscaled)} - \mu_i$) , where the mean of process variable i (μ_i) can be evaluated with equation 2.14. Once the standard deviations of process variables i(σ_i) and mean of process variable i (μ_i) are known, the unscaled and uncentered process data matrix ($\mathbf{X}_{i,j}^{(NOC:Unscaled)}$), can be scaled and centered by using equation 2.16.

Eigen decomposition of the co-variance matrix

Eigenvalue decomposition of the covariance matrix maps from vector spaces $\mathbf{V} \to \mathbf{W}$ for the special case where $\mathbf{V} = \mathbf{W}$, meaning that the obtained mapping function is a linear operator [Dellaert, 2008]. For visualization purposes can be imagined at a rotation in the observation space onto the new basis. The PCA algorithm involves the eigendecomposition to the covariance matrix which holds the covariance between pairs of monitored process variables. The eigenvalues and eigenvectors of the covariance matrix provide insight into the data structure [Abdi, 2007]. The eigenvectors obtained contain the weightings used in defining the principal axes and the eigenvalues the variances in these directions.

Directions of variance

Principal components axes refer to the main directions of variance and principal component scores refer to the projection of data onto the new axes. A linear combination just means that a weighted combination can describe every point on the principal axes in terms of the original axis.

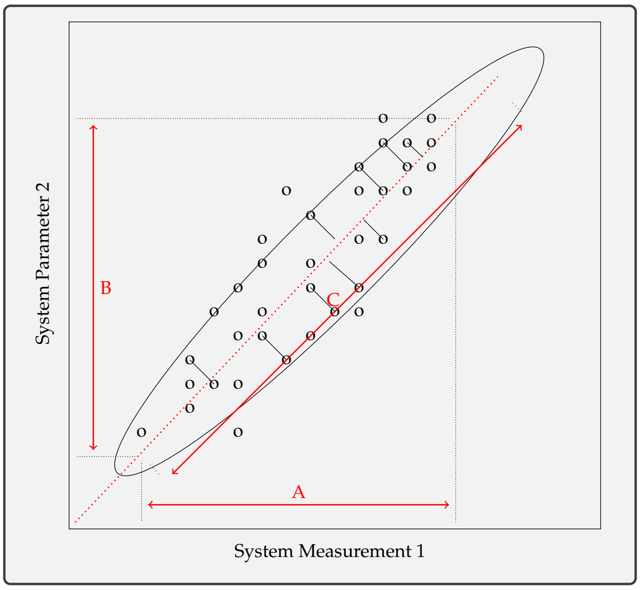


FIGURE 2.5: 2 dimensional PCA

The hypothetical case of a two variable system in figure 2.5. This serves as an intuitive graphical representation of the concept which can be extended to any number of dimensions.

Mapping from higher to a lower dimensional space is dimensional reduction [Lu et al., 2007]. In PCA this is achieved by selecting a subset of the extracted features in the feature space. The advantages of dimensional reduction are summarized below.

- If a lower dimensional space of three or less extracted features can sufficiently describe the variation in the system, then, this space can be plotted. This allows for visualization of the data which can be utilized by operators and managers. The visualization is used in pattern recognition. [Aldrich and Auret, 2013]
- Data compression allows for dealing with a huge amount of data.

Feature extraction

$$\mathbf{CP} = \mathbf{\Lambda P} \tag{2.17}$$

The projected matrix $\mathbf{P}$ (matrix made up of projected variables as columns which are linear combinations original data) can be found with equation .
The matrix $\mathbf{\Lambda}$ contains the eigenvalues corresponding to the different loading vectors (eigenvectors) in order of greatest to smallest, corresponding to the variance in the principal components (new variables as columns of the loading vectors) in the loading matrix.

$$\mathbf{T} = \mathbf{XP}* \tag{2.18}$$

Mapping of the original data $\mathbf{X}$ to the space $\mathbf{P}^*$ can be done with equation 2.18.

$$\hat{\mathbf{X}} = \mathbf{T}\mathbf{P}{*}^T \tag{2.19}$$

The reconstructed data matrix $\hat{\mathbf{X}}$ is evaluated by multiplying the scores matrix $\mathbf{T}$ by the transpose of the loading matrix i.e. $\mathbf{P}{*}^T$

$$\mathbf{E} = \mathbf{X} - \hat{\mathbf{X}} \tag{2.20}$$

The residual matrix $\mathbf{E}$ is equal to the difference between the between the original data matrix $\mathbf{X}$ and the reconstructed data matrix $\hat{\mathbf{X}}$ as shown in equation 2.20.

$$\mathbf{P}^* \in \mathbf{P} \tag{2.21}$$

The dimensional reduction is achieved by selecting only a subset of principal component axes to project data onto. Therefore the matrix of retained projected vectors $\mathbf{P}^*$ is a subset of the original matrix $\mathbf{P}$ (2.21). By retaining only some of the projected vectors, the matrix P^* contains a fraction of the total variance seen in the original data, $\mathbf{P}$ contains all of it.

$$Portion\ explained\ by\ componant\ j\ = \frac{\lambda_j}{\sum_j^m \lambda_j} \tag{2.22}$$

Eigenvalues are the variance in the principal component directions. These directions which are defined by corresponding unit eigenvectors. The variance in the data can, therefore, be concentrated into a few newly constructed variables by defining the new variable axes correctly.

Diagnostics

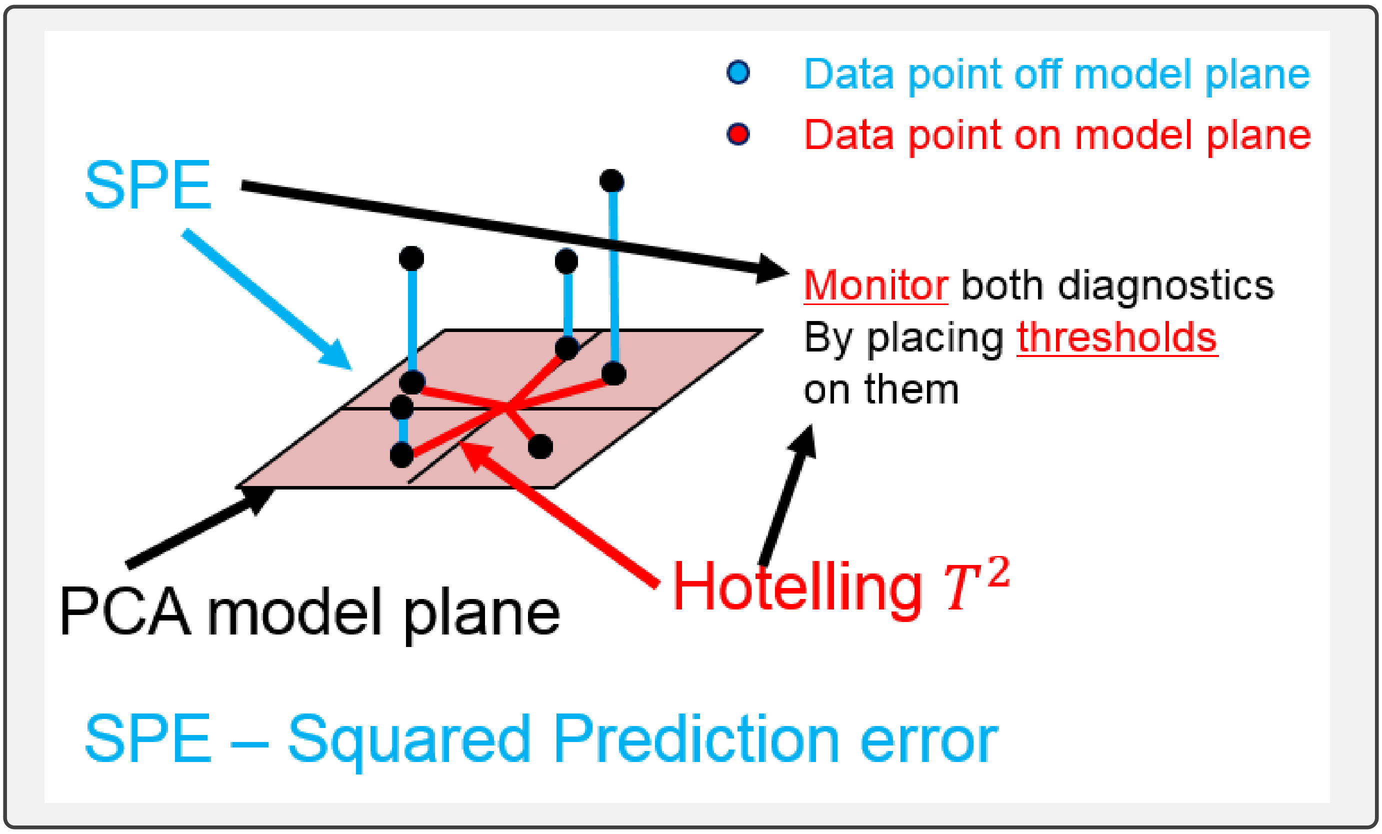


FIGURE 2.6: Hotelling's T^2 and SPE diagnostics

Figure 2.6 shows is a visual representation of the two monitoring diagnostics, SPE and Hotelling's T^2 statistic in blue and red respectively. The SPE is interpreted as the error between the position of the original data point and its predicted position according to the model. The error between these two values increases as the direction of variance changes relative to the directions of variance defined by the model. This can be visualized by the dots moving further away from the model plane. Hotelling's T^2 statistic, on the other hand, measures the magnitude of the variation in the trends captured by the model. This diagnostic increases when the relationships between variables remain the same but the variance within that relationship increases. This can be visualized as the data points moving further away from the center of the model plane.

Hotelling's T^2 statistic

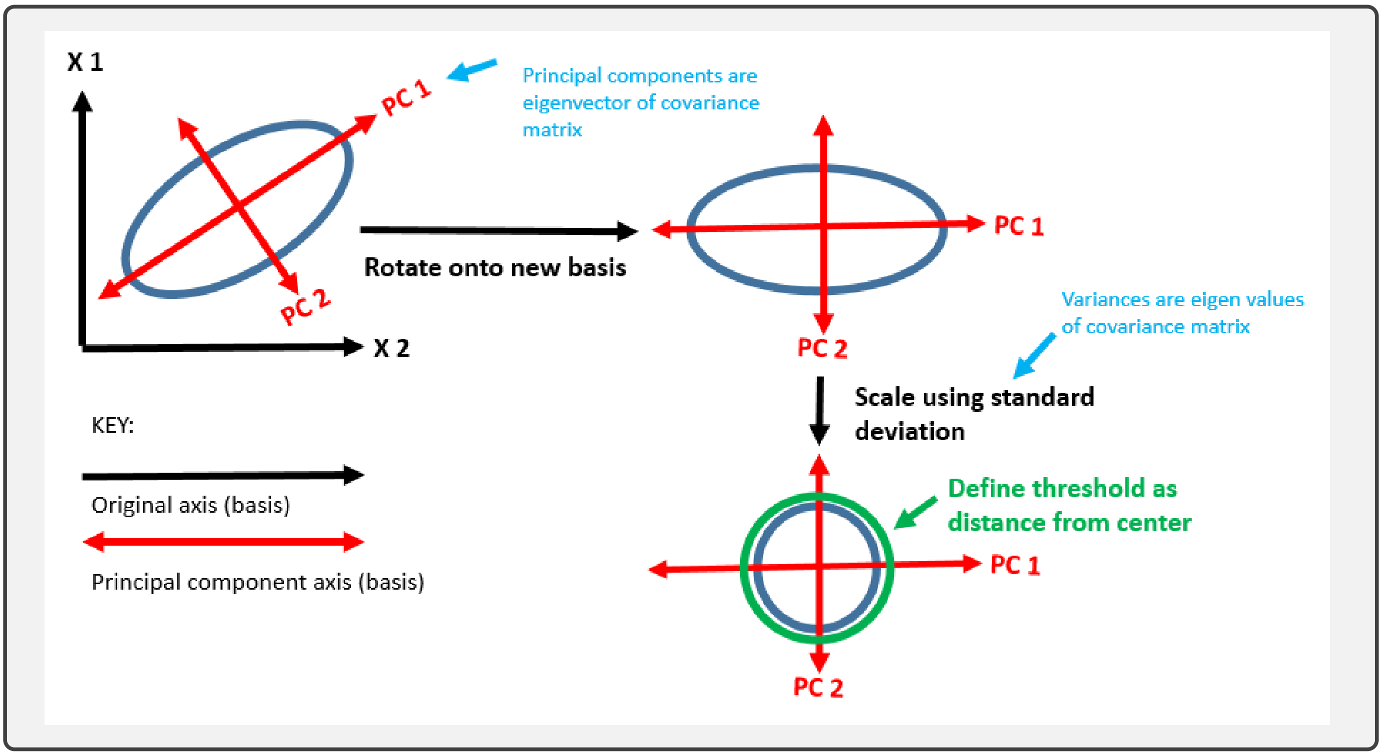


FIGURE 2.7: Hotelling's T^2 statistic threshold

In chemical systems, there are relationships between variables. The consequence of these relationships is that variables co-vary with one another. Unlike univariate monitoring, multivariate monitoring takes into account this co-variation. Relationships between variables lead to shaped data cluster[1]. Figure 2.7 illustrates this concept. On the left, a shaped data cluster due to a linear relationship between variables is projected in the observation space. Using Principal component analysis [2], the data set is rotated onto a new set of axes called the principal component axes where there is no correlation between the data as shown in the middle figure. Then using the standard deviation in principal component space, the data is normalized [3]. Setting a threshold on the squared [4] distance from the center of the data cluster, is equivalent to forming an elliptical threshold in in the original observation space. This results in a tighter threshold with less space for the data to move away from the training data without exceeding a threshold than in the space than that shown in 2.3

Normal and special cause variation

The terminology used in describing the source of variations is briefly explained. Common cause variation refers to the variation from known phenomena which are captured in the training stage.

[1]Ellipsoid for linear relationships. However, nonlinear relationships form other shapes
[2]This will be formally introduced in section 2.3.2
[3]This converts the data from an elliptical to a circular shape
[4]Squaring is necessary to avoid positive and negative from canceling one another out

Specifically, this refers to the relationships that produce deterministic variation because of constraints such as conservation and control algorithms imposed during normal operation. This is contrasted special cause variation which is a result of some previously unseen (during training) phenomena however still deterministic for i.e. because of a fault. Fault detection relies on the ability of the classifier to distinguish special cause variation from common cause variation. Additionally, there is stochastic variation (random variation) which is present during both normal operation, and during fault events, the source of this variation are unknown. An advantage of feature extraction is that the random variation can be separated from the deterministic variation.

2.3.3 Fault detection

Fault detection is reliant on a fault detection statistic. To have good detection performance, certain characteristics of this statistic are desirable. Listed below are the characteristics as well as how they may be quantified.

- Robustness - Quantified by calculating the false alarm rate.
- Sensitivity - Quantified by the missed detection rate of the faults 1 to 10.
- promptness - Detection delays

2.3.4 Fault Identification

Fault diagnosis is complicated by the following aspects [Russel et al., 2000]:

- There are many measured variables.
- Many of these variables deviate largely from their nominal value in a short period.
- Chemical Processes are complex and integrated.

The purpose of fault identification is to narrow down the variables that are considered by an operator during fault diagnosis. An approach to fault identification is to plot of the contributions of the monitored process variables to the diagnostic spaces [Russel et al., 2000]. This method is applicable in both the residual and the feature space diagnostics.

2.3.5 Performance measures

Detection performance depends on the detection method and thresholds selected. A poor choice of either can result in a bad performance. The purpose of quantifying performance is to assess the success of classification or to compare performance of different methods. Detection performance can be measured in terms of false alarm rate (FAR), true alarm rate (TAR), missing alarm rate (MAR), detection delay (DD), alarm run length (ARL). Additionally, the trade-off between TAR and FAR at different thresholds can be visualized on the receiver operator curve. The area under this curve (AUC) can be evaluated as a threshold independent performance parameter.

FAR, TAR and ROC

In the case of a simulation, knowledge of the true and classified state of the system can be known. Table 2.1 below shows the different scenarios that may arise.

TABLE 2.1: Alarm classifications

		Actual State of system	
		No fault has occured	A fault has occured
Classifier result	A fault has occured	False positive - The classifier detects a fault in the system when there is none.	True positive - The classifier correctly detects a fault in the system
	No fault has occured	True negative - The classifier correctly determines that no fault has occured.	False negative - The classifier has missed a fault that has occured

Once the data has been labeled, it can be tallied and the TAR and FAR calculated from equations 2.23 and 2.25.

$$FAR = \frac{\sum False\ Positive}{\sum True\ state\ negative} \tag{2.23}$$

$$TAR = \frac{\sum True\ positive}{\sum True\ state\ positive} \tag{2.24}$$

Figure 2.8 shows typical distributions of fault and normal samples on the left and the ROC curve on the left. The vertical lines that intersect the overlapping distributions on the left represent different possible choices of the threshold. The selection of the threshold ranges from liberal to conservative and correspond to different positions on the ROC curve.

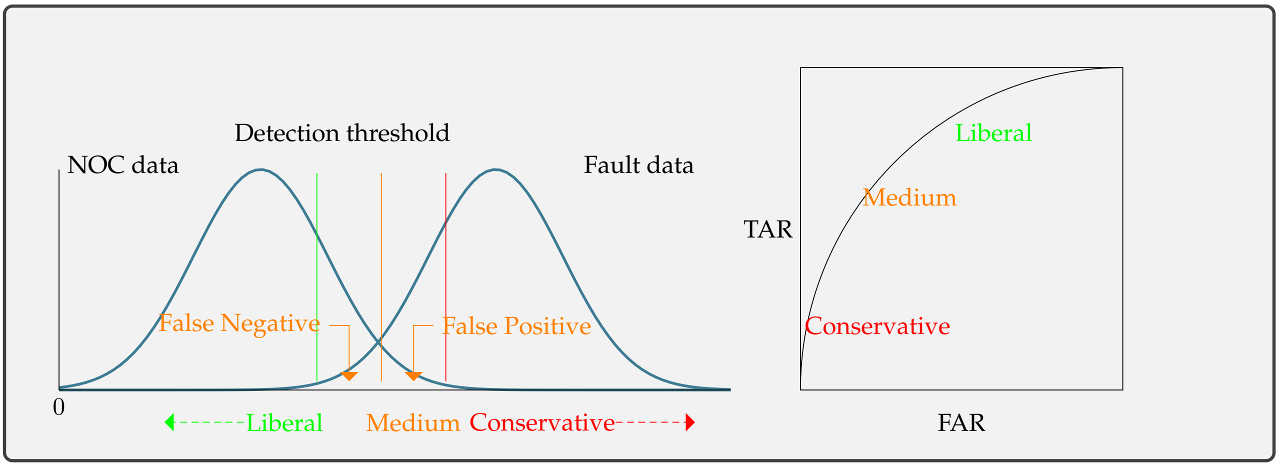


FIGURE 2.8: ROC curve showing relationship between FAR and TAR at different threshold choices

$$TAR = f_{TAR}(\theta) \tag{2.25}$$

$$FAR = f_{FAR}(\theta) \tag{2.26}$$

Both the true alarm rate and the the false alarm rate are functions of the detection threshold [Aldrich and Auret, 201 as implied in equations 2.25 and 2.26. Therefore, by choosing different threshold values, θ, a set of FAR and TAR can be calculated and plotted to generate a receiver operator curve (ROC) as shown graphically in figure 2.8. Then depending on the desired tradeoff between FAR and TAR, a threshold can be selected corresponding to a point on the ROC.

AUC

The AUC of the ROC is a useful parameter as it is independent of the selected threshold. Therefore is may be interpreted as a measure of how well the method is suited to the system or how easy to detect the fault is.

Detection delays

The detection delay refers to the number of missed sample that occur before detection is declared. Shorted detection delays are desired as these lead to faster response times.

Alarm run lengths

The alarm run length refers to the number of samples before an alarm is made. Applying this to true cases, i.e. when an alarm is made, and in fact, there is a fault (true positive – see table 2.1) The smaller the ARL_{TRUE} the better the performance.

MAR

The fraction of known fault samples that are classified as normal samples is know as the MAR. It is desired that this parameter is low.

Chapter 3

Objectives

The purpose of this project is to investigate using simulation the selection of an appropriate monitoring strategy for the PAR system. The objectives presented are formulated around achieving the aim of this investigation which is restated here.

To evaluate the PCA algorithm as the basis for statistical monitoring on the PAR system.

The first objective is to implement and validate the PAR model. This purpose of this objective is to obtain a validated model that is capable of dynamically simulating the system's responses. This functionality is necessary for the simulation of normal operating and fault data which can be used as benchmark data for testing a monitoring strategies performance.

The second objective is to design and implement an improved control strategy. The control strategy can be assessed in terms of control performance parameters and the ability to maintain stable operation.

The third objective is to model 6 fault scenarios presented by [Kauffman, 1990] The purpose of this objective is to generate fault data. This data is used in testing the performance of a monitoring strategy.

The fourth objective is to design, implement and assess a process monitoring strategy that can be used to detect faults and identify the variables that are most closely related to them. This lets the operator know when a fault occurs and provides the cause variable, which is valuable information during diagnosis. In addition the performance results obtained by meeting this objective can be used to comment on the suitability of the PCA based approach to the PAR system.

Chapter 4

Methodology

In this chapter, the method followed to achieve the objectives outlined in the previous chapter is given. The method is divided along the same three themes of modeling and simulation in section 4.1, control in section 4.2 and monitoring in section 4.3. Although the sections are sequential, there is a degree of disconnectedness between them. An overview of how all the methods relate one another is presented graphically in figure 4.1.

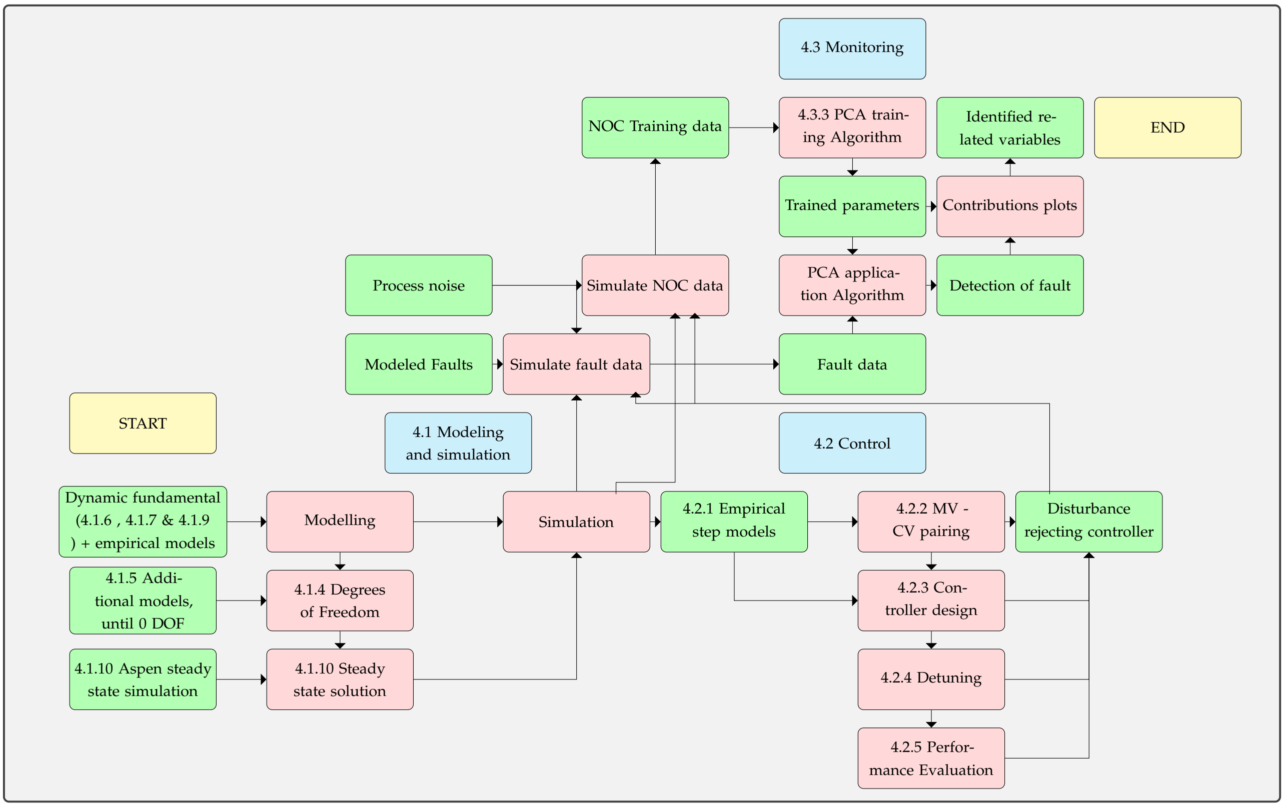


FIGURE 4.1: Overview of methodology

Section 4.1 assesses the models obtained from the literature regarding suitability and completeness. The degrees of freedom are calculated and where under-specified new models are formulated. This step is necessary to constrain a single steady state solution. In 4.1.10 the Aspen steady state simulator is used to a simulate a steady state solution so that the initial values and control set points in the PAR simulation can be specified. Section 4.1.11 provides the method for building the steady state simulation. Following this, the method of validating the simulation is explained in 4.1.12. Once validated, the simulation is used to conduct step tests. The output of these step tests provides the basis for formulating empirical linear relationships between each MV and CV. Based on these relationships, MV's and CV's are optimally paired using the relative gain array (RGA) approach. SISO tuning using the direct synthesis method, followed by detuning (for interaction) is performed to obtain the control structures and parameters for the MIMO control structure. Performance evaluation of the control structure is quantified and stability achieved. The control structure, now capable of rejecting disturbances is incorporated into the simulation. The simulation is then run with process noise introduced as a disturbance. Automated control ensures that the system remains stable allowing time series profiles to be collected for all variables. The data characterizes normal operation and is used to train a classifier. The classifier should be capable of distinguishing NOC data from fault data. Similarly, fault data is then simulated by introducing faults into the simulation; the classifier is then applied to classify the fault data based on parameters learned from the NOC data. The performance of the fault detection algorithm is then evaluated. In addition to detection of faults, the algorithm is used to determine which variable caused the fault and corrective suggestions that may be implemented by the operator are provided based on which variable is identified.

4.1 Modeling and simulation Methodololgy

A fundamental modeling procedure obtained from [Marlin, 2000] is presented below, the objective of following the procedure evaluates the suitability and completeness of the model obtained from literature [Kauffman, 1990].

4.1.1 Define goals

The goal of the model is to enable the simulation of realistic data. This is used to characterize the normal operating conditions and fault condition time series data. Specifically, the data must sufficiently capture the underlying relationships between the monitored variables. By containing non-deterministic variation propagates through the variables in a cause and effect manner.

The models must be able to capture the dynamic responses of monitored variables to simulated faults over a wide range of conditions. In this respect, the fundamental models are well suited. Empirical models however used in heat capacities are limited at certain extremes. The assumption is made that this will not affect the monitoring performance. Significant deviation must occur before ranges of applicability of empirical models are reached, by which time detection should occur.

4.1.2 Prepare information

The model consists of two system volumes, the gas reacting mixture inside of the vessel and the carbon steel reactor shell. The control volumes are treated as lumped parameter systems which imply that properties inside the system volumes do not vary with position [Marlin, 2000].

The simplification of a lumped parameter system for the shell is employed as the shell thickness is not significant. Furthermore, there is no desire to know the shell temperature profile. The reacting gas volume is regarded as suspended catalyst systems are well mixed. Both these assumptions are in line with the desired outcome of the model.

Since lumped parameter assumptions are made the macroscopic behavior of the system is available, which for monitoring purposes is good enough. Note, when data is gathered on a real physical system often relies on a single sensor in a single location. Therefore the position varying behavior of the property may never be measured.

4.1.3 Model Formulation

Both constitutive and conservation models, used in describing the system are obtained from literature [Kauffman, 1990]. The conservation equations account for the conservation of material and energy, providing relationships between the main variables which are monitored (e.g. Temperature, flow rates, volumes, etc.). These equations are required in their dynamic form, as dynamic behavior (time series profiles) of the process variables need to be captured both during normal operation and fault simulation. Normal operation, although stable and operating around the region of the steady state cannot be considered truly steady. This is because of constant noise disturbance and rejection by automated control action. The variation contained within the normal operation is common cause variation. As the models constrain variables to one another, covariance structures are expected. It is these structures that multivariate methods attempt to consider. Since the reacting gas system is well mixed, the material balance equations are ordinary differential equations [Marlin, 2000].

4.1.4 A degrees of freedom analysis

A degree of freedom analysis is necessary to determine whether the number of independent equations is sufficient to determine a solution to the model. The degrees of freedom of the system was calculated by subtracting the number of independent equations (NE) from the number of dependent variables (NV) [Marlin, 2000] as shown in equation 4.1.

$$DOF = NV - NE \tag{4.1}$$

Included into the degrees of freedom analysis are constitutive and conservative equations obtained from [Kauffman, 1990]. The degrees of freedom analysis revealed that the system was unconstrained, prompting the addition of further equations which relate the monitored process variables.

4.1.5 Decreasing DOF to 0

The ideal gas law 4.2 is used as the equation of state, relating temperature, pressure and volume.

$$PV = nRT \tag{4.2}$$

Using Hess's Law 4.3 heats of formation data obtained from NIST is used to calculate the heats of reaction at standard state pressure.

$$\Delta H^o_{RXN,ref} = \sum \Delta v_i H_{f,} \tag{4.3}$$

Heat capacities as temperature functions for all gaseous species NIST were used to account for the temperature dependence of the heat of reaction in equation 4.4 . As only discrete data was available, polynomials were fitted through the heat capacities to obtain an empirical heat capacity models.

$$\Delta H_{RXN} = \Delta H^o_{RXN,ref} + \int_{Ref.}^{T} Cp(T)dT \tag{4.4}$$

4.1.6 Component material balance

The number of mol of each of the species in the reactor is described by equations 4.5 to 4.12. All kinetic constants are functions of temperature, which is solved with the energy balance on the gaseous species.

$$\frac{dN_{NA}}{dt} = F_{NA,in} - F_{NA,out} - (k_1 + k_2)N_{NA} \tag{4.5}$$

$$\frac{dN_{PA}}{dt} = -F_{PA,out} + k_1 N_{NA} + k_3 N_{NQ} - k_4 N_{PA} \tag{4.6}$$

$$\frac{dN_{NQ}}{dt} = -F_{NQ,out} + k_2 N_{NA} - k_3 N_{NQ} \tag{4.7}$$

$$\frac{dN_{MA}}{dt} = -F_{MA,out} + k_4 N_{PA} \tag{4.8}$$

$$\frac{dN_{O_2}}{dt} = F_{O_2,in} - F_{O_2,out} - (4\frac{1}{2}k_1 + 1\frac{1}{2}k_2)N_{NA} - 3k_3 N_{NQ} - 4\frac{1}{2}k_4 N_{PA} \tag{4.9}$$

$$\frac{N_{N_2}}{dt} = F_{N_2,in} - F_{N_2,out} \tag{4.10}$$

$$\frac{dN_{CO_2}}{dt} = -F_{CO_2,out} + 2k_1 N_{NA} + 2k_3 N_{NQ} + 4k_4 N_{PA} \tag{4.11}$$

$$\frac{dN_{H_2O}}{dt} = -F_{H_2O} + (2k_1 + k_2) N_{NA} + k_3 N_{NQ} + k_4 N_{PA} \tag{4.12}$$

4.1.7 Energy balances

The temperature of the reacting gas mixture is described by the ODE energy balance given in equation 4.13. Since the heat capacity of gasses cannot be assumed to be independent of temperature, temperature dependent heat capacities were used.

$$\begin{aligned} &\frac{d}{dt}\left[\sum_n N_n \int_{T_a}^{T} Cp_n dT + M_C \int_{T_a}^{T} Cp_C dT\right] = \\ &\sum_n \left[F_{n,in} \int_{T_a}^{T_o} - F_{n,out} \int_{T_a}^{T} Cp_n dT\right] - Q_C - Q_V + \sum_m (-\Delta H_m) k_m N_j \end{aligned} \tag{4.13}$$

4.1.8 Kinetics equations

The set of kinetic equations 4.1.8 taken from literature [Kauffman, 1990] were not consistent with other data found in literature [Saleh and Wachs, 1987]. Therefore the reaction constants models given in 4.15 are used in place of 4.1.8 from [Kauffman, 1990].

$$\begin{aligned} k_1 &= e^{-1.481+0.055T} \\ k_2 &= e^{-1.481+0.055T} \\ k_3 &= e^{-0.92+0.0645T} \\ k_4 &= e^{-4.747+0.0268T} \end{aligned} \tag{4.14}$$

$$\begin{aligned} k_1 &= e^{-1.481+\frac{0.055}{T}} \\ k_2 &= e^{-1.481+\frac{0.055}{T}} \\ k_3 &= e^{-0.92+\frac{0.0645}{T}} \\ k_4 &= e^{-4.747+\frac{0.0268}{T}} \end{aligned} \tag{4.15}$$

4.1.9 Vessel energy balance

The lumped system model that describes the temperature of the vessel wall is given in 4.16.

$$\frac{dT_V}{dt} = \frac{A_v}{M_V Cp_V}\left[h_f(T - T_V) - \frac{(T_V - T_a)}{\frac{1}{h_a} + \frac{\delta x_{ins}}{k_{ins}}}\right] \tag{4.16}$$

4.1.10 Steady state solution

After reducing the degrees of freedom of the model to 0 through introduction of additional constraints. The steady state solution can be solved for. The steady state values are required to initialize the numerical simulation and decide on the control set points.

The dynamic balances were reduced to their steady state form by setting the accumulation terms to 0. Where possible, the system of equations was then broken into smaller systems of equations with 0 DOF and solved for. With the remaining unsolved system, an aspen simulation was constructed and solved for. When simulated in the Simulink, then dynamic simulation still did not reach steady state, most probably due to numerical error. To correct for this, the control was set to manual and the flow rate iteratively adjusted until the energy removed is equal to the energy released from the reaction.

4.1.11 Programming Simulation

Simulink, a numerical simulation environment that allows for graphical programming was used to create the simulation. Figure 4.2 is a visual representation of the interaction between the different models and control structure. The temperature signal obtained by solving the energy balance ODE, which is then used by the material balance as the kinetic constants are functions of temperature. The pressure is controlled by manipulating the outlet flow rate and the temperature is controlled by manipulating the coolant flow rate which affects the heat loss term in the energy balance. The set points for the temperature and pressure are obtained from the steady state solution.

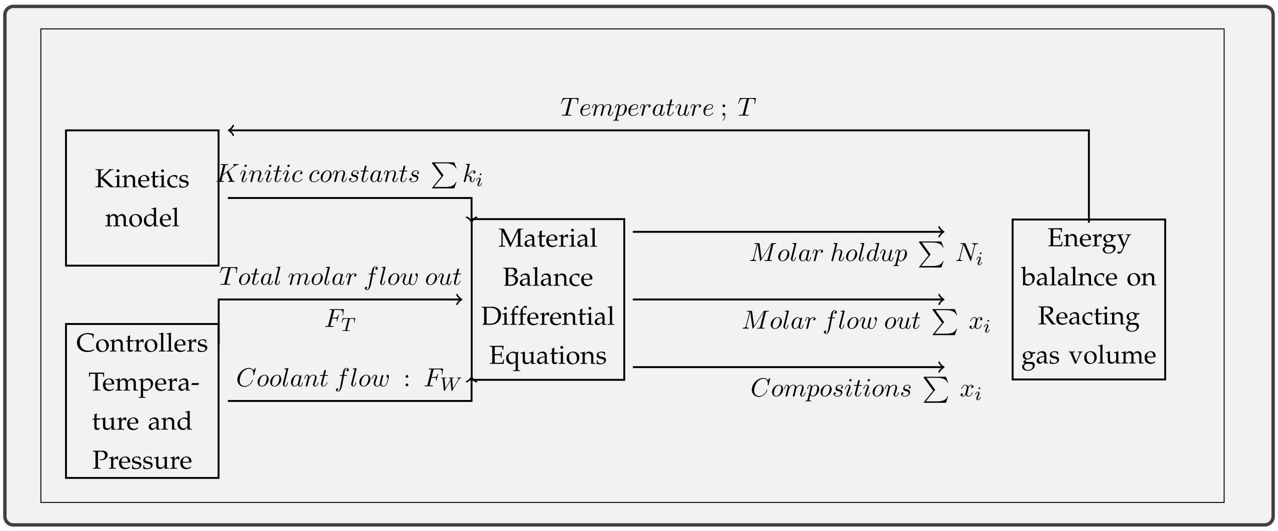


FIGURE 4.2: Interaction between subsystems in simulation

4.1.12 Validate model

The kinetic models were adapted from those originally suggested by [Kauffman, 1990] as they were found to be unsuitable. Therefore, quantitative validation of the simulated faults was not possible, and a qualitative approach was used instead. Six faults obtained from [Kauffman, 1990] were simulated and the dynamic responses of monitored process variables (i.e. Temperature, pressure) were plotted against time. The dynamic time responses were then interpreted from an engineering knowledge perspective in order the validate the model. The interpretation and discussion of these responses are presented in section 5.2.

4.2 Control

The objective related to control is to design and implement a control structure, then to assess control performance of it and ensure that it allows the system to reach stability. The approach taken is summarized in 4.3 below. Since the system has multiple inputs and outputs, the pairing of controlled and manipulated variables is necessary. The method of achieving this is to use the relative gain array approach. This method requires that models relating the controlled and manipulated variables be known, these are determined empirically. The controller tuning method implemented is the direct synthesis method which also requires these models. Controller tuning is broken up into two stages. First, the control loops based on the outcome of pairing are tuned independently , ignoring the interaction between the loops. Then to account for the interaction , de-tuning, and fine tuning methods are applied. Control performance is assessed in terms of integral absolute error and variance.

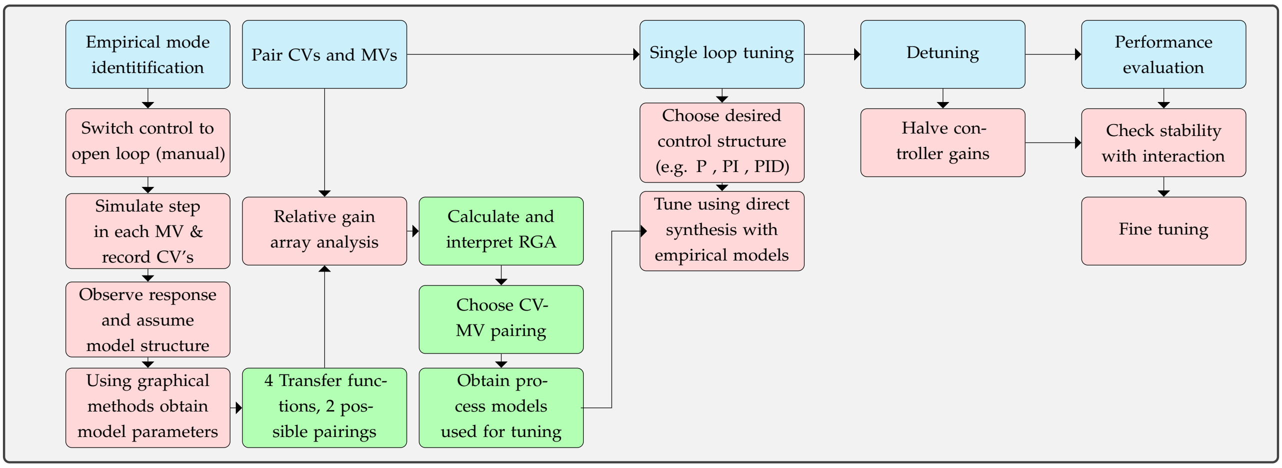
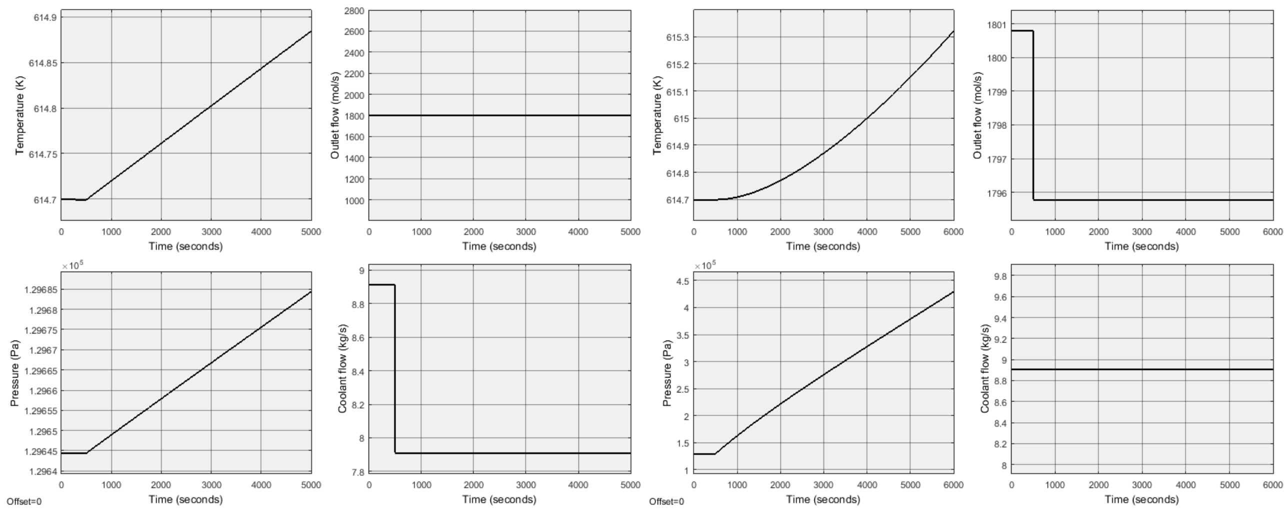


FIGURE 4.3: Control approach overview

4.2.1 Empirical model identification

As previously stated, models that relate the controlled and manipulated variables are required by both the relative gain array pairing and the direct synthesis single loop tuning methods. These models are obtained empirically by graphical means and result in linear models which are considered acceptable in accuracy for control purposes. The following procedure was followed when obtaining the models. First, the automatic control algorithm is changed to manual mode meaning that there is no automated feedback control. Step input changes in the manipulated variables are then introduced, and the response curves of the controlled variables are captured graphically as shown in figure 4.4.



(A) Coolant flow rate step change (B) Outlet flow rate step change

FIGURE 4.4: Open Loop step test results

By visual inspection of figure 4.4, the responses can be identified approximate integrator systems as there is no indication of an intrinsic feed back which will allow for CV's to reach a new steady state. The integrator model parameter can be obtained from the slopes of the output (y) of the responses as shown in Laplace domain model 4.17. Note, the slope should be independent of the magnitude of the MV (u) change, this can be achieved by normalizing the outputs (i.e. dividing by the magnitude of the inputs Δu.)

$$G_P(s) = \frac{\frac{\Delta y}{\Delta t}}{\Delta us} = \frac{K_P}{s} \tag{4.17}$$

The following linear process models were obtained in this way are presented below , where the $G_{P,21}$ refers to the relationship between CV_2 and MV_1 and MV_1 is the coolant flow rate , MV_2 is the outlet gas flow rate, CV_1 is the temperature and CV_2 is the pressure:

$$G_{P,11} = \frac{-0.000043}{s} \tag{4.18}$$

$$G_{P,12} = \frac{-0.00035}{s} \tag{4.19}$$

$$G_{P,21} = \frac{-0.000095x10^2}{s} \tag{4.20}$$

$$G_{P,22} = \frac{-11}{s} \tag{4.21}$$

4.2.2 Relative gain array

The relative gain array method is used to decide which manipulated variables should be used to control which controlled variables. This methodology makes use of the theory presented in section 2.2.3 and the empirical models obtained in the previous section.

Typically with self-regulating systems, the RGA is obtained using the steady gains as an indication of the steady state impact that an MV has on a CV. In the case of an integrating system, however, the gain is undefined as the system does not reach a new steady state. [Marlin, 2000] suggests that overcome this, the rate of change of the CV is treated as the controlled variable, rather than the controlled variable itself. This means that the change in slope from steady state to non-steady is taken as the equivalent gain. Using this approach, the next the RGA is constructed.

$$\mathbf{K} = RGA = \begin{bmatrix} -0.000043 & -0.000035 \\ -0.000095x10^2 & -11 \end{bmatrix} \tag{4.22}$$

$$\lambda_{11} = \frac{1}{1 - \frac{(0.000095x10^2)(0.000035)}{(0.000043)(11)}} \tag{4.23}$$

$$RGA = \begin{bmatrix} 1.0007 & -0.0007 \\ -0.0007 & 1.0007 \end{bmatrix} \tag{4.24}$$

Positive relative gains equal to 1.0007 indicate little interaction. Therefore it is optimal to pair the cooling water and temperature related by $G_{P,11}$ and the outlet flow rate and pressure re $G_{P,22}$. Although this was the natural pairing, the procedure is valuable as the natural pairing is not always the optimal pairing.

4.2.3 SISO tuning : Direct synthesis

As previously stated the loops are first tuned independently not accounting for interaction. The pairings obtained from the previous section 4.2.2 are used to define the loops and the empirical models that related them are used as the basis for tuning. The single loop tuning method used is the direct synthesis approach obtained from [Chen and Seborg, 2002].

Starting at the closed loop transfer function for a disturbance given by 4.25 , the form of the process model 4.26 and the desired form of the controller, a PI controller is chosen for its ability to eliminate the offset. A PID controller was not considered appropriate as both the temperature and pressure have a large amount of noise in the simulation.

$$(\frac{y}{d}) = \frac{G_P}{1 + G_P G_C} \tag{4.25}$$

$$G_P = \frac{K_P}{s} \tag{4.26}$$

$$G_C = Kc(1 + \frac{1}{\tau_I s}) \tag{4.27}$$

These three equations can be combined and simplified to give 4.28 which suggests that if a PI controller is desired, then a reasonable assumption for the desired closed loop transfer function is of the same form shown in 4.28.

$$\frac{y}{d} = \frac{Ks}{K_C K s + \frac{K_P K_c}{\tau_I} + s^2} \tag{4.28}$$

Therefore the desired transfer function is stated 4.29.

$$(\frac{y}{d})_{desired} = \frac{K_d s}{(\tau_c s + 1)^2} = \frac{K_{K_d}}{\tau^2 s^2 + 2\tau_c s + 1} \tag{4.29}$$

By comparing 4.29 and 4.28 it can be seen that the following three equations 4.30 4.31 and 4.32 must hold

$$K_P = K_d \tag{4.30}$$

$$K_C = \frac{-2}{K_P} \tag{4.31}$$

$$1 = \frac{K_P K_c}{\tau_I} \tag{4.32}$$

Combining 4.31 and 4.32 yields equation 4.33

$$\tau_I = -2 \tag{4.33}$$

$$K_c = \frac{-2}{K_P} \tag{4.34}$$

Applying theses two equations to the empirically obtained transfer functions yields two PI controllers.

$$G_c = \frac{1}{-0.000043}(1 + \frac{1}{-2s}) \tag{4.35}$$

4.2.4 Detuning and fine tuning

Initial tuning parameters obtained in the previous section do not consider control interaction. This section evaluates the control performance of these parameters and includes de-tuning and fine tuning steps that do take control interaction into account. Following this, control performance is re-evaluated. The goal is to achieve stability in both CV's simultaneously as well as good performance in disturbance attenuation.

Per [Marlin, 2000], trial and error tuning is often used in practice when tuning multi-variable loops. Additional insight gain from open loop step test results can also be utilized. These showed that a change in coolant has a negligible impact on the pressure, however, the sensitivity of temperature to changes in outlet gas flow rate was more significant. Based on this observation, the approach taken in de-tuning and fine tuning was to decrease the gain in the pressure control loop and increase the gain in the temperature control loop.

The expected outcome was that de-tuning of the pressure loop would lower interference in the temperature loop while increasing the gain in the temperature loop will not affect the pressure loop. The approach to employing this method is to run a simulation without noise, introduce a disturbance and to compare the performance of the controllers with varying gains of each loop.

4.2.5 Control performance

To assess the success of the controller design, the integral absolute error and the standard deviation of the controlled variables are calculated as performance parameters. It is desired that both are minimized.

Integral absolute error

To evaluate the integral absolute error of the controlled variables, a disturbance is introduced into the simulation with the controllers in automatic (closed loop) mode. The accumulated absolute error calculated as the difference between the controlled variable and its set point.

Stochastic variation

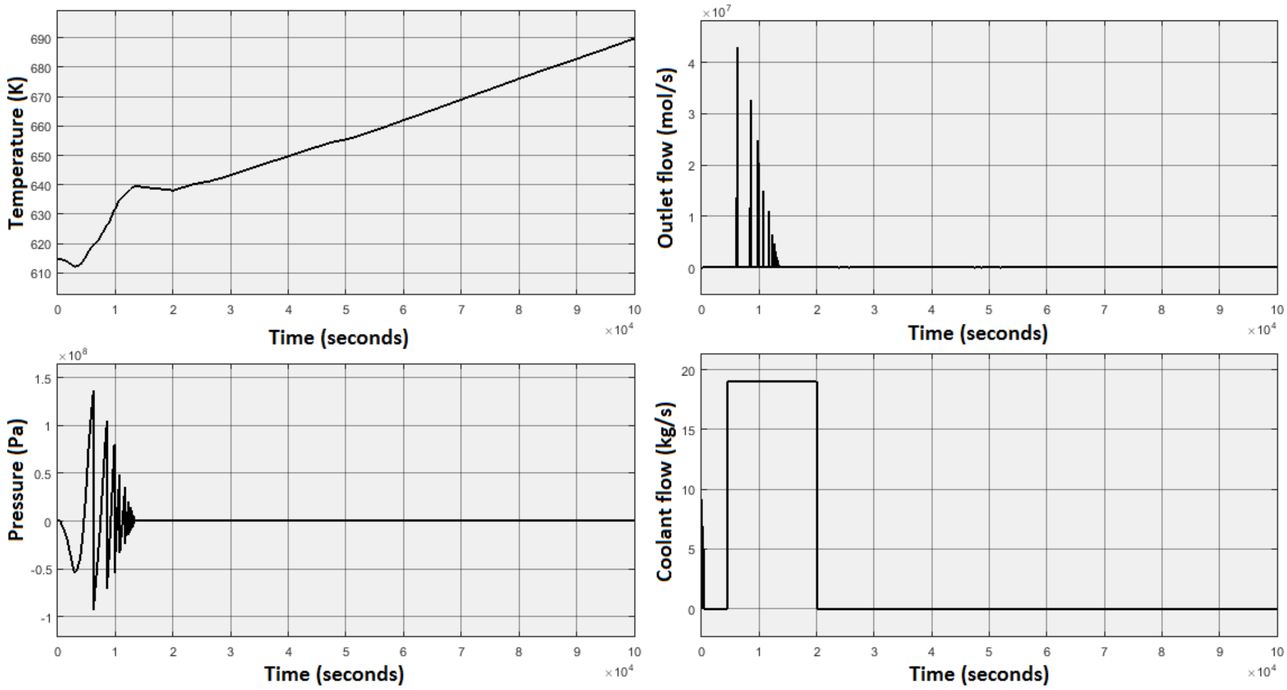
The purpose of the controller in the context of this investigation is to reject stochastic variation and maintain stability. Its performance is measured regarding its ability to do this. This requires simulating noise into the system and the calculating the standard deviation (average deviation from mean) of the CV's and MV's better performance can be interpreted by a lower standard deviation.

4.3 Monitoring

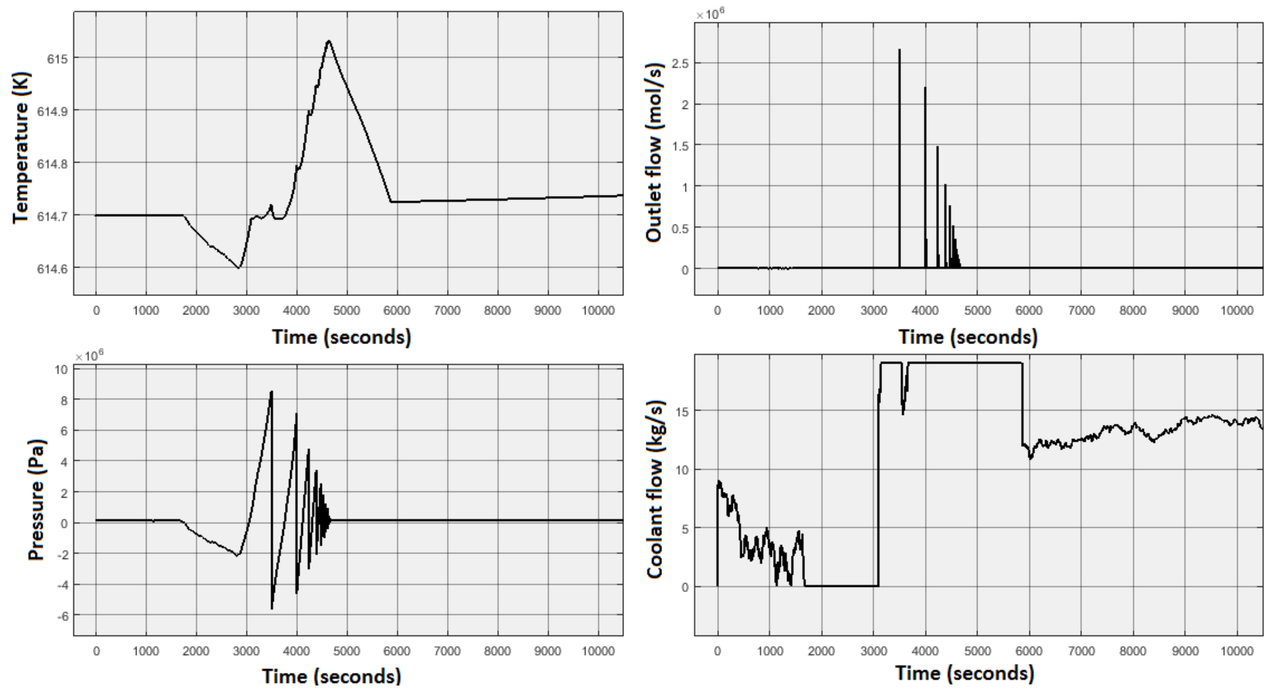
The monitoring of process variables can be used to detect when faults occur and to identify which variables are most affected. Normal operating condition data was simulated to train the classification models and threshold values, which could then be applied to simulated fault data.

4.3.1 Normal operating condition simulation

Process noise was added to the process simulation as a disturbance, to simulate normal operating conditions. This introduces variability into the data. Trial and error adjustment of the noise magnitude was then done until controller saturation did not occur as seen in Figures 4.5 and 4.6.

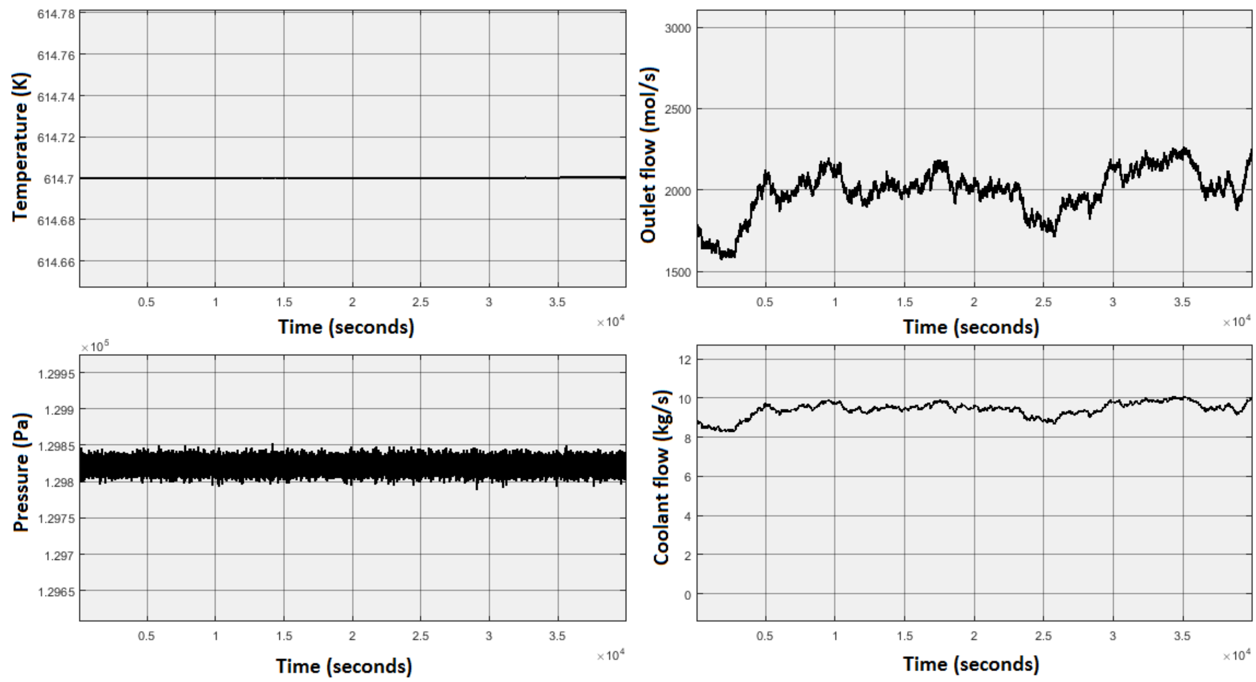


(A) First iteration : unstable

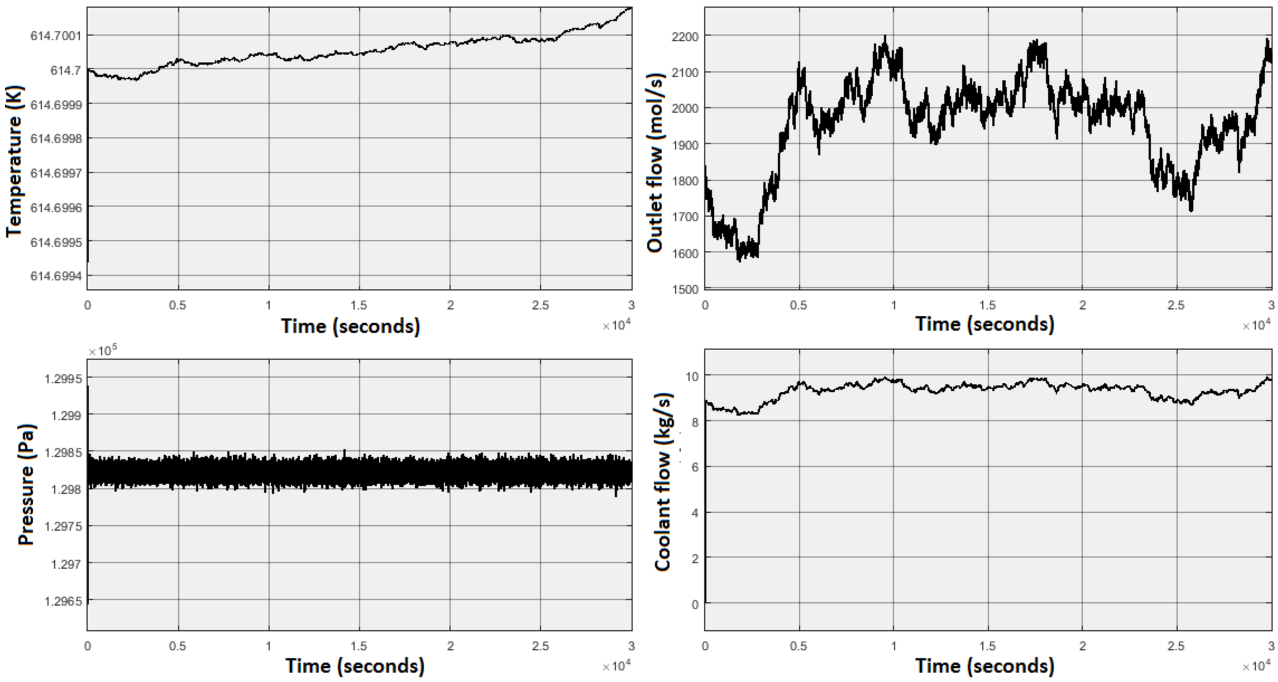


(B) Second iteration: unstable

FIGURE 4.5: Noise addition iterations 1 & 2



(A) Third iteration: stable



(B) Fourth iteration: stable

FIGURE 4.6: Noise addition iterations 3 & 4

The time series data of the 15 variables listed in table 4.1 were used to train the classification model and diagnostic thresholds. The sample time was set to every second so that a large amount of training data was obtained, necessary to properly capture the underlying data structure. Real sensors and probes cannot necessarily keep up with this sampling time, which is noted.

TABLE 4.1: Process Variables

Variable	Description	Variable	Description
1	Reacting gas temperature	9	CO_2 composition
2	Reactor shell temperature	10	N_2 composition
3	Coolant flow rate	11	O_2 composition
4	Pressure insdie vessel	12	MA composition
5	Total molar flow rate at outlet	13	NQ composition
6	Molar flow rate of NA at inlet	14	PA composition
7	Molar flow rate of air at inlet	15	H_2O composition
8	NA composition		

Normal operating condition data is not technically steady as there is variation in it, however, is stable. It contains paths between the steady state which should not be classified as faults and is, therefore, desirable as training data.

4.3.2 Faults simulation

TABLE 4.2: Process Faults

Fault	Cause variable/s	Fault Description	Type
1	Coolant flow (3)	No coolant flow	Step
2	NA (6) or air flow (7)	Ratio control fails high (NA high)	Step
3	NA (6) or air flow (7)	Ratio control fails low (NA low)	Step
4	Total Molar flow out (5)	Outlet flow valve fails open	Step
5	Total Molar flow out (5)	Outlet flow valve fails closed	Step
5	Coolant flow (5)	Coolant flow valve fails open	Step

Table 4.2 summarizes the faults that are simulated. All faults are step changes which are set to occur at a specified time in the simulation after steady has been reached. The results of these simulations are presented in section 5.2 and are used to evaluate the monitoring performance of the PCA-based monitoring strategy. Furthermore, these results are used in validating the simulation.

4.3.3 Training stage

The simulated normal operating condition data is used to train the classification model. The framework for training the model is given below in 4.7. The model can then be used to distinguish normal from fault samples in the application phase. Noise and control action ensure that the data has variability in it, but remains stable.

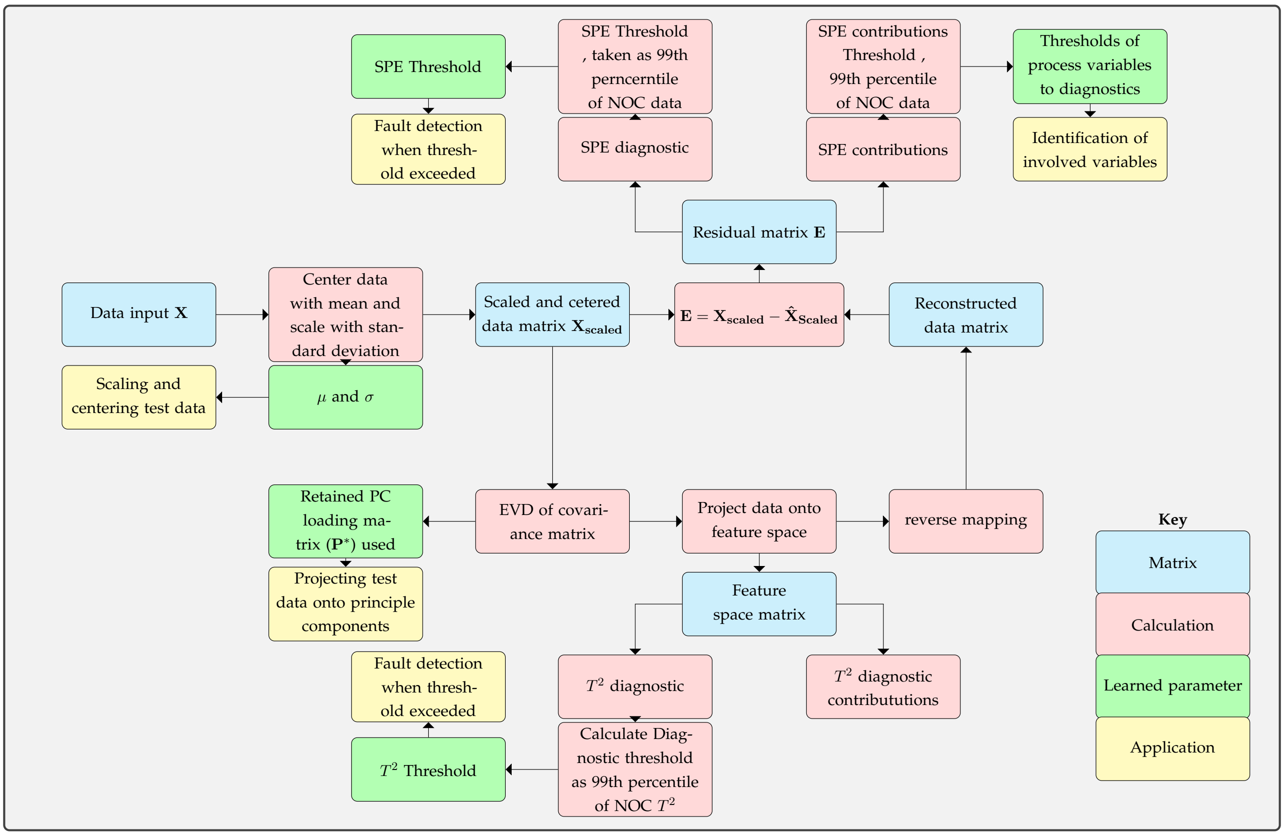


FIGURE 4.7: General offline training Procedure

The desired output of the training stage can be summarized as follows:

- Using equations 2.14 and 2.15 the scaling and centering parameters can be calculated.
- Eigen decomposition of the covariance matrix is used to obtain the eigenvectors and eigenvalues. These define the directions of most variance and the variance of those directions respectively.
- The number of retained principal component axes in the form of a reduced coefficients matrix. [1]
- Using the normal operating condition data, a distribution of Hotelling's T^2 statistic values are generated. The 99th percentile of this distribution is then used as the threshold value.
- Similarly, a distribution of the sum of the squares of the prediction error is obtained, and the diagnostic is also set at the 99th percentile.
- For identification purpose thresholds are placed on the contributions of individual variables to both the residual space diagnostic.

[1] The coefficients matrix and the eigenvectors matrix are the same things. It contains the coefficients that constrain the orthogonal directions of most variance.

Number of retained variables

A subset of the extracted features is retained in the feature space. This separates deterministic variation from non-deterministic variation (random variation due to noise). The scree plot is used as a graphical guide to selecting a sensible cut off explained variation, per [Jolliffe, 2002] this is usually between 70% and 80%. Alternatively, the cut-off can be chosen at the 'elbow' which occurs at the transition from steep to non-steep.

Diagnostic thresholds for detection

The derived diagnostics in the feature and residual spaces are used for monitoring the system. Empirical thresholds were placed on these diagnostics, that if exceeded would trigger an alarm.

The objective of setting diagnostic thresholds is to determine a threshold that will not result in triggering an alarm under NOC. However, any variation more than the NOC variation (due to noise), will trigger an alarm. The threshold in both the T^2 space and the SPE space were set to the empirically determined 99th percentile. No assumptions about the distribution of the diagnostics were made as there were uncertainties about the impact of possible autocorrelation in variables on the i.i.d assumption. To monitor the feature space and residual space, Hotelling's T^2 statistic and SPE are used respectively.

Thresholds on variable contributions

Variable contributions thresholds can be placed on both the contributions plots of the residual space diagnostic [2]. Thresholds were empirically set to the 99th percentile [3]. To simplify the contribution plot thresholds, the contributions of new process data are divided by the learned thresholds. Threshold values exceeding one, therefore, exceed the threshold for that variable and are classified as variables related to the fault.

4.3.4 Application stage

The parameters obtained in offline training are applied to the new un-scaled process data during online application. The unscaled data is first subjected to the scaling and centering procedure to ensure equally weighted contributions of all variables. The learned extraction model is then applied to map the data from the observation space to the feature space. In application, the PCA algorithm programmed into Matlab was run again, however, instead of recalculating: (1) The means and the standard deviations of the variables, (2) the eigenvalues (variance of new features) and eigenvectors (new basis directions), (3) number of retained PC axes and (4) thresholds. Those learned during the training stage are used instead.

[2] The feature space in not considered in this study

[3] An alternative would be to assume an underlying distribution and then determine the 99th percentile para-metrically

4.3.5 Performance evaluation

Performance parameters were calculated so that conclusions about the suitability of PCA to the PAR system could be made. The performance is quantified with missing alarm rate (MAR), false alarm rate (FAR), true alarm rate (TAR), alarm run length (ARL), the area under the curve (AUC) of the receiver operator curve (ROC). It is necessary to know the true state of the system and the classified state of the system to calculate most of these parameters.

Knowledge of when the fault was simulated was used to label each sample as either fault or normal operating condition data. This information describes the true state of the system.

The PCA algorithm was applied to fault data, using the learned mapping functions. The diagnostics calculated from the fault data were then compared to learned threshold values and used classify the data. If the calculated value of the diagnostic exceeded that of the threshold, the sample was classified as a fault sample.

The TAR versus FAR for the set of all possible threshold choices was used to plot the ROC curve. This plot is independent of the threshold chosen and therefore does not allow a poor choice of a threshold to influence the performance evaluation. The curve is quantified by numerically integrating the area under it.

Chapter 5

Results and interpretation of analysis

In this section, the results generated from the previous methodologies are presented and discussed according to the structure shown in figure 5.1. This provides the methods used in generating each result in the first column, the question each result aims to answer in the second, where to find each result in this chapter in the third and how the result is used in the fourth. The last result addresses the aim of this report, which is the evaluation of PCA as a monitoring strategy.

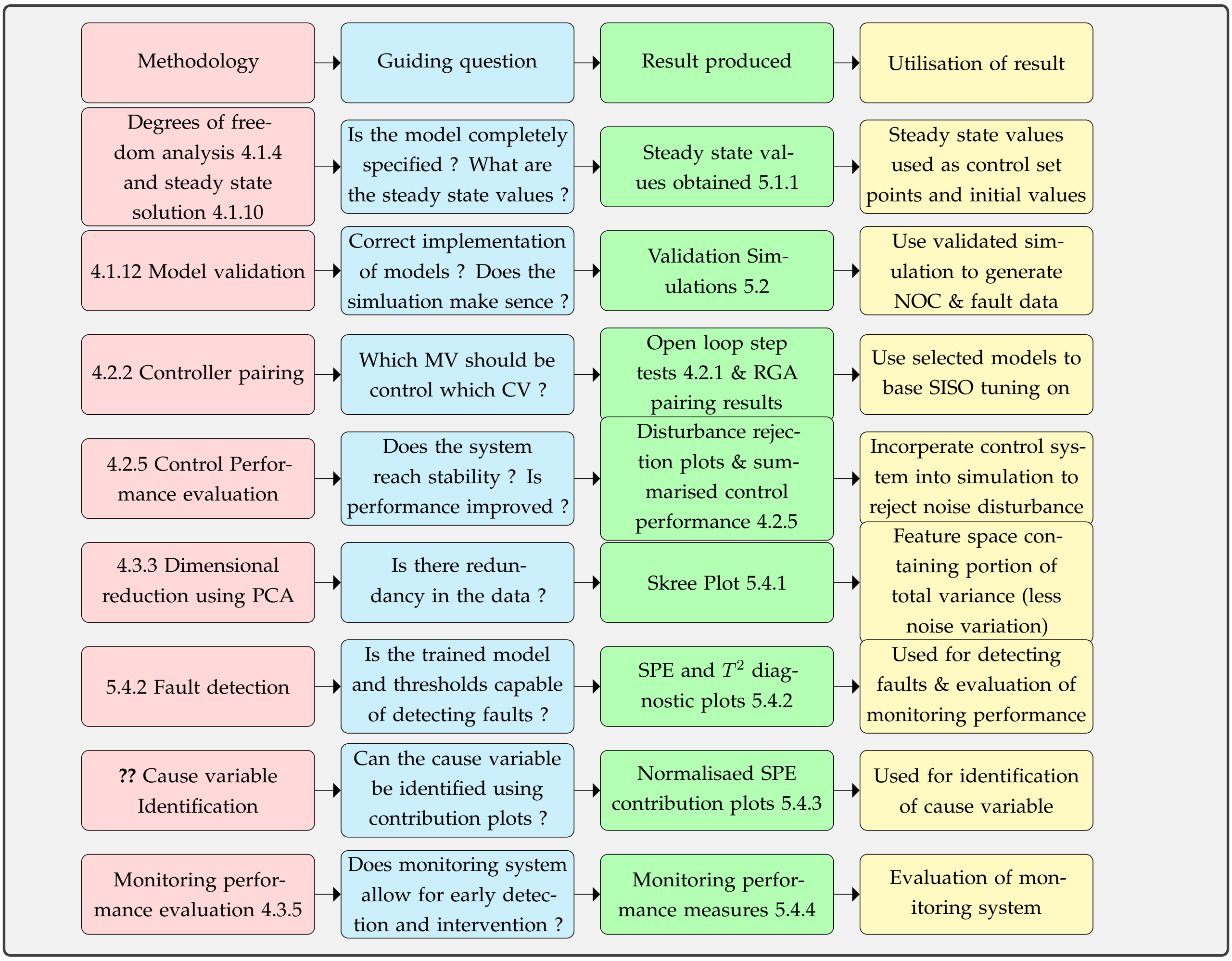


FIGURE 5.1: Summary of Results produced from methodology in Chapter 4

5.1 Modeling

5.1.1 Steady state values

TABLE 5.1: Steady state values obtained

Variable	Description	Steady state value	Variable	Description	Steady state value
1	Reacting gas temperature	614.7 (K)	9	CO_2 composition	0.019
2	Reactor shell temperature	445.82 (K)	10	N_2 composition	0.78
3	Coolant flow rate	8.91 ($\frac{kg}{s}$)	11	O_2 composition	0.16
4	Pressure inside vessel	129821.95 Pa	12	MA composition	0.0004
5	Total molar flow rate at outlet	1800.77 ($\frac{mol}{s}$)	13	NQ composition	0.0017
6	Molar flow rate of NA at inlet	26.74 ($\frac{mol}{s}$)	14	PA composition	0.0083
7	Molar flow rate of air at inlet	1783.08 ($\frac{mol}{s}$)	15	H_2O composition	0.02
8	NA composition	0.0044			

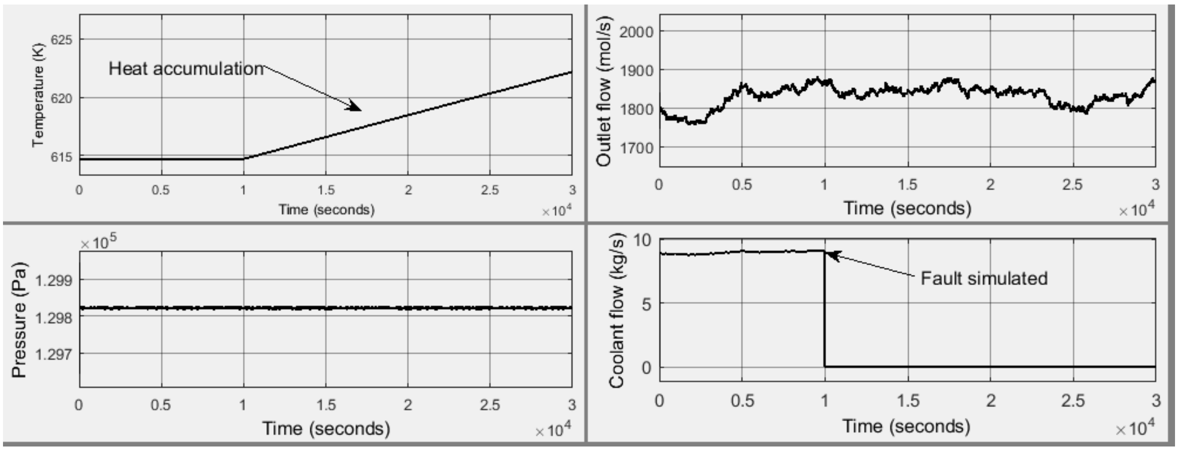
The steady state values obtained from the simulation are summarized in Table 5.1. These values are in the range of the steady state values presented in the literature. All values are sensible and are therefore considered valid.

5.2 Simulation validation

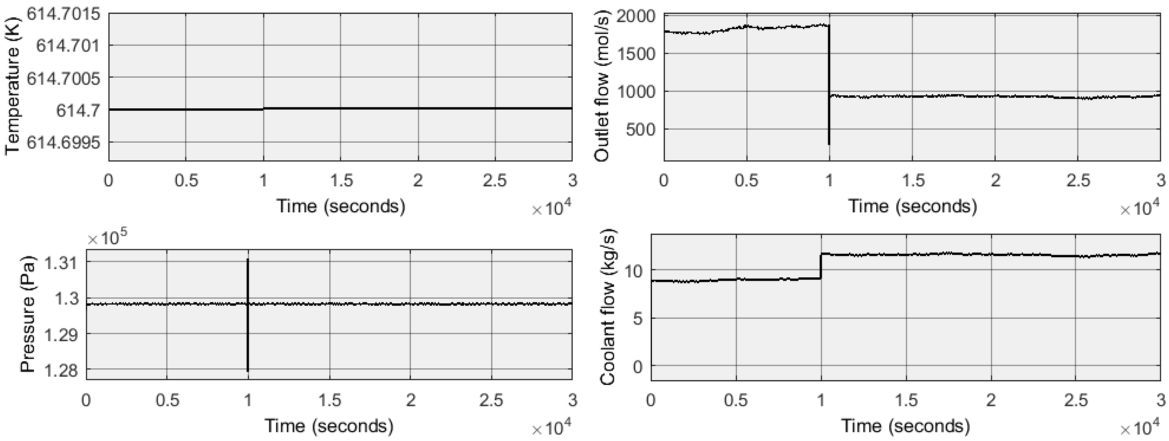
The results of 6 [1] fault scenarios are presented in figures 5.2a to 5.4. The interpretation of these results is used to determine whether the simulation produces correct outputs for the selected process variables: temperature, pressure, outlet flow rate and coolant flow rate. The method of validation is to qualitatively assess these process variables from a chemical engineering understanding of the process models [2] and to conclude whether the outputs are sensible or not.

[1] Due to Simulink block limit, the number of faults was decreased from 10 to 6

[2] The initial approach to matching the dynamic responses of [Kauffman, 1990] was not possible as the model change in 4.1.8 were necessary



(A) Fault 1: Loss of coolant



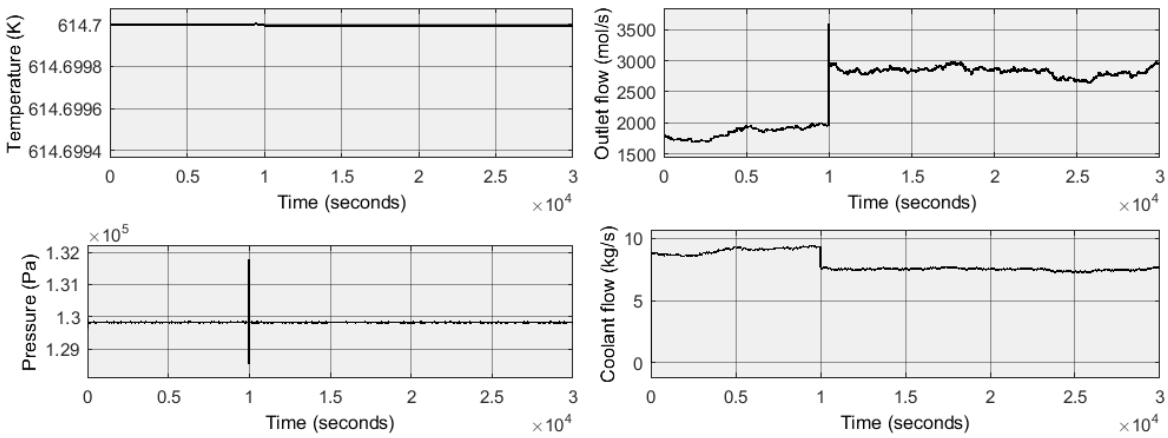
(B) Fault 2: NA/air ratio controller fails high

FIGURE 5.2: Validation results for faults 1 and 2

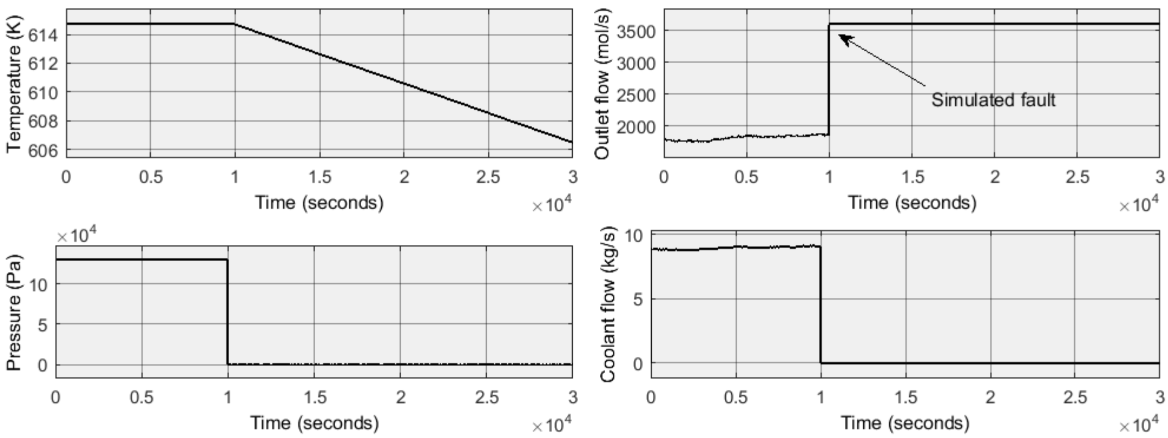
The first simulated fault was to stop the cooling water to the reactor, on a plant, this may occur if a valve fails closed. [3]. In fault 1, figure 5.3 step change in the coolant flow rate can be seen. In the temperature of the reacting gas increases, this is due to an accumulation of energy released from the exothermic reaction as the coolant water is no longer removing this excess heat from the system. There are no significant changes in the pressure or outlet from the rate which indicates that they are relatively independent of the coolant flow rate. All responses to this fault are as expected.

In the second simulated fault, a step change in the feed ratio of NA/air is made to simulate the ratio controller failing high; this may occur if the ratio control fails high. In response, the cooling water flow rate increases due to reaction rate increasing. Moreover, the outlet gas flow rate decreases. The explanation for the coolant flow increasing is that the reaction rate increases with increasing NA, causing the temperature to increase, which is offset by increasing the coolant flow rate. The outlet gas flow rate increases as more air is entering, therefore to keep the pressure at its set point, more gas must leave.

[3]Refer back to 2.2 for a full list of possible reasons



(A) Fault 3: NA/air ratio controller fails low

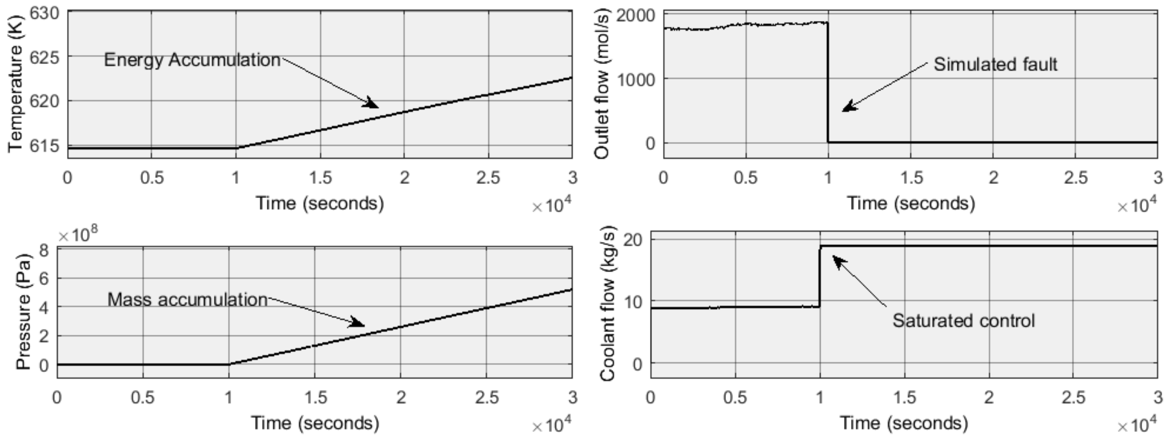


(B) Fault 4: Outlet valve fail open

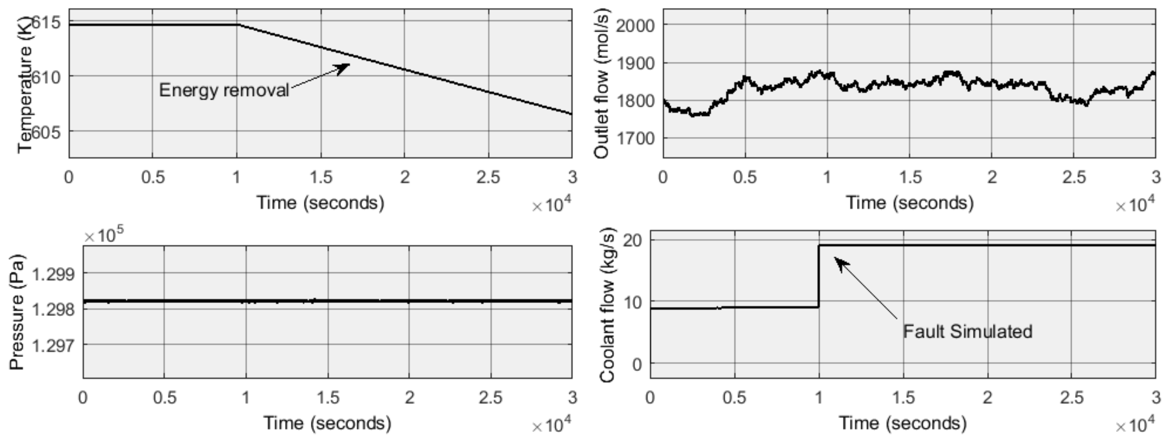
FIGURE 5.3: Validation results for faults 3 and 4

In the third fault simulation, feed ratio failing low is simulated, the exact reverse of the second faults result are expected.

In the fourth fault, the outlet flow rate is increased to its maximum, simulating the outlet valve failing open. The pressure and temperature decrease and since the coolant flow rate controls the temperature, it too decreases until saturation at 0. The model is incapable of considering that the fact that pressure would not realistically reduce to 0, however, other than that, all is as expected.



(A) Fault 5: Outlet valve fail closed



(B) Fault 6: Coolant flow valve fails open

FIGURE 5.4: Validation results for faults 5 and 6

The fifth simulation shows the outlet gas control valve failing shut. As expected, both temperature and pressure increase due to mass and energy accumulation, the coolant flow rate decrease to stabilize the temperature, however, saturates almost instantly. This fault is regarded as the most dangerous and as stated by [Kauffman, 1990], if the pressure release valve fails, there is a possibility of the vessel rupturing. From a design perspective, using a fail open control valve in the outlet gas stream is preferable as failing closed could lead to potential harm of personnel and equipment.

The sixth simulation shows the responses to the coolant control valve failing open. As with the failing closed case, the pressure is unaffected and as expected the temperature decreases as more heat is being removed that the reactor than is being given off by the reaction.

Except for faults 2 and 3, the magnitude of the faults overwhelmed the controllers, leading to saturation in a very short time, implying that operator intervention is necessary to restore the process to its pre-fault condition.

5.3 Control

5.3.1 Control structure summary

The control structure arrived at is summarized in table 5.2 below. From the RGA analysis, it was concluded that the coolant flow rate/temperature and outlet gas flow rate/pressure pairing lead to the least interaction. Initial control parameters were obtained from Direct Synthesis, a trial and error procedure lead to stability in both CV's simultaneously. Control performance is given below. The control performance measures given are the integral absolute error, which represents the cumulative deviation of the controlled variables. The second performance parameter is the variance of the CV around the mean, the lower the variance around the mean the better the control performance as it means that the average deviation from the set point squared is lower.

TABLE 5.2: Control Performance

Performance criteria CV_1= P , CV_2=T	K_{C1} = 0.126 K_{C2}=0.0508	K_{C1} =-0.909 K_{C2} =23255.81 τ_{I1}=-2 τ_{I2}=-2	K_{C1} =-0.909 K_{C2}=232558.13 τ_{I1}=-2 τ_{I2}=-2
AIE CV_1	2.974$x10^4$	7.98	6.35
AIE CV_2	0.6802	0.023	0.02
Variance CV_1		0.8836	0.6656
Variance CV_2		$1.6 * 10^{-13}$	$1 * 10^{-13}$
Stability CV_1	No	Yes	Yes
Stability CV_2	No	Yes	Yes

The control performance presented in table 5.2 highlight the improvements in control as a consequence of the new control design.

The addition of the integral term into the control structure improved performance by integrating the error, thus leading to an elimination of steady-state offset.

5.4 Statistical process control

This section presents the results of fault detection and identification of the six simulated faults described in table 4.2. Detection performance is characterized by detection delays, missing alarm rates, and false alarm rates which are discussed regarding their implications on a plant. Fault identification results are generated to see how well the cause and effect variables can be identified from all possible variables, information that can be utilized in fault diagnosis.

5.4.1 Scree plot

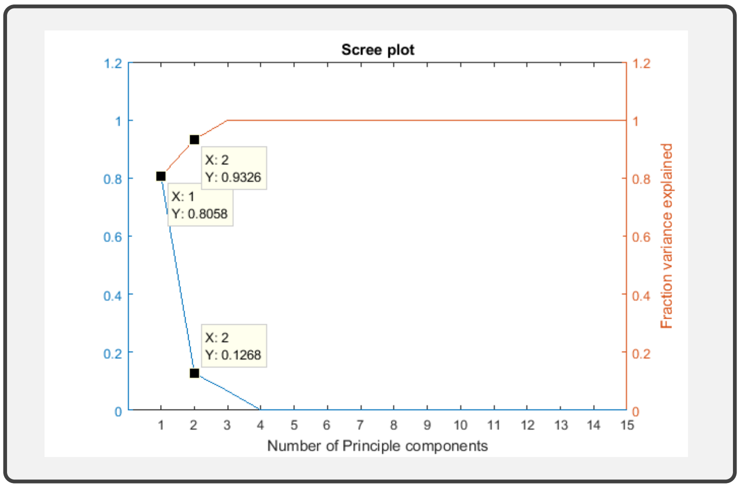


FIGURE 5.5: Scree plot

The scree plot is given in figure 5.5 as a graphical representation of the contribution of principle components to the total variability in the data. It is used to decide how many extracted features to maintain. It can be seen in figure 5.5 that by retaining only 2 out of a possible 15 available features [4], 93% of all the variance can be explained in the feature space. The other 7% is assumed to be a consequence of noise [5] , however, may also be attributed to underlying non-linear relationships which are not taken into account. [6]

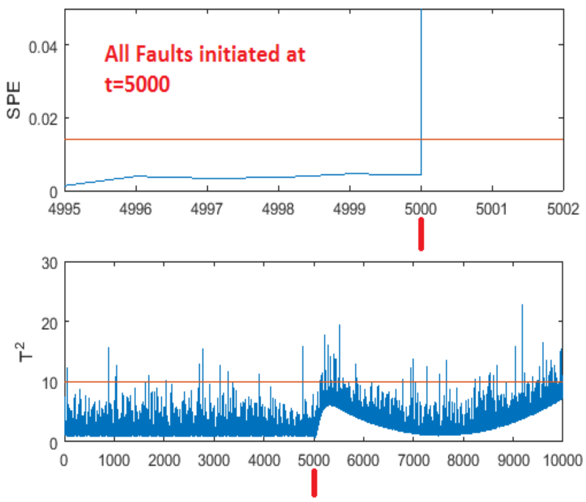
5.4.2 Diagnostic monitoring charts

Figures 5.6 , 5.7 and 5.8 show SPE and T^2 diagnostic monitoring charts are for all six fault simulations. Diagnostic monitoring charts graphically track the residual and feature space diagnostics through time and are used detecting abnormal events.

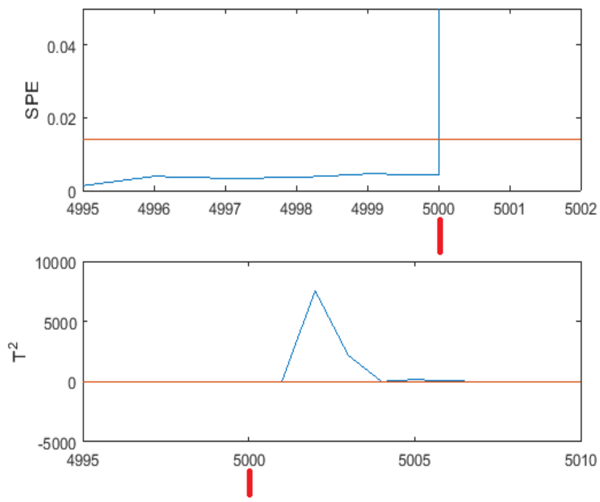
[4] As the feature selection method being used is PCA, the extracted features can also be referred to as principal components or PC axes

[5] Stochastic variation that is not attributed to any causal relationship between two process variables

[6] A non-linear feature extraction method would be used to take this variation into account.



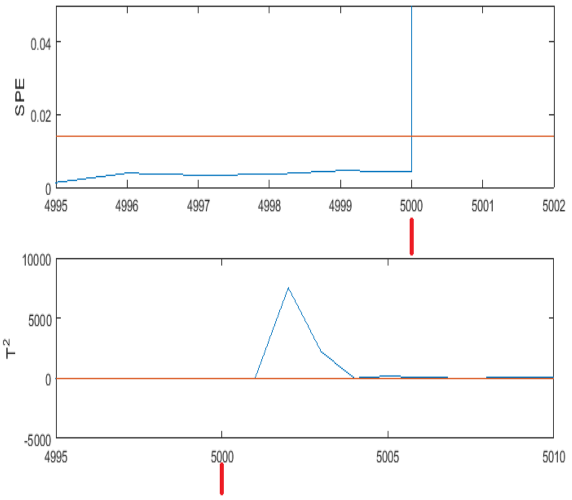
(A) Fault 1: Loss of coolant



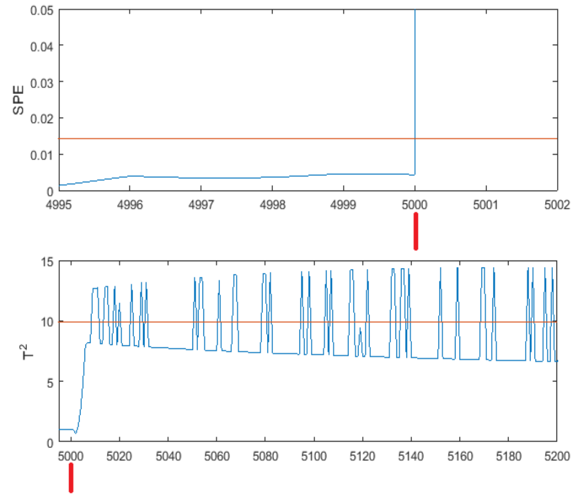
(B) Fault 2: NA/air ratio controller fails high

FIGURE 5.6: Fault 1 and 2

The orange horizontal lines indicate thresholds and the red vertical lines at t= 5000 indicate when the fault was initiated. In all six simulations, the SPE threshold was broken immediately, without any detection delay. Detection in the feature space was also achieved, however with lower performance and a detection delay. SPE detection results from large reconstruction errors due to changes in the relationships between variables. The performance of the SPE monitoring charts is explained by the immediate (step change) and large magnitude changes of the fault. Faults of this size are easy to detect, and it is possible that similar performance would be achieved by univariate methods, showing this, however, requires additional investigation. The usefulness of this method may be in detecting smaller time evolving faults; this too requires additional investigation.

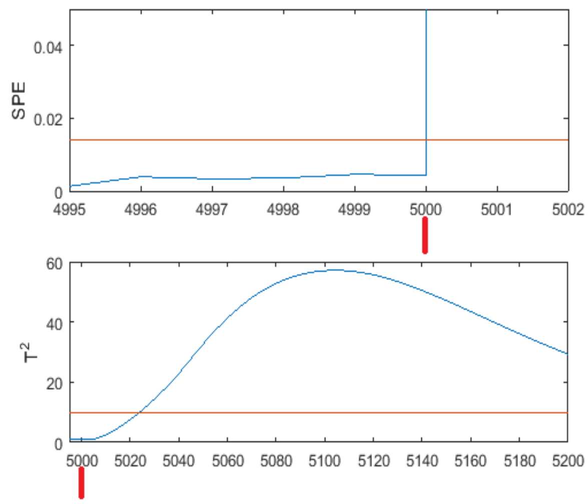


(A) Fault 3: NA/air ratio controller fails high

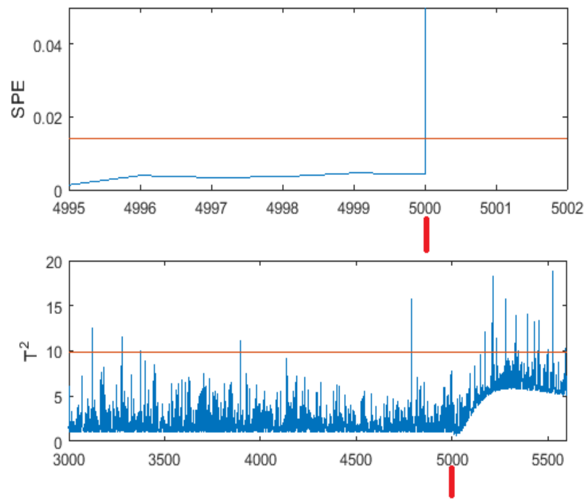


(B) Fault 4: Outlet valve fail open

FIGURE 5.7: Fault: 3 and 4



(A) Fault 5: Outlet valve fail closed



(B) Fault 6: Coolant flow valve fails open

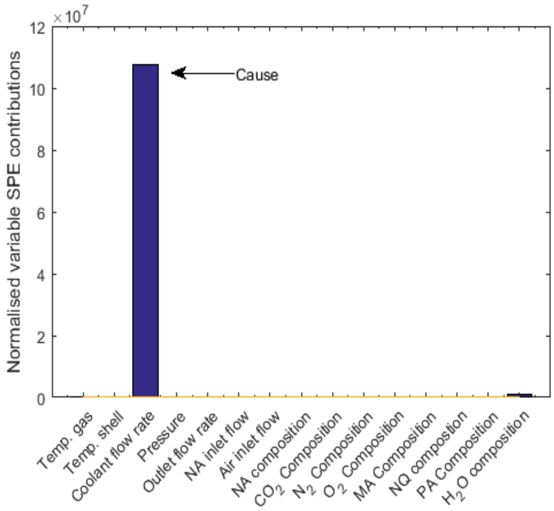
FIGURE 5.8: Fault 5 and 6

For the first fault, the flow rate decreased from its nominal value to zero instantly. This change breaks the existing relationship between the temperature and the coolant imposed via the automatic control algorithm. Similarly, in the second and third faults, the ratio of the feed streams changes, resulting in another changed relationship and detection in the SPE space. The same reasoning applies to the outlet flow rate which is related to the pressure during normal operation, however, during a fault 4 and 5, this relationship is broken. The trends in T^2 diagnostic are harder to interpret. The initial increase in T^2 followed by a decrease in all faults (except with fault one) may indicate a sort of internal feedback mechanism imposed within the model structure. However, this is only speculation.

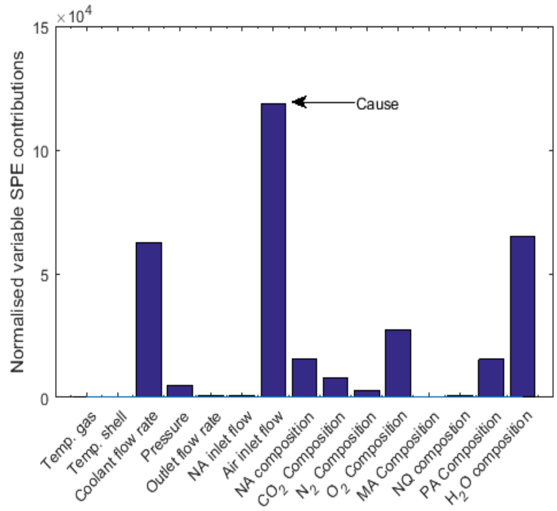
Using this technique, all six faults would be immediately detected proving that this could be successfully deployed as a monitoring solution.

5.4.3 Cause variable Identification

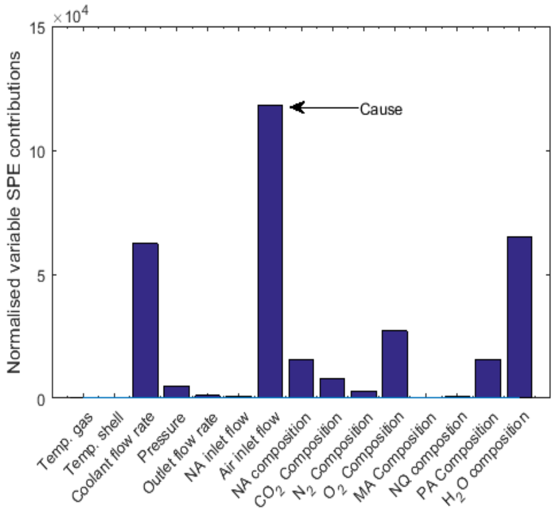
The normalized contribution plot the SPE diagnostic for each of the six faults is given in figure 5.9 with thresholds normalized to one and an arrow to indicate the real cause variable in each fault.



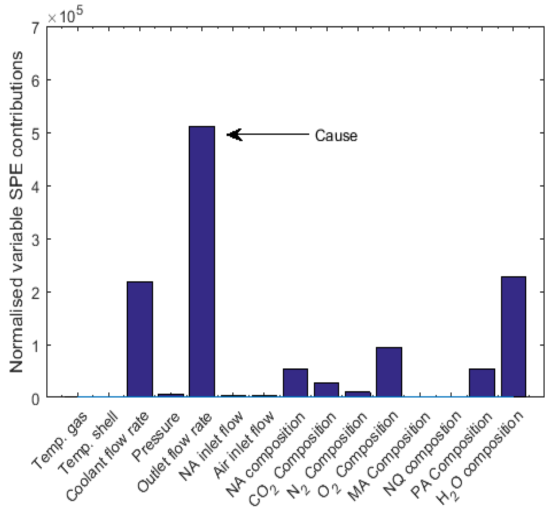
(A) Fault 1: Loss of coolant



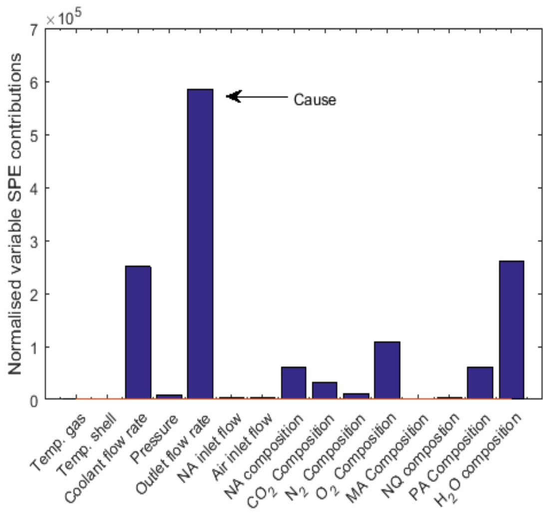
(B) Fault 2: NA/air ratio controller fails high



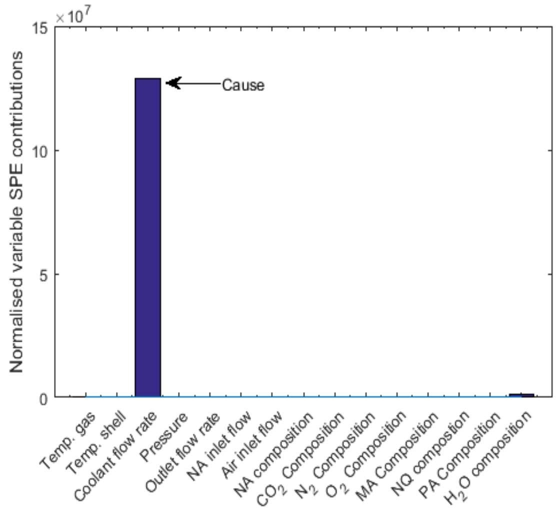
(C) Fault 3: NA/air ratio controller fails low



(D) Fault 4: Outlet valve fail open



(E) Fault 5: Outlet valve fail closed



(F) Fault 6: Coolant flow valve fails open

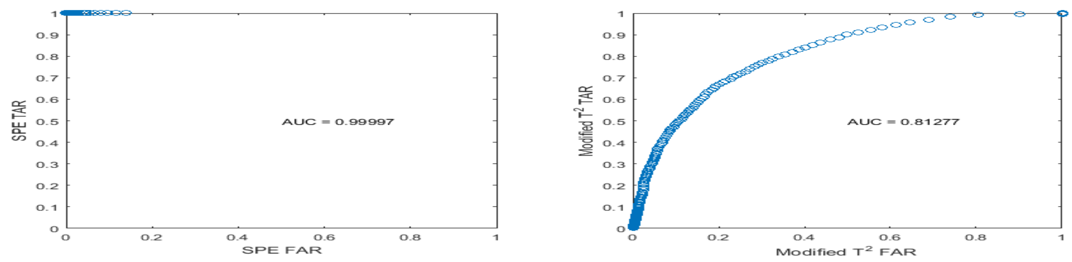
FIGURE 5.9: Contribution plots for all 6 faults at 1 (sec) after the fault is simulated

In every one of the six faults, the highest contribution is the actual cause variable. This is the best case scenario as it allows an operator to immediately identify the cause variable, leaving the maximum amount of time for diagnosing which fault caused this variable to deviate. Additionally, variable contributions other than the cause variable increase above the threshold, this is expected, as causal relationships exist between variables and those contributions represent the effect variables. Note, cause, and effect can occur simultaneously as time delays were not programmed into the simulation, however, would take place in a real system.

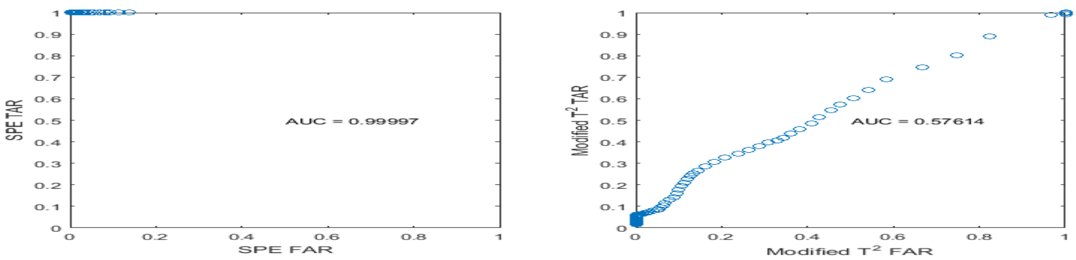
5.4.4 Monitoring Performance

Reciver operator curves

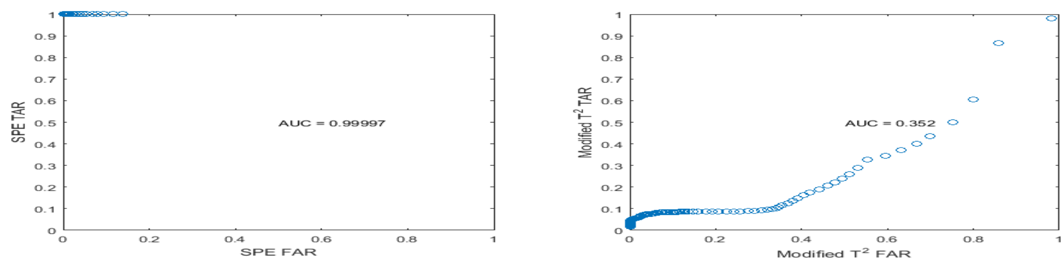
Figure 5.10 is the receiver operator curve (ROC) for all six faults for both.



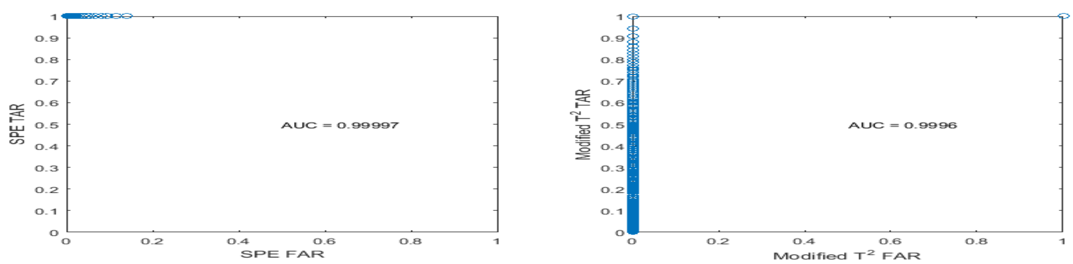
(A) Fault 1: Loss of coolant



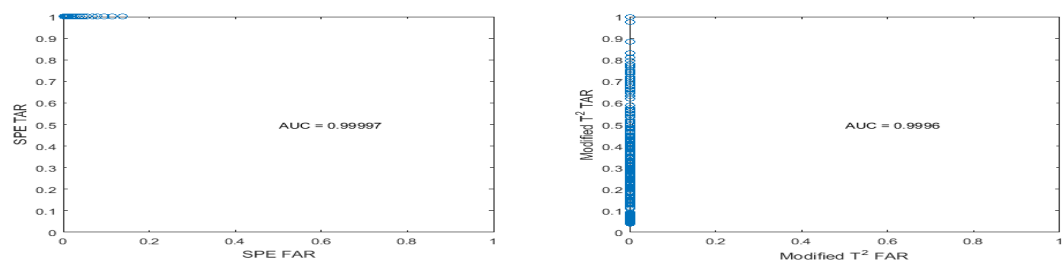
(B) Fault 2: NA/air ratio controller fails high



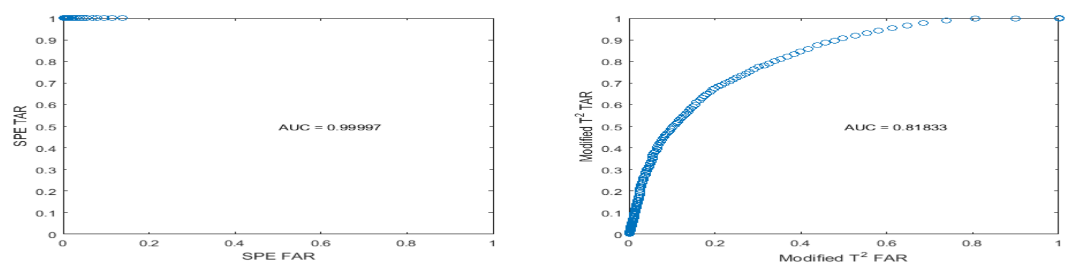
(C) Fault 3: NA/air ratio controller fails low



(D) Fault 4: Outlet valve fail open



(E) Fault 5: Outlet valve fail closed



(F) Fault 6: Coolant flow valve fails open

FIGURE 5.10: Receiver operator curves for all 6 faults in both SPE and T^2

The ROC curves show the false alarm rate (FAR) plotted against the true alarm rate (TAR) for several different choices of the threshold. Ideally, the FAR is close to zero, and, the TAR, close to one. As seen in figure 5.10 the SPE diagnostic ROC has multiple points that lie on, or close to this ideal region. This observation implies that several choices of threshold result in perfect classification indicating that there is a large numerical difference between the SPE diagnostic of fault and normal samples with little to no overlap of distributions. This implication confirms the notion that the size of the faults makes them easy to classify rather than the suitability of the method. Smaller, time evolving faults would have to be investigated to make a conclusion about the suitability of the method to the system.

Performance in the feature space is not ideal and is, therefore, worth discussion. The ROC curve generated for fault one, and six represent the typical trade-off that is expected as explained in 2.3.5. The curve lies above the diagonal, indicating that it is better than guessing. The optimal selection of threshold would depend on the desired performance, most often the point closest to the top left corner. If it is desired to have a low FAR because operators are overwhelmed with constant alarms, then a selection of threshold close to the left-hand side of the curve may be chosen and if detection is desired regardless of the number of false alarms set off then somewhere toward the top of the curve is suggested. In a chemical processing plant, due to the high number of alarms expected from automated control in addition to monitoring, it is recommended that a threshold corresponding to a lower FAR be chosen.

The ROC curve generated by fault 2 represents a classifier that would be only slightly better than guessing with an AUC of close to 0.5 and a curve which passes almost along the horizontal.

The third ROC curve represents a classifier that performs worse than random guessing. A suggested option [Aldrich and Auret, 2013] for such a classifier would be to reverse the classifier such that any sample above the threshold is classified as normal. This suggestion, however, would not be practical unless this were the only fault that could occur.

The ROC curve generated by faults four and five show the same trend, and by choosing the right threshold, the classifier can achieve a perfect performance.

Performance parameters

Table 5.3 summarizes the performance measures for both diagnostics in the monitoring strategy. The measures presented are the detection delay (DD), the alarm run length (ARL), the missing alarm rate (MAR), the false alarm rate (FAR), the true alarm rate (TAR) and the area under the receiver operator curve (AUC).

TABLE 5.3: Monitoring performance parameters

T^2/SPE	DD	ARL	MAR	FAR	TAR	AUC
Fault 1	200/0	10/-	0.9/0	0.4/0.01	0.75/1	0.81/0.99
Fault 2	2/0	3/-	0.8/0	0.6/0.01	0.6/1	0.58/0.99
Fault 3	2/0	3/-	0.8/0	0.2/0.01	0.4/1	0.35/0.99
Fault 4	5/0	10/-	0.55/0	0.01/0.01	0.8/1	0.99/0.99
Fault 5	20/0	200/-	0.45/0	0.01/0.01	0.8/1	0.99/0.99
Fault 6	200/0	100/-	0.4/0	0.4/0.01	0.6/1	0.82/0.99

Detection delays

Table 5.3 shows that there is no detection delay in the SPE monitoring space and that there are varying detection delays in the T^2 space. SPE outperforming T^2 as a monitoring diagnostic is because the type of fault that is selected causes changes in the relationships between variables. This reason holds true for all performance parameters and is not discussed further. The instant detection delay for all faults means that detection is not a limiting step in recovery action.

Alarm run length

Table 5.3 shows once a fault occurs the alarm will not go off unless manually switched off. There is no indication that the SPE will go back below the threshold, even if T^2 does.

Missing alarm rate

Table 5.3 shows that no alarms are missed in the SPE space and that performance in T^2 varies. Since either diagnostic may activate an alarm, no alarms will be missed if this strategy is deployed.

False alarm rate

Note although the choice of a 99th percentile ensures a false detection rate of 0.01, it does not necessarily imply that there must be false alarms[7] during NOC. By programming the alarm only to be activated only if, for example, five samples are detected in a row, the real false alarms heard by the operator during NOC may be heavily diminished. The obvious motivation for doing this is that too many false alarms may cause operators to become unresponsive or overwhelmed. For example, if an actual alarm were activated incorrectly every 100 samples on average for the sampling time of 1 second, there would be an alarm going off at least once every 2 minutes from the monitoring system alone.

[7] Referring to physical alarms that operators will hear

True alarm rate

Table 5.3 again as expected shows perfect true alarm rates for the SPE monitoring space and varying performance in the T^2 space.

Area under curve

Table 5.3 shows that the AUC is 0.99 for all faults in the SPE monitoring space. This means there is ideal performance regardless of the choice of threshold further confirming that the faults are easy to detect.

5.5 Process recovery actions

Following the successful detection of a fault, an operator can use the contribution plot (see figure 5.9) to identify the cause variable after which, the fault diagram is given in section 2.1.2 can be used to troubleshoot. For example, if the cause variable is identified as the cooling flow water, the possible thing to look for are: V-14 closed by mistake, V-13 closed by mistake, an incorrect set point causing TCV-14 to close, the controller failing to cause TCV-14 to close, TCV-14 to fail closed or the upstream valves of pump P-201 A or B may be closed by mistake. A P&ID reproduced from [Kauffman, 1990] is provided in the Appendix B.

Chapter 6

Conclusions and recommendations

The aim of this study was to evaluate the performance of the linear PCA algorithm as the feature extraction technique in the fault diagnosis framework. The purpose of this aim is to establish a suitable monitoring method for the PAR system.

All objectives defined for this project were achieved. The first objective was to implement and validate the closed loop PAR model. An adaption to the initial model was made as a degree of freedom analysis revealed that the model was under-constrained. Furthermore, a comparison with published literature showed that the kinetics model was incorrect. Therefore, instead of matching the dynamic response curves to those found in literature, the model was validated qualitatively. Time series responses of the main process variables to simulated faults were interpreted and it was found that all responses were sensible. Consequently the simulation was considered validated.

The second objective was to design, implement and assess an improved control strategy. The controllers were improved from P to PI feedback controllers which allowed for steady state offset to be eliminated. The design of the control system was achieved by pairing the controlled and manipulated variables with the RGA approach, then using direct synthesis approach in single loop tuning. To account for interaction, the tuning constants were de-tuned. The designed feedback controllers were implemented in controlling the PAR model in the Simulink environment and assessed with the relative performance measure IAE and standard deviation. Overall system stability was achieved and steady state offset eliminated.

The third objective was to model and simulated six selected faults. These were successfully implemented with sensible response curves generated.

The fourth objective was to design, implement and assess a process monitoring strategy, allowing for detection and identification of the simulated fault scenarios. This objective was achieved. PCA model parameters were trained using simulated steady state data. The scree plot method was used in selecting the number of extracted features. Perfect detection performance and identification were achieved for all simulated faults.

The results presented in this paper successfully demonstrated that the PCA algorithm is a viable monitoring approach for the PAR system. Fault classification performance was near perfect, with no detection delay. Cause variable identification was also successful in all six faults. This monitoring strategy could, therefore, be successfully deployed onto the PAR system to monitor these six faults.

It was, however, also concluded that the good performance presented, is due to the magnitude of the simulated faults, making them easy to detect. This fact complicates making a conclusion about the suitability of the method to the system. For faults of this magnitude, it is unclear if multivariate methods offer any advantage in performance over univariate methods, or if performance in both cases would be perfect. A comparison of performance between these two strategies would be necessary to make this conclusion.

To improve on this aspect of the study, smaller faults, should be investigated to check the utility of the method for detecting more difficult, slower evolving faults, not just dramatic faults. These should bring the sdata to a region of detection where different methods have different performance.

Furthermore, by investigating only one fault monitoring strategy limited conclusions that can be made. No judgment can be made as to whether applying this method to this system offers any advantages over other methods.

Appendix A

Minutes of meeting

Department of Process Engineering
Final Year Project (CE 478 | MP 478) – Project Approval Form

Name of Supervisor	Student Name and Number
Dr L Auret	JL Pickard (16565088)

Project Title

Fault modelling and diagnosis for a phthalic anhydride reactor

Project Description and Objectives

The overall aim of the project is to devise process monitoring strategies to detect and identify faults (abnormal events) that may lead to catastrophic failure of a phthalic anhydride reactor (PAR). The scope of the project is limited to a PAR dynamic model (Kauffman and Chen, 1990). The objectives are the following:

- Implement and validate the dynamic PHR model.
- Design, implement and assess an improved control strategy for the PHR.
- Model ten fault scenarios presented by Kauffman and Chen (1990).
- Design, implement and assess process monitoring strategies for early detection and identification of the ten fault scenarios.

Project Outcome and Deliverables

The following requirements have to be met for the project to be considered successful:

- Successful implementation and validation of closed-loop PAR model (with base case control): matching dynamic responses in Kauffman and Chen (1990).
- Successful design and implementation of improved control strategy for PAR model: system stability achieved, and strategy assessed in terms of control performance measures.
- Modelling and simulation of ten fault scenarios in PAR model, as specified by Kauffman and Chen (1990).
- Successful design and implementation of monitoring strategies for PAR model: sensible selection of univariate and/or multivariate monitoring strategy and evaluation of monitoring performance.
- Suggestion of possible process recovery actions on successful detection and identification of fault scenarios.

Project Characteristics and Requirements

Applicability to Chemical Engineering: The student must engage with selected knowledge in the research literature of the chemical engineering discipline. Briefly describe the relevance of this project to chemical engineering.

Dynamic modelling, control and process monitoring are significant chemical engineering activities.

References: Are sufficient literature sources available and accessible to support this topic? Provide at least two examples.

The references appropriate for this project cover topics on dynamic modelling and simulation, process control, and monitoring. These topics are generally well-covered in undergraduate modelling and control textbooks, e.g.:

- Seborg, D.E., Edgar, T.F., Mellichamp, D.A., Doyle, F.J. 2011. Process dynamics and control. Third edition. Wiley.

The specific system to be modelled is presented in the following paper:

- Kauffman, D., Chen, H. 1990. Fault-dynamic modelling of a phthalic anhydride reactor. Journal of Loss Prevention in the Process Industries. 3, 386 – 394.

Infrastructure, Resources and Funding: Are there special infrastructure, resource or funding requirements for this project? If so, specify how these will be provided.

No special infrastructure. In terms of resources: a MATLAB student licence will be purchased for the student, for installation on their personal computer. Funding will be required for the student licence.

ECSA Exit Level Outcomes

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Final Year Project (CE 478 | MP 478) – Project Approval Form

2. Application of scientific and engineering knowledge: Apply knowledge of mathematics, natural sciences, engineering fundamentals and an engineering speciality to solve complex engineering problems.

Knowledge of the following areas of mathematics and/or natural science and/or engineering fundamentals shall be applied:
- Dynamic modelling and simulation, based on ordinary differential equations.
- Process control strategy design and testing.
- Statistical techniques for process monitoring.

Sufficient complexity shall be captured in:
- Complexity of simulation model.
- Thorough validation of simulation model.
- Control design approach and control performance assessment.
- Nature and implementation of statistical monitoring techniques.

4. Investigations, experiments and data analysis: Demonstrate competence to design and conduct investigations and experiments.

Investigations:
- Identification of appropriate monitoring strategies.

Experiments:
- Model implementation and model validation simulations.
- Control strategy implementation and simulations.
- Fault scenario implementation and simulations.
- Monitoring implementation and simulations.

Data analysis:
- Model validation analyses.
- Control performance analyses.
- Monitoring performance analyses.

6. Professional and technical communication: Demonstrate competence to communicate effectively, both orally and in writing, with engineering audiences and the community at large.

A well-structured, well-written, professional technical report shall be submitted for assessment. In addition, oral and poster presentations shall be delivered to examiners as part of the formal assessment.

8. Individual, team and multidisciplinary work: Demonstrate competence to work effectively as an individual, in teams and in multidisciplinary environments.

The student shall work under the guidance of a supervisor. The supervisor shall provide sound, professional advice and administrative support, but shall not do the work on behalf of the student. The student shall therefore demonstrate competence to interact, devise and conduct the investigation effectively as an individual, as follows:
- Keeping record of all minutes of meetings; adhering to deadlines, etc.
- Do all simulation work and subsequent analyses of results on his/her own.
- Write all reports on his/her own.

9. Independent learning ability: Demonstrate competence to engage in independent learning through well-developed learning skills.

The student shall engage, independently and without formal lecturing, with new theoretical and/or practical concepts. Key concepts and skills to be mastered independently are:
- Fault modelling.
- Process monitoring: techniques and performance analyses.

Criteria for continuation of project (items to be delivered by June)

Department of Process Engineering
Final Year Project (CE 478 | MP 478) – Project Approval Form

- Closed-loop PAR simulation (base case control and improved).
- Model validation results.
- At least three fault scenarios modelled.

Sign-off: This project has been registered and reviewed by the Department of Process Engineering, and accepted as suitable for a Final Year Project.

	Signature	Date
Supervisor		24/02/2016
Student		24/02/2016
Coordinator	A.J. Burger	2016-02-27

Department of Process Engineering

Final Year Project (CE 478 | MP 478) – Short Minutes of Meeting

Name	Signature	Date
Johann Pickard		12/2/2016
Dr Auret		12/2/2016 03/03/2016

Problems experienced and progress made since previous meeting

- Not applicable, first meeting
- Discussed
    o Control charts for the purpose of detecting faults
    o Univariate methods
    o Multivariate methods
- Noise in simulation
- Hotellings Tsq statistic

Decisions, as well as actions to be taken after meeting	Responsible	Deadline
- Read up about multi and univariate methods		Continuous
- Possible approach, PCA		Continuous
- Read up about Hotelling's Tsq statistic		Continuous

All parties present must sign these short minutes at the end of the meeting. Scan the signed document and send an electronic copy to your supervisor within 48 hours after the meeting. The original must be included in an appendix of your final report.

Department of Process Engineering
Final Year Project (CE 478 | MP 478) – Short Minutes of Meeting

Name	Signature	Date
Johann Pickard		4/3/2016
Dr Auret		4/3/2016 03/11/2016

Problems experienced and progress made since previous meeting
- Uncertain of how a fault is identified once detected - Question: does PCA allow you to choose the number of measuring devices - Question: Are we looking for patterns in the monitoring charts   o Western electric and Nelson control rules - Question: is corrective action automated

Decisions, as well as actions to be taken after meeting	Responsible	Deadline
- Read up about identification (contribution plots)		Continuous
- Response not automated, compile list of operator responses		NA
- PCA is dimensional reduction not selecting number of dimensions		NA
- Read up about PCA		Continuous
- Read up about what a diagnostic is		Continuous

All parties present must sign these short minutes at the end of the meeting. Scan the signed document and send an electronic copy to your supervisor within 48 hours after the meeting. The original must be included in an appendix of your final report.

Department of Process Engineering
Final Year Project (CE 478 | MP 478) – Short Minutes of Meeting

Name	Signature	Date
Johann Pickard		8/4/2016
Dr Auret		8/4/2016 03/11/2016

Problems experienced and progress made since previous meeting
- Degrees of freedom in model - Additional equations required - Lots of missing data (heat capacities, heats of reactions) - Should detection require that both thresholds SPE and Tsq be broken? - Why is there an error in PCA model? - Quantifying detection

Decisions, as well as actions to be taken after meeting	Responsible	Deadline
- Additional model required to constrain system, try ideal gas law		Next meeting
- Determine all missing data, heats of reaction etc from literature		Continuous
- Read up about performance quantification		Continuous
- Read up about EWMA		Continuous
- Read up about selecting subset of features, explained variance		Continuous
- SPE and Tsq detect different changes		Continuous

All parties present must sign these short minutes at the end of the meeting. Scan the signed document and send an electronic copy to your supervisor within 48 hours after the meeting. The original must be included in an appendix of your final report.

Department of Process Engineering
Final Year Project (CE 478 | MP 478) – Short Minutes of Meeting

Name	Signature	Date
Johann Pickard		22/6/2016
Dr Auret	R Auret 22/09/2016	~~22/6/2016~~

Problems experienced and progress made since previous meeting
- Identified unit error bugs in code - Identified sign error in code cause massive error - Identified missing information relating to cooling utility focus on one case

Decisions, as well as actions to be taken after meeting	Responsible	Deadline
- Simplification of cooling water cases -Only consider single case of cooling water ✓ - Make as many additional simplifying assumptions as necessary ✓		29/6/2016
- Email weekly progress emails ✓		Continuous

All parties present must sign these short minutes at the end of the meeting. Scan the signed document and send an electronic copy to your supervisor within 48 hours after the meeting. The original must be included in an appendix of your final report.

Department of Process Engineering
Final Year Project (CE 478 | MP 478) – Short Minutes of Meeting

Name	Signature	Date
Johann Pickard		6/5/2016
Dr Auret	L Auret	6/5/2015 3/11/2016

Problems experienced and progress made since previous meeting
- Heat capacity as a function of temperature in Simulink - Changing between cooling cases - Validating model - Bugs in Simulink

Decisions, as well as actions to be taken after meeting	Responsible	Deadline
- Use logic blocks in Simulink, to switch between cooling cases - Model validation by comparison with curves generated in original article - Decomposing the signal to solve for temperature - Definite integral for heat capacity integration		

All parties present must sign these short minutes at the end of the meeting. Scan the signed document and send an electronic copy to your supervisor within 48 hours after the meeting. The original must be included in an appendix of your final report.

Department of Process Engineering
Final Year Project (CE 478 | MP 478) – Short Minutes of Meeting

Name	Signature	Date
Johann Pickard		15/9/2016
Dr Auret	L Auret 26/09/2016	~~15/9/2016~~

Problems experienced and progress made since previous meeting

- Discussed project scope with regard to principle component analysis.
  o Reconstruction of Hotelling's T^2 not in scope. Contributions
  o Difference between supervised and unsupervised learning.
  o Supervised learning not in scope ✓
- Discussed simplification of kinetic model. (earlier)
- Layout of showing model interaction in visio rather than Simulink.
- Agreed to reduce number of faults due to block limit on student version of Simulink.
Structure of report [illegible] (earlier)

Decisions, as well as actions to be taken after meeting	Responsible	Deadline
- Agreed to hand in a skeleton structure of the report		23/09/2016
- Simplification of kinetic model.		
o Irregular output from literature model from test which project is based		23/09/2016
- Prelinary literature report. ✗ (handwritten correction: "imi")		23/09/2016
- Discussed project scope with regard to principle component analysis.		
o Reconstruction of Hotelling's T^2 not in scope.		NA
o Difference between supervised and unsupervised learning established that supervised learning is out of scope.		NA

All parties present must sign these short minutes at the end of the meeting. Scan the signed document and send an electronic copy to your supervisor within 48 hours after the meeting. The original must be included in an appendix of your final report.

Department of Process Engineering
Final Year Project (CE 478 | MP 478) – Short Minutes of Meeting

Name	Signature	Date
Johann Pickard		26/9/2017
Dr Auret	L Auret 7/10/2016	26/9/2017

Problems experienced and progress made since previous meeting
- Inclusion of time delays (in relation controller tuning) - Choosing a tuning method DS - Discussion on aims, what is expected - Algebraic loop problem when including integral block in PI controller (only happen when I do this)

Decisions, as well as actions to be taken after meeting	Responsible	Deadline
- Read up on direct synthesis tuning method from Seborg - Added direct synthesis to methods - Read up on Ciacone tuning and added to methods - Read up on graphical empirical model identification and put in methods - Updated aim of investigation in repot - Motivation and background for introduction written.	?	?

All parties present must sign these short minutes at the end of the meeting. Scan the signed document and send an electronic copy to your supervisor within 48 hours after the meeting. The original must be included in an appendix of your final report.

Department of Process Engineering
Final Year Project (CE 478 | MP 478) – Short Minutes of Meeting Date of meeting

Name	Signature	Date
Johann Pickard		17/10/2016
Dr Auret	L Auret	17/10/2016

Problems experienced and progress made since previous meeting
- ~~Understanding parametric distribution assumption.~~ - Setting confidence intervals at 99th percentile. → contribution plot - Distinguishing between identified cause and effect variables. ✓ - Unsure of how much to emphasize/not emphasize control tying into objectives; use control design procedure

Decisions, as well as actions to be taken after meeting	Responsible	Deadline
- Not focus on distinguishing between cause and effect in "diagnosis step" unless time at the end	✓	NA
- Use either average or 99th percentile in setting up thresholds.		10/17/2016

All parties present must sign these short minutes at the end of the meeting. Scan the signed document and send an electronic copy to your supervisor within 48 hours after the meeting. The original must be included in an appendix of your final report.

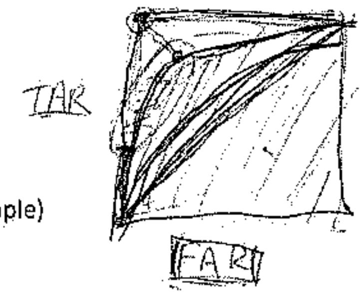
Department of Process Engineering
Final Year Project (CE 478 | MP 478) – Short Minutes of Meeting

Name	Signature	Date
Johann Pickard		27/10/2016
Dr Auret	Auret	27/10/2016

Problems experienced and progress made since previous meeting

- Questions about
  - I.i.d assumption
  - Central limit theorem
  - Hotteling Tsq geometrical interpretation clarification — Hotelling's
  - Including code into report (methodology)
  - ROC quantifies overlap?
  - Necessary to determine autocorrelation (plot against previous sample) — outside scope
  - Definition of Chi square distribution
    - Degrees of freedom
  - Assuming underlying parametric vs empirical
  - Law large numbers
  - Where do we scale by std dev in Hotelling ?
- Progress made
  - Controllers works (analytical expression obtained from direct synthesis)
  - NOC simulation working
  - Fault simulation working
  - Training parameters obtained
    - Thresholds set empirically at 99th percentile
  - MIMO pairing done using RGA (Derivatives of CVS used as CVS)

$m = 15$
$a = 3$

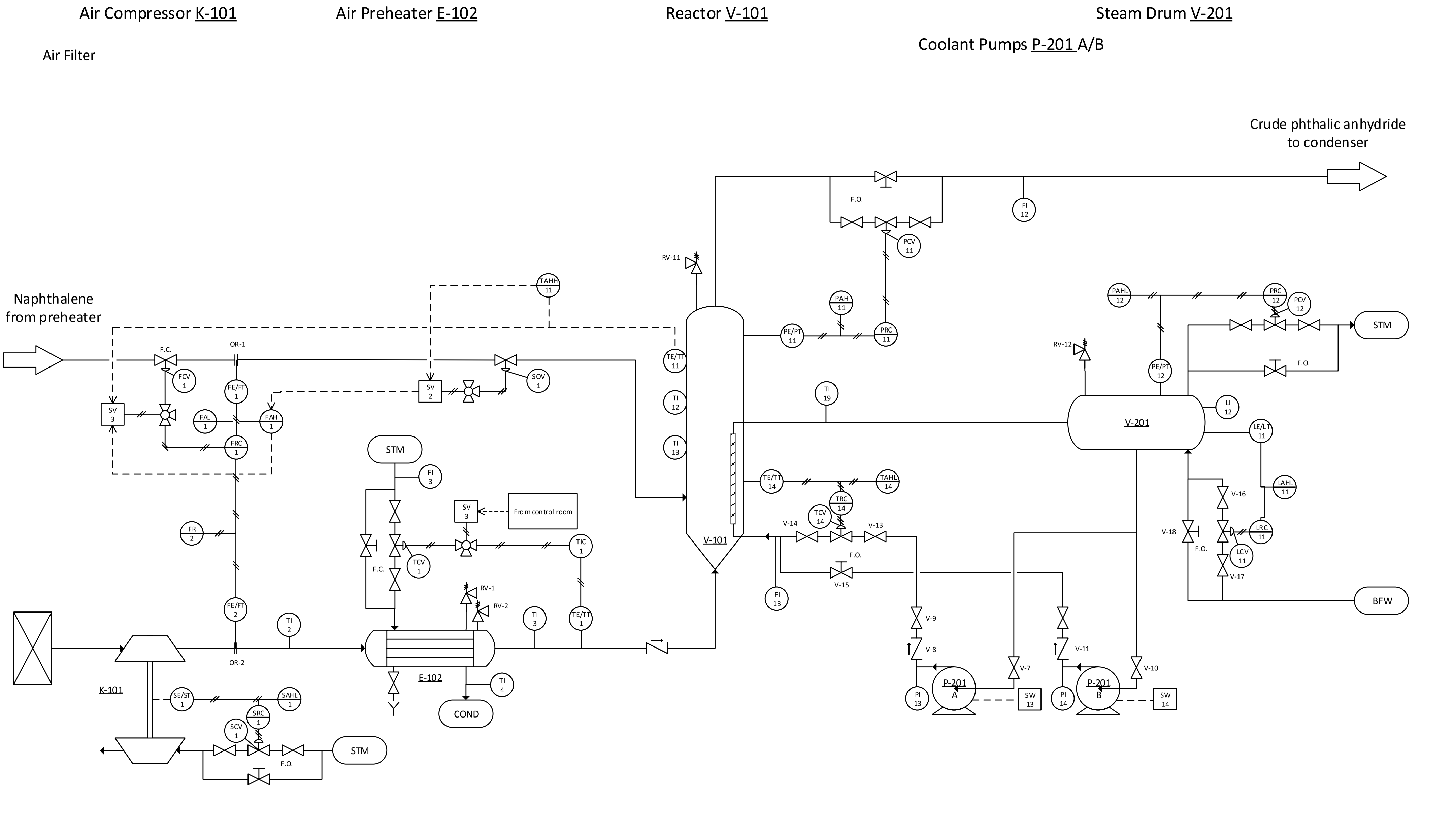


Decisions, as well as actions to be taken after meeting	Responsible	Deadline
Finish draft	JP	31/10

All parties present must sign these short minutes at the end of the meeting. Scan the signed document and send an electronic copy to your supervisor within 48 hours after the meeting. The original must be included in an appendix of your final report.

Appendix B

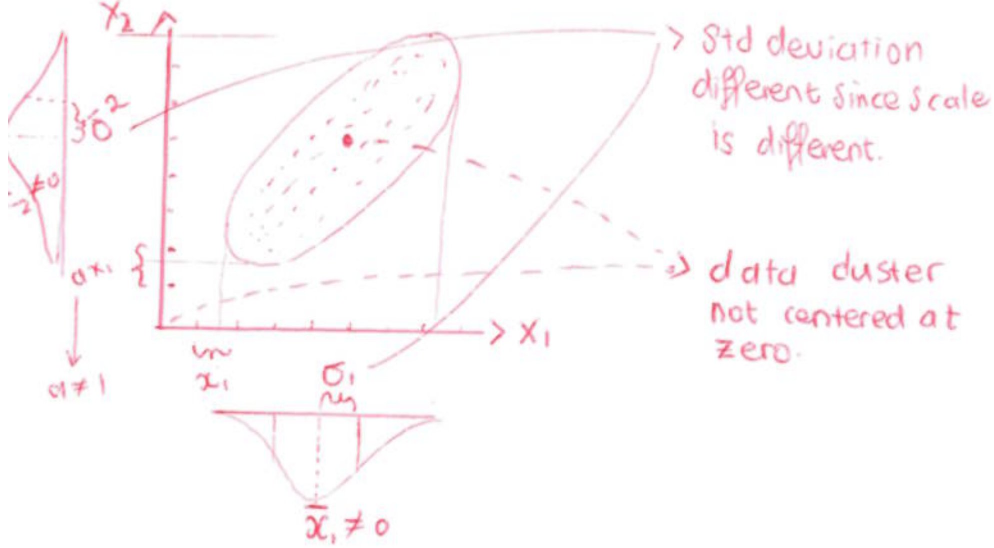
Piping and instrumentation diagram



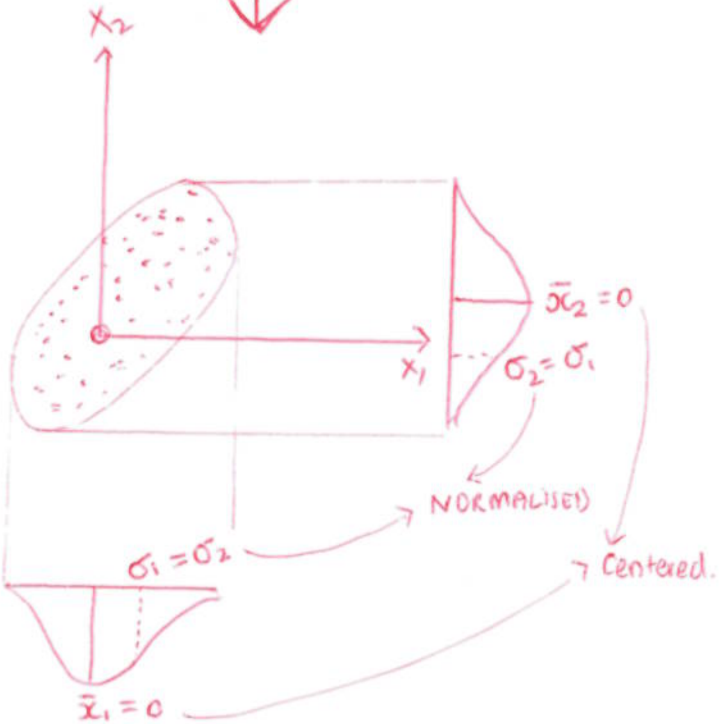
Description:	P&ID of Phthalic Anhydride Reactor
Drawn by:	Johann Pickard
Student number:	16565088

Appendix C

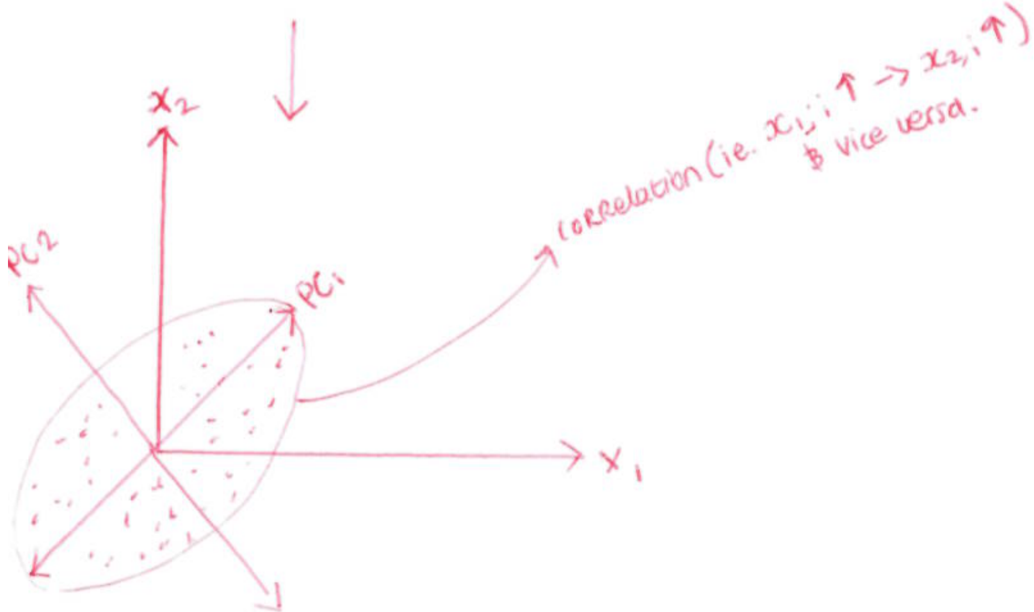
Graphical explanations



X_2
σ^2
$\bar{x}_2 \neq 0$
$a x_1$
$a \neq 1$
X_1
x_1
σ_1
$\bar{x}_1 \neq 0$
Std deviation different since scale is different.
data cluster not centered at zero.

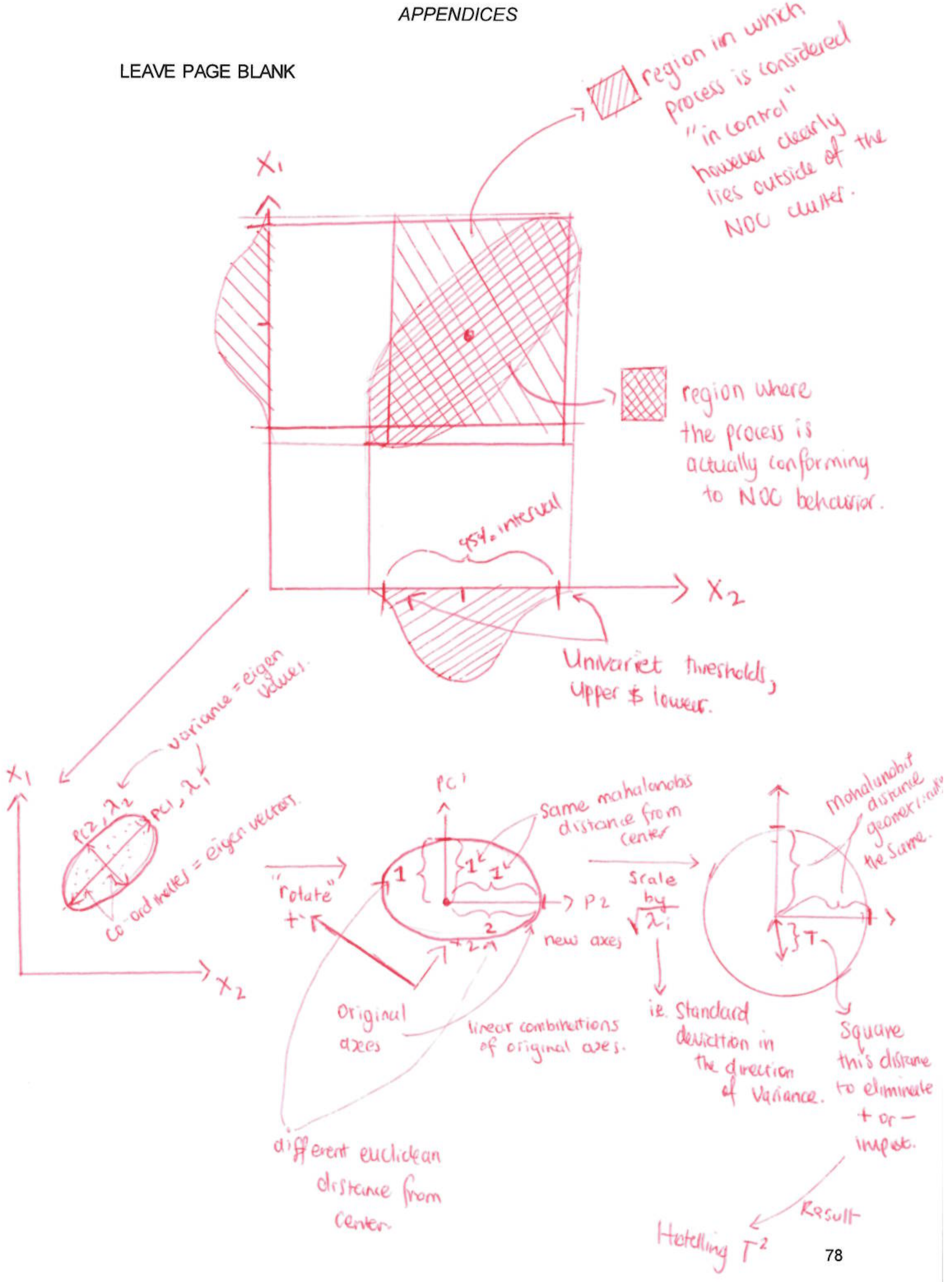


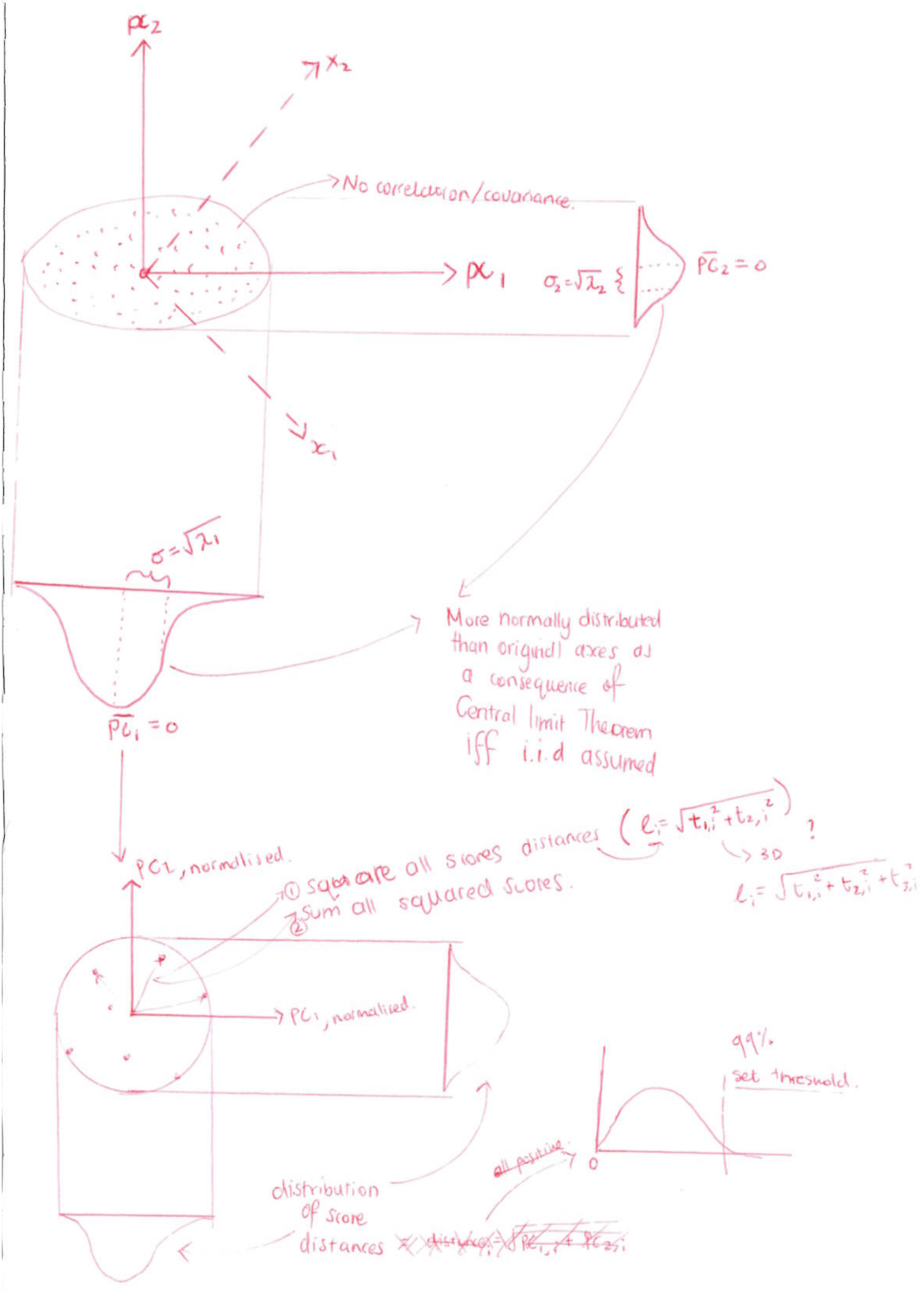
X_2
X_1
$\bar{x}_2 = 0$
$\sigma_2 = \sigma_1$
NORMALISED
$\sigma_1 = \sigma_2$
Centered.
$\bar{x}_1 = 0$



X_2
PC2
PC1
X_1
correlation (ie. $x_{1,i} \uparrow \rightarrow x_{2,i} \uparrow$) & vice versa.

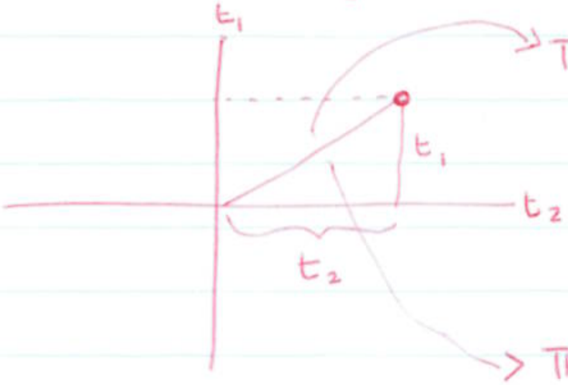
LEAVE PAGE BLANK





PC_2
x_2
No correlation/covariance.
PC_1
$\sigma_2 = \sqrt{\lambda_2}$
$\overline{PC_2} = 0$
x_1
$\sigma = \sqrt{\lambda_1}$
More normally distributed than original axes as a consequence of Central limit Theorem iff i.i.d assumed
$\overline{PC_1} = 0$
PC2, normalised.
① square all scores
② Sum all squared scores.
distances $\left(l_i = \sqrt{t_{1,i}^2 + t_{2,i}^2} \right)$?
3D
$l_i = \sqrt{t_{1,i}^2 + t_{2,i}^2 + t_{3,i}^2}$
PC1, normalised.
99%
set threshold.
~~all positive~~
0
distribution of score distances ~~distance = $\sqrt{PC_{1,i}^2 + PC_{2,i}^2}$~~

Hotelling T^2



$$T^2 = t_1^2 + t_2^2$$

This distance from the center squared.

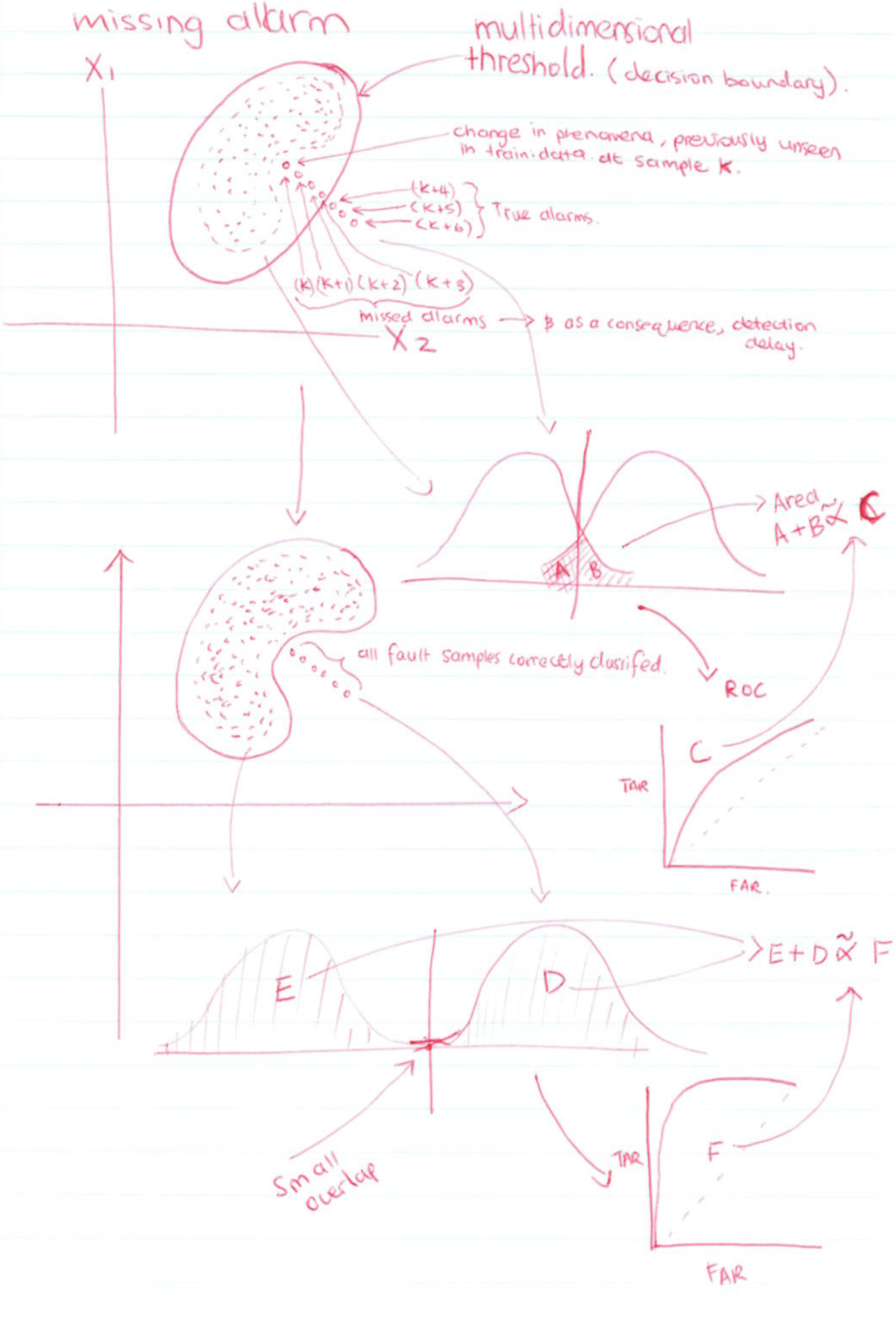
1 sample

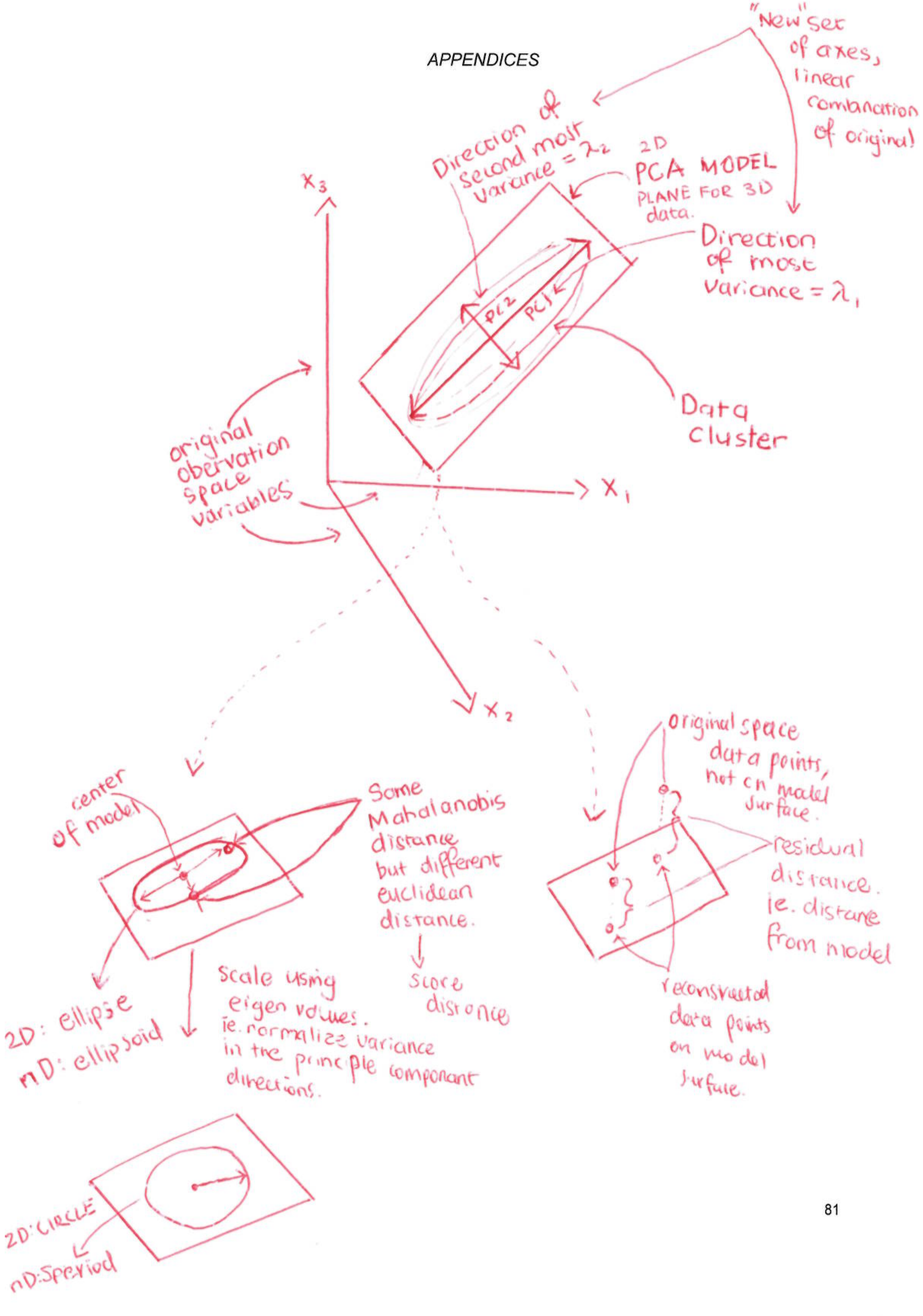
NOTE

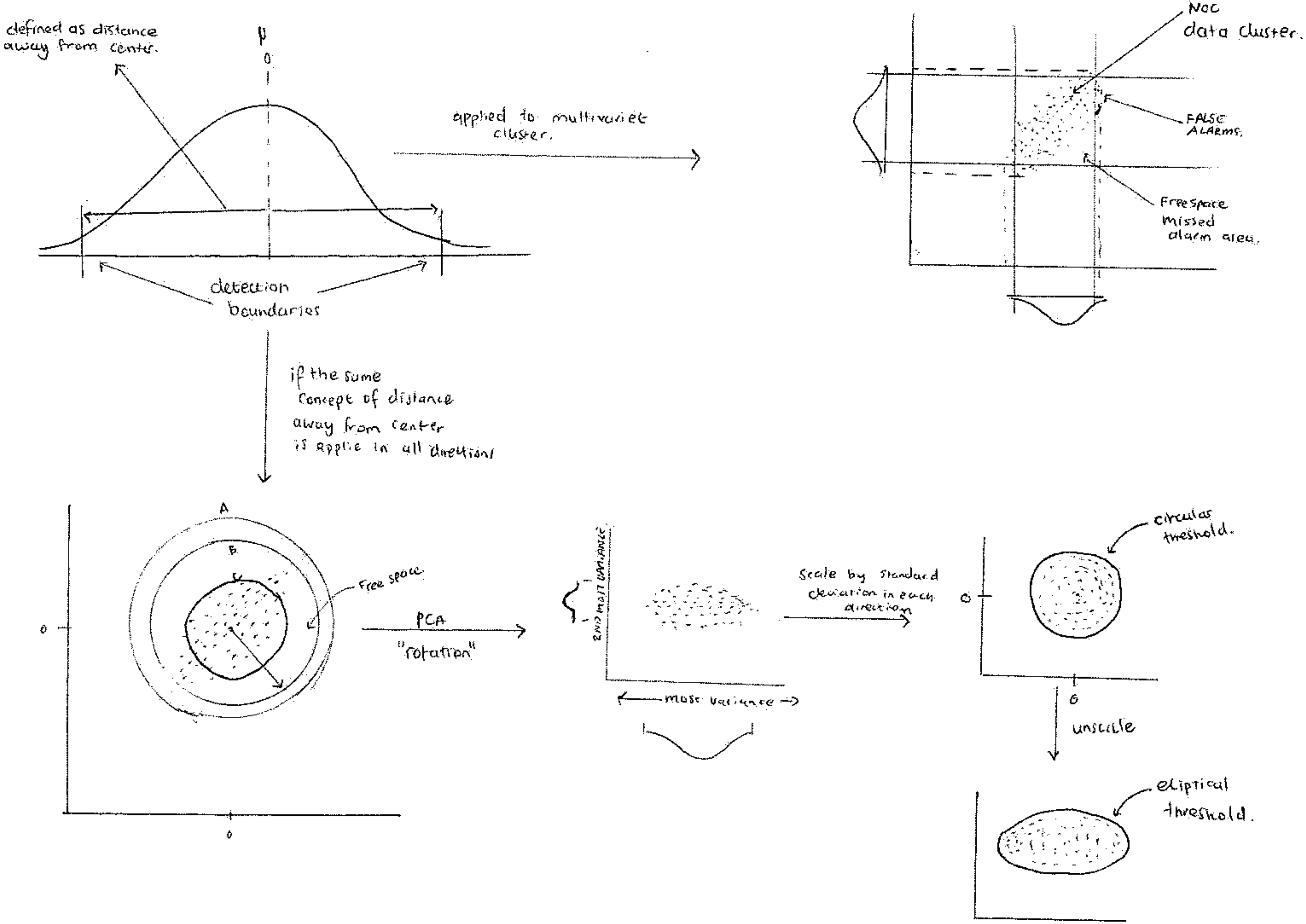
Since all distances are squared, all samples of T^2 will be +, meaning the distribution is no longer normal. (if assumed to initially be).

~~FALSE ALARM~~

missing alarm




"New" set of axes, linear combanation of original
Direction of second most variance = λ_2
2D PCA MODEL
PLANE FOR 3D data.
Direction of most variance = λ_1
PC2
PC1
Data cluster
x_3
x_1
x_2
original obervation space variables
center of model
Some Mahalanobis distance but different euclidean distance.
score distance
Scale using eigen values. ie. normalize variance in the principle componant directions.
2D: ellipse
nD: ellipsoid
2D: CIRCLE
nD: Speriod
original space data points, not on model surface.
residual distance. ie. distance from model
reconstructed data points on model surface.


defined as distance away from center.
μ
0
detection boundaries
applied to multivariet cluster.
Noc data cluster.
FALSE ALARMS.
Freespace missed alarm area.
if the same concept of distance away from center is applie in all directions
A
B
Free space
0
0
PCA
"rotation"
2ND MOST VARIANCE
most variance
Scale by standard deviation in each direction
circular threshold.
0
0
unscale
eliptical threshold.

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