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Identification of Desired Operational Spaces via Numerical Methods

by

Prevlen Rambalee

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of the requirements for the degree

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Identification of Desired Operational Spaces via Numerical Methods

Synopsis

Plant efficiency and profitability are becoming increasingly important and operating at the most optimal point is a necessity. The definition of proper operational bounds on output variables such as product quality, production rates etc., is critical for plant optimisation. The use of operational bounds that do not lie within the region of the output operational space of the plant can result in the control system attempting to operate the plant in a non attainable region. The use of operational bounds that lie within the bounds of the output operational space of the plant and if the output operational space is non convex can also result in the control system attempting to operate the plant in a non attainable region. This results in non feasible optimisation.

A numerical intersection algorithm has been developed that identifies the feasible region of operation known as the desired operational space. This is accomplished by finding the intersection of the required operational space and the achievable output operational space. The algorithm was simulated and evaluated on a case study under various scenarios. These scenarios included specifying operational bounds that lie partially within the bounds of the achievable operational space and also specifying operational bounds that lie within the bounds of the operational space which was non convex. The results yielded a desired operational space with bounds that were guaranteed to lie within an attainable region on the output operational space. The desired operational space bounds were also simplified into a rectangle with high and low limits that can be readily used in control systems.

Keywords: constraints, feasible regions, intersection algorithms, optimisation, desired output space.

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Lastly to my pillar of strength, my wife Kershnie. Thank you for all the understanding, patience, love and laughs throughout all the long nights and weekends.

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NOMENCLATURE

Acronyms

DOS Desired Operational Space

HCl Hydrochloric Acid

IOS Input Operational Space

KPM Key Performance Metric

Max Maximum Value

Min Minimum Value

MPC Model Predictive Control

OCI Output Controllability Index

OOS Output Operational Space

ROS Required Operational Space

RTO Real Time Optimisation

Symbols

Bs Bin Size

G Plant Model

No Number

R Matrix Size

X Input Variable Matrix

Y Output Variable Matrix

$\cap$ intersected with

$\supset$ super set

$\notin$ not an element

η Feasible Region

$\tilde{\eta}$ Non Feasible Region

ϵ Utilisation of a Region

τ Time in seconds

μ Representing a function

Subscripts

l Lower bound of variable

u Upper bound of variable

i Element of matrix

n Normalised value

CHAPTER 1

INTRODUCTION

1.1 Background

The ability of a plant to operate efficiently and on desired specifications is becoming increasingly important. The global competitive market requires cost effective, quality products therefore production facilities around the world are constantly optimising processes. Optimisation of a plant involves gaining maximum utilisation of current equipment while being safe and economically efficient. This requires identifying bounds for key plant output parameters and operating within desired bounds. These output parameters are typically measurements such as product quality, temperatures, product flows etc. The output parameters of the plant are a function of and limited by input parameters, such as valve positions, pump speeds, etc. The bounds on the input parameters can be a result of various factors such as physical equipment limitations, safety constraints etc. These bounds define a region known as the input operational space, IOS, of the plant. Simulating the IOS in a steady state model of the plant will result in output parameters forming a region known as the output operational space, OOS. This is illustrated using a two input, two output plant in Figure 1.1;

The inputs, X_1 and X_2, in Figure 1.1.(a), form the IOS, where the constraints on the input variables are;

$$X_{1l} < X_1 < X_{1u} \tag{1.1}$$

where X_{1l} and X_{1u} are lower and upper bounds of input X_1.

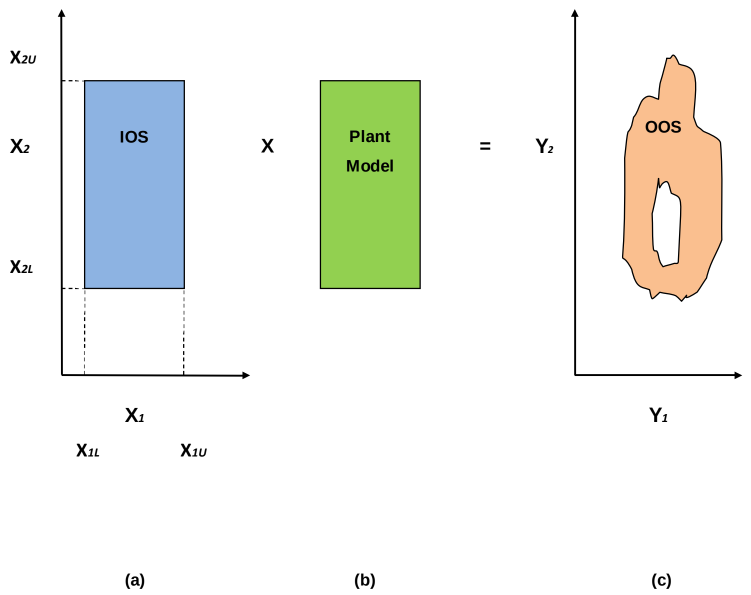

Figure 1.1: Plant IOS and OOS regions.

$$X_{2l} < X_2 < X_{2u} \tag{1.2}$$

where X_{2l} and X_{2u} are lower and upper bounds of input X_2.

Simulation of the steady state plant model with inputs within the constraints of the IOS generates the OOS region. The OOS region is generated as follows;

$$OOS = G(X) \tag{1.3}$$

where G represents a linear plant model in Figure 1.1.(b), as a function of the IOS parameters. The plant model, G, is representative of a linear systems as in nonlinear systems, the input space may not map the output space in some non linear systems as one set of inputs may have more than one associated output points and the above OOS region would not be valid.

The outputs, Y_1 and Y_2, in Figure 1.1.(c), form the OOS. The OOS region has an irregular shape and includes a region within the boundaries that is non attainable. Operational bounds on outputs Y_1 and Y_2 due to requirements such as production, product quality, economics, down or up stream requirements form the region known as the required operational space, ROS and typically the ROS region is defined by upper and lower bounds. In Figure 1.2, a ROS region is superimposed on the OOS region identified in Figure 1.1.(c);

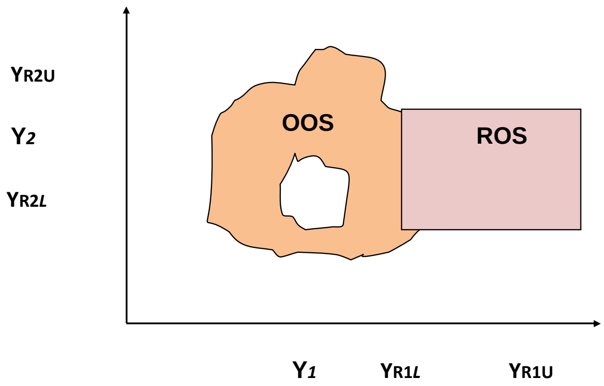

Figure 1.2: Plant ROS and OOS regions.

The ROS region bounds, for outputs, Y_1 and Y_2, in Figure 1.2, are as follows;

$$Y_{1Rl} < Y_1 < Y_{1Ru} \tag{1.4}$$

where Y_{1Rl} and Y_{1Ru} are lower and upper bounds of output Y_1.

$$Y_{2Rl} < Y_2 < Y_{2Ru} \tag{1.5}$$

where Y_{2Rl} and Y_{2Ru} are lower and upper bounds of output Y_2.

It is desirable to operate the plant within bounds such that OOS $\cap$ ROS. The ROS region can lie in one of three areas regarding the OOS region as shown in Figure 1.3,

In Figure 1.3 the regions can be described as follows:

- ROS lies entirely outside the OOS, Figure 1.3.(a).

- ROS lies partially or completely inside the OOS and the OOS is convex, Figure 1.3.(b).

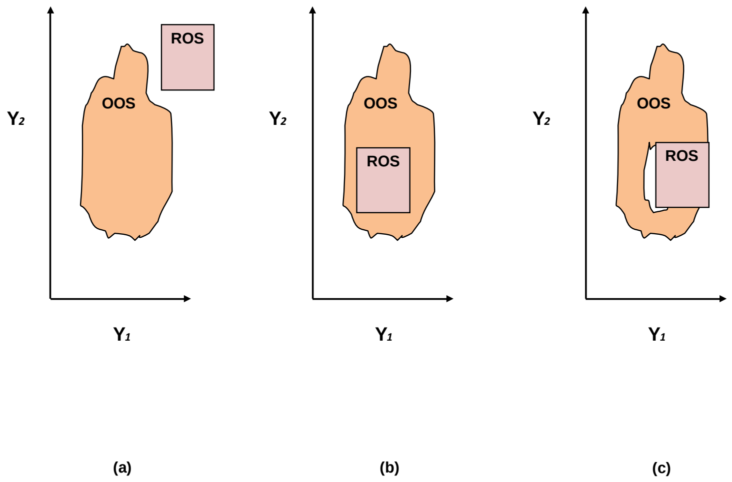

Figure 1.3: Various ROS and OOS region of intersections.

- ROS lies partially or completely inside the OOS and the OOS region is non convex, Figure 1.3.(c).

The parameters of the ROS region are used as bounds for control systems either directly or via optimisation algorithms. The control system cannot operate the plant in an ROS region entirely outside the OOS region, Figure 1.3.(a), however the control system will operate the plant if the ROS region lies entirely within a convex area of the OOS region, Figure 1.3.(b). If the control system was given ROS parameters that lie partially inside the OOS region, the control system will try to operate in the non attainable region and will not achieve required outcomes. The same is true if the ROS region lies partially or completely inside a non convex OOS region, Figure 1.3.(c).

1.2 Problem Statement

It is required to identify the largest region that both satisfies ROS region requirements whilst still feasible by being part of the OOS region. If the ROS region has infeasibility the new common region will be smaller. Optimisation algorithms would prefer larger regions and if the optimal point lies within a non attainable region the control system will try and achieve the closest attainable operational point. This would suggest that finding a region that is attainable both in the ROS and OOS region has very little value apart from giving the control system achievable limits. However if the ROS bounds of operation are non attainable and these bounds are used in optimisation for deliverable's such as production rates, quality, etc., unrealistic expectations are made and this can severely affect operations and profitability. A motivating case study by Makkonen & Lahdelma (2003) on the optimisation of a non convex power generation unit highlights the need for optimisation bounds that accurately represent the process. The European electricity market has changed to smaller competing power generating companies as opposed to previously large monopolised companies. These companies must now optimise processes to meet hourly spot market variations and adhere to emission regulations whilst realising maximum profitability under this competitive environment. These power plant feed costs, electricity prices, electricity demand are extremely volatile such that production optimisation and planning is based on the spot price and short term forward prices. There are also penalties associated for slack and surplus energy production. Makkonen & Lahdelma (2003) considered a combined power and heat plant which comprised of a boiler, a back pressure turbine with an optional reduction bypass, condensing operation and auxiliary cooling.

The OOS region for the combined power plant is shown in Figure 1.4. Areas two and three are only available if the auxiliary cooling circuit is operating. The auxiliary cooling circuit enables the plant to produce more power. If the auxiliary cooling circuit is not operational, part of the ROS shown in Figure 1.4 is unattainable. This can result in optimisation requiring a specific power output that the control system cannot achieve and will result in sub optimal operation leading loss in revenue due to penalties or increased operational costs. Therefore finding the largest feasible region between the ROS and OOS region is sometimes required.

1.3 Objective

Optimisation algorithms including advanced controls require constraints on plant parameters to operate the plant within the desired regions. Incorrect definition of these constraint parameters could result in the optimisation requiring the control system to operate the plant in an unattainable region. As shown in Figure 1.1 a simulation of the

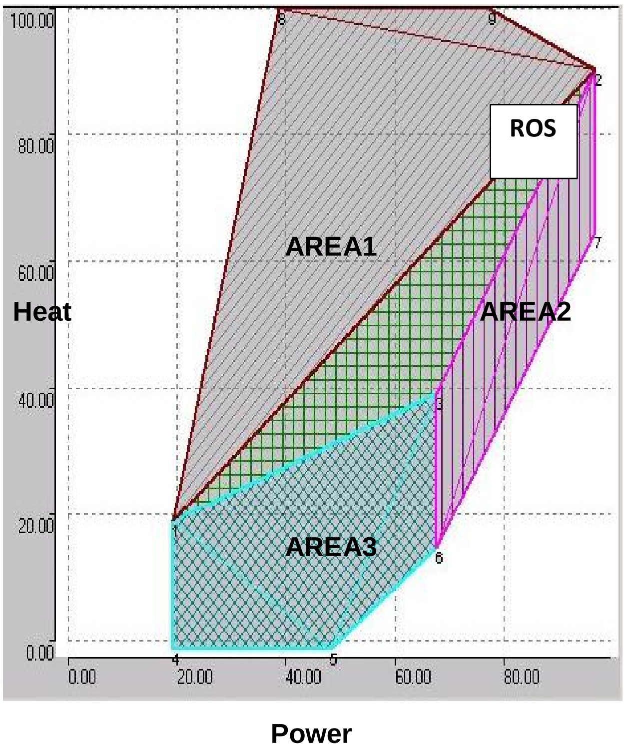

Figure 1.4: Power plant heat versus power generation.

plant model with the IOS constraints can be used to identify the OOS region. The constraints that define the ROS region can originate from various sources and as shown in Figure 1.3 may not necessarily lie within the OOS region. This can be overcome by identifying a region known as the desired output space, DOS. The DOS is the common region between the ROS and the OOS and is determined by finding the geometric intersection of the OOS and ROS regions. The DOS is defined as follows;

$$DOS = OOS \cap ROS \tag{1.6}$$

The resulting DOS region is illustrated in Figure 1.5;

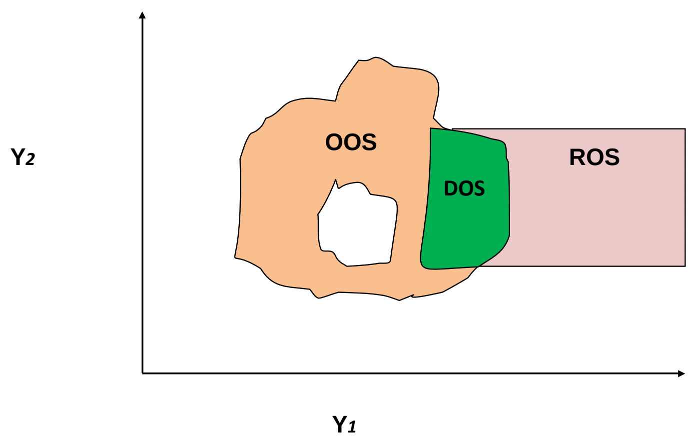

Figure 1.5: Identifying plant DOS region.

In Figure 1.5 the ROS region is positioned within non attainable parts of the OOS region. The DOS region, represented by the green shaded area in Figure 1.5, finds the region such that equation 1.6 is satisfied. The DOS region can also be irregular in shape which could prove difficult for control systems that require upper and lower bounds of operation. This can be overcome by finding the largest set of upper and lower bounds within the DOS region, as depicted in Figure 1.6;

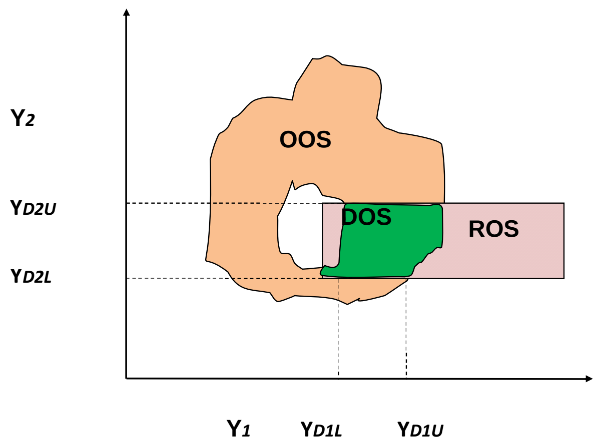

Figure 1.6: DOS region upper and lower bounds.

The DOS region bounds, for outputs, Y_1 and Y_2, in Figure 1.6, are as follows;

$$Y_{1Dl} < Y_1 < Y_{1Du} \tag{1.7}$$

where Y_{1Dl} and Y_{1Du} are lower and upper bounds of output Y_1.

$$Y_{2Dl} < Y_2 < Y_{2Du} \tag{1.8}$$

where Y_{2Dl} and Y_{2Du} are lower and upper bounds of output Y_2.

The objective of this study is to develop a method of identifying the DOS region via numerical methods.

1.4 Method

To achieve the objective of identifying the DOS region via numerical methods, the following approach was used in this study;

Literature Review

The literature review study was approached as follows;

- Review previous controllability assessments methods that have been developed. Identify the shortcomings of previous work in relation to the identification of the DOS region, this is accomplished via a gap analysis.
- A feasible DOS regions is mainly required for plant optimisation therefore approaches to plant optimisation in different industries were reviewed. Common key aspects are summarised to form a generic approach to plant optimisation.
- Concepts around optimisation are reviewed in further detail, this includes objective functions, optimisation techniques, uncertainty and real time optimisation.
- Based on the above analysis of optimisation approaches, developing the DOS region requires modelling and simulating the plant. The different methods of process simulation are reviewed and important aspects of simulating this process model are discussed.
- This study proposes the identification of the DOS regions via numerical methods by reviewing geometric intersection and analysing various techniques that were previously developed.

Experimental

Based on the information analysed in the literature review the algorithm was developed and tested on a case study in the following manner;

- A HCL flash system was chosen as the case study. The parameters and specifications of the circuit are specified.
- The case study was modelled and simulated based on the analysis of the literature study.
- The simulation provided results to allow the intersection test. The data was pre-processed to increase efficiency of the intersection as identified in the literature study.

- Post processing of the intersection algorithm.
- Key performance metrics are defined to evaluate the success of the proposed technique.

Results

The proposed algorithm to numerically identify the DOS was tested and evaluated on the case study as follows;

- The simulated case study was analysed i.e. the OOS region.
- Three sets of ROS regions were used to evaluate the intersection algorithm. The ROS parameters included a feasible region, partially feasible region and a non convex region.
- For each of the above parameter sets the results were evaluated in accordance to the key performance metrics defined.

Discussion

The discussion summarises the approach to numerically identify the DOS region and includes the results obtained through the case study and recommendations for future work are discussed.

CHAPTER 2

LITERATURE

The literature review for this study reviews plant operability, optimisation approaches in industries, principles of optimisation and geometric intersections.

2.1 Plant Operability

Prior to optimising a plant it is required to identify if the process is operable and controllable within the bounds defined by the DOS region. A process is defined as operable (Georgakis *et al*, 2003) if in the presence of disturbances and without violating any process constraints, the desired steady state and dynamic performance of the process are met with the available IOS. A process is defined as controllable if the ability of the IOS keeps the process under steady state conditions in the presence of disturbances.

Several controllability assessment methods have been developed over the past three decades. This section will review these methods and highlight the differences in their applicability through a GAP analysis. The controllability assessment techniques include the following:

- Time Domain analysis (Kuo & Golnaraghi, 2003 233-317).
- The use of open loop frequency response characteristics by the use of Bode and Nyquist criterion (Seborg, Edgar & Mellichamp, 2004 376-383).
- The measure of resiliency using the Morari Resiliency Index (Lyuben,1990 573-575).
- Relative gain arrays, RGA, to determine multi-variable interaction (Marlin, 2000 334-337).

- Singular value decomposition with the use of condition number (Skogestad & Postlethwaiteet, 1996 66-69).
- Steady State Feasibility using the Output controllability Index (Georgakis *et al*, (2003)).

The above analysis techniques aid in the understanding of the process operability. The first three techniques are commonly used on single input single output analysis whereby the latter three techniques are used in multivariate analysis.

Time Domain Analysis

Involves evaluating the system's responses with respect to time. A reference signal is applied to the system and the performance of the system is evaluated by its time response. Typically a unit step signal is used as an input for time response evaluations. The following parameters are evaluated with regards to time domain analysis:

- Maximum overshoot: this is the difference between the maximum output and steady state value. Maximum overshoot is used to measure relative stability of the control system; a large maximum overshoot is usually undesirable.
- Time Delay: time required for the step response to reach 50% of its final value.
- Rise time: time required for the step response to rise from 10% to 90% of its final value. The quicker the rise time the more likely the system will suffer from overshoot. Similarly a slow rise time will result in the system taking an extended period to reach steady state.
- Steady state error: discrepancy between the output and the reference input signal when steady state is reached.

The above parameters are useful in evaluating and design control systems. The stability and performance of the system can be determined by analysing the time domain characteristics.

Frequency Domain Analysis

Frequency Domain Analysis is a graphical method and it indicates how the output response characteristic of a system depends on the frequency of the input signal. The frequency response characteristics are calculated from the transfer function of the linear process. Typically a sinusoidal input is used to obtain the frequency response which is represented graphically via techniques such as the Bode and Nyquist diagrams.

Bode: Bode diagrams provide information about the amplitude ratio and phase angle of the system as a function of frequency i.e. amplitude ratio vs. frequency and phase vs. frequency. The amplitude ratio is defined as the ratio of the output magnitude over the input magnitude and the phase angle is the phase difference between the input and output signal. A critical frequency is defined whereby the phase of the system = -180 degC and the gain crossover frequency is defined when the gain =1. The control system will become unstable if it operates at frequencies above the critical or crossover frequency. The Bode analysis provides information about the control system stability and design.

Nyquist: Provides a polar plot of the gain and phase of the system. A Nyquist diagram can be constructed directly from the gain and phase of the system for different frequencies. The Nyquist plot uses the point (-1,0) and the number of times the plot encircles this point. The Nqyuist plot can be used to analyse the stability of control systems and can also be used for the design of control systems to ensure the process is stable.

Morari Resiliency Index

The MRI gives an indication of the inherent controllability of a process. It is based on the relationship between how invertible the transfer function matrix of a system is and its resilience. The MRI is defined as the minimum singular value of the process. The larger the minimum singular value the easier the plant is to control. This is based on the fact that every controller tries to invert the plant directly or indirectly to find the suitable inputs that will keep the plant at its set point. According to the MRI there are four fundamental factors preventing the inversion of the process. These include right-half-plane zeros, time delays, constraints on the input variables, and model uncertainty.

Relative Gain Array

In multivariate systems there are several single loop controllers which have interaction whereby a process input affects more than one process output. Therefore the range and controllability of multivariate systems are influenced by process interactions. This range defines an operating window for the feasible steady state process variables that can be achieved with the available equipment. A quantitative measure interaction is known as the relative gain array, RGA. The RGA is a matrix composed of elements defined as ratios of open loop to closed loop gains i.e. a matrix of relative gains. The analysis of RGA's can be used to pair input and output variables for control system designs and large RGA elements indicate the plant is difficult to control due to interaction or sensitivity to uncertainty.

Singular Values

Directions in multivariate systems are important as it provides information about the system gains. Singular value decomposition of the system indicates the input direction, output directions and the singular values. The singular values indicate the strongest and weakest directions of the process. This identifies which direction the plant is more easily controllable. The system condition number is another analysis which provide information about the system controllability. The condition number is the ratio between the maximum and minimum singular values. A large condition number will indicate controllability problems.

Output Controllability Index

A technique presented by Vinson & Georgakis (2000) is a steady state controllability measure called the output controllability index, OCI, which determines the steady state feasibility of the ROS region based on the OOS region. The OCI uses the plant input-output relationship to determine the limited range the input has on achieving the objectives of the process. The OCI is intended to be a single number to evaluate process controllability and operability. The OCI is defined as follows;

$$OCI = \mu(OOS\frac{R}{O}S)/\mu(ROS) \tag{2.1}$$

where μ represents a function calculating the size of the space for example, in two dimensions, it represents the area, and in three dimensions, it represents the volume. If the OOS space is not large enough to cover the ROS space then the controllability of the process is less than a 100 % thus resulting in a OCI less than 100%. This would imply the IOS would require to be extended to allow the ROS region to be controllable over the OOS region. For illustration, let us consider a continuous process where two (binary) streams of different compositions are mixed. The input variables in the problem are the two feed stream flow rates, F1 and F2. The outputs of interest are the product flow rate F and its composition x: The OOS shown in Figure 2.1 is derived from the IOS given in the in set of the same figure. If the OOS calculated is compared with DOS and the OI is less than 1, the IOS is not sufficiently large enough to deliver all the outputs in ROS.

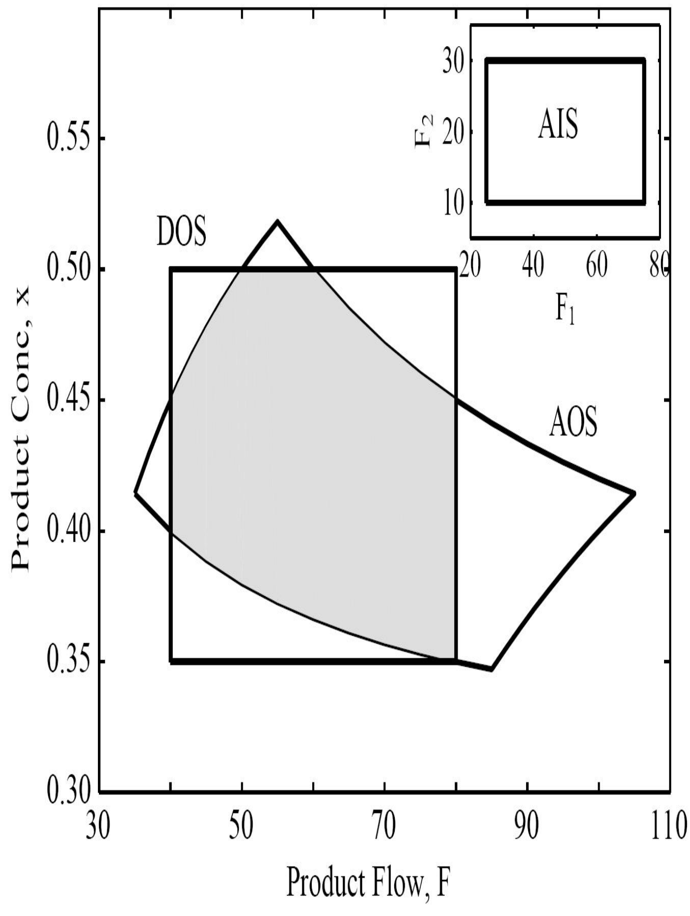

Figure 2.1: Achievable output space of a binary mixing system.

Georgakis *et al* (2003) have evaluated the OCI with other controllability measures such as RGA, singular value, condition number, etc., and have demonstrated that the OCI is superior to the compared techniques. The OCI highlights aspects of the process design which require to be changed thus making a useful tool during initial process design.

In the case of an existing plant where process design changes are not always possible the OCI does not identify the bounds of a feasible region of operation such as the DOS region. The OCI provides open loop feasibility of both linear and non linear processes. In industry non-linear processes are generally controlled using linear controllers, Sentosa, Bao & Lee (2009) have proposed a technique to evaluate whether a steady state region within the non linear process is attainable using linear feedback control. The technique defines the largest set of initial steady-state operating points in the IOS from which the closed loop system with linear control is guaranteed to converge to the feasible steady-state within OOS region. It was noted that the results are only theoretical and cannot be readily used in practise.

Other methods that have been developed on operability include (Georgakis *et al*, 2003):

- Swartz (1996) presented a computational framework for plant operability assessment. The formulation takes the form of a convex optimisation problem and utilises Q-parametrisation to search over all stabilising linear feedback controllers. The solution obtained represents an upper bound on the performance of all linear stabilising feedback controllers.

- Another class of operability tools and measures are those that utilise nonlinear models. The concept of a flexibility index was introduced by Swaney and Grossmann (1985a) for quantifying the steady-state operability of nonlinear processes. This is defined as the maximum normalized uncertainty in its parameters that a process can tolerate without violating any constraints.

- Bahri, Bandoni, and Romagnoli (1996) formulated an optimisation-based approach for making sure that the plant is operable in the presence of disturbances. They moved the nominal operating point away from the constraints so that the constraints would not become active even when disturbances enter the plant. If the objective function is given in terms of economic factors, the cost difference between optimum point and back-off point quantifies the maximum savings that can be obtained by decreasing the process variability by either reducing the magnitudes of the disturbances or installing a control system

The above analysis techniques highlight the importance of ROS region being a feasible part of the OOS region for the implementation of plant optimisation. Optimisation on a plant that is not controllable or has limited operatability will provide little or no benefits.

GAP Analysis

The DOS region of intersection is defined as OOS $\cap$ ROS, however in the case when OOS $\notin$ ROS, will result in a plant with limited operability. Fisher, Doherty & Douglas (1988) suggested that lack of operability can be rectified by;

- Modifying plant flow sheets to include more or improved manipulated variables.
- Over-designing certain pieces of equipment to compensate for the complete range of disturbances.
- Ignoring the optimisation of least important variables.

There have been several controllability assessment methods developed as discussed previously hence a GAP analysis was performed to identify the areas of improvement. In order for a plant to have the ability to operate efficiently and on desired specifications it requires the following from a controllability assessment technique:

- The process must be controllable.
- The level of controllability must be identified.
- The design of controls system to provide stable performance when maintaining required set points.
- Identify available spaces of operation for optimisation algorithms.
- Provide bounds of operation for optimisation algorithms.

Time domain and frequency domain analysis will address process controllability, level of controllability and provide required information for the control system design. These analyses are typically used for SISO control systems and do not address optimisation.

The MRI, RGA and singular will address process controllability and the level of controllability. These analyses can be used on multivariate systems however do not address optimisation.

The OCI index does address optimisation and does not analyse control system stability or control system design. It however does identify the available achievable output space and the limitations of the plant input variables.

The time domain, frequency domain, MRI, RGA and singular values are more relevant to control system stability and design. The OCI and other optimisation techniques are used once the system is controllable and stable. These optimisation techniques do not provide feasible bounds of operation. Generally plants are required to operate optimally within bounds defined by the end user i.e. the ROS region. This ROS region defined by the end user may not necessarily have gone through rigorous checks for feasibility. This creates a gap as no technique identifies the DOS region based on the ROS and OOS region. The closest analysis is the OCI which identifies the IOS regions that requires changes to ensure the ROS is attainable within the OOS regions. All above techniques do not explicitly provide solutions for non convex OOS operating spaces that are not feasible. The next section will address methods and key concepts concerning plant optimisation.

2.2 Plant Optimisation

Once the process is analysed for controllability and the various analysis have been performed to ensure the process control system can keep the plant stable, optimisation can occur. Optimisation involves changing process parameters such as feed conditions, product and utility prices as well as equipment parameters so that the economically optimal operating conditions of the process is realised. Thus optimisation requires the continual adjustment of the plant operating point to coincide with the economic optimum (Young, Baker & Swart, 2004). Several methods and techniques have been used in the process of optimising plants around the world and these techniques vary with the type of industry and specific plant requirements. This section will review the various approaches to optimisation in different industries and a general optimisation methodology is summarised. The industries reviewed and their optimisation objectives are as follows;

- Chemical - IOS Limitations (Diaz *et al*, 1996)
- Chemical - Environmental (Zhang, Pike & Hertwiget, 1995)
- Power - OOS Accuracy (El-Nagger, Alrashidi & Al-Othman, 2009)

- Nuclear - Efficiency (Sayyaadi & Sabzaligol, 2009)
- Mining - Throughput (Svedensten & Evertsson, 2005)
- Petrochemical - Real Time Optimisation (Van Wyk & Pope, 1991)

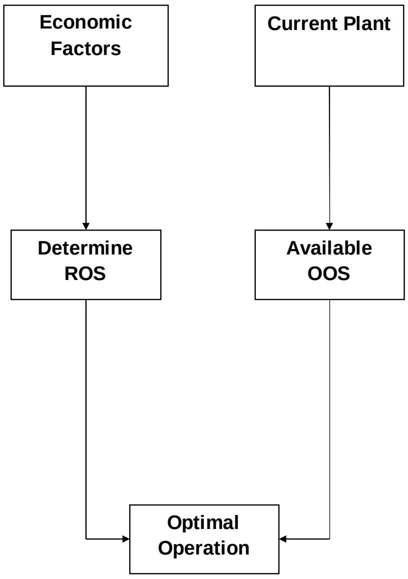

Figure 2.2: Approach to plant optimisation.

In Figure 2.2 economic factors determine the parameters that define the ROS, the available plant results in the OOS and based on thess plant optimisation occurs. The following case studies have been reviewed to identify approaches taken by various plants when performing optimisation as Figure 2.2 suggests.

Chemical Industry - IOS Limitations

In the chemical industry Diaz *et al* (1996) have studied the optimisation of an ethane extraction plant to achieve higher production rates and reduce operating costs. The ethane extraction plant consists of a final demethanizer that produces ethane gas which is compressed through three stages and delivered as sales gas. The compressors are driven by gas turbines and form a large part of the plant operating costs. It was required to determine if design alternatives to the current plant offer higher recoveries and lower operating costs which would result in a better operating plant. In order to achieve this goal a mathematical model of the current plant was built and simulated. The model used was extended from a previous model. The simulation of the plant model included constraints such as process specifications and bounds on equipment capacities, the IOS region. To evaluate profitability, an economic objective function was considered in the simulator used. The analysis indicated the optimal economic point of the plant achieves maximum production in spite of compressor operational costs. The results have also shown that the feed is a bottleneck to the plant. The cooling capacity of the plant was insufficient for higher feed rates. Increasing feed rates reduces the recovery of the current plant, thus adding additional capacity to cool the feed will result in higher production and plant profitability. The impact of additional cooling capacity is shown in Figure 2.3 below

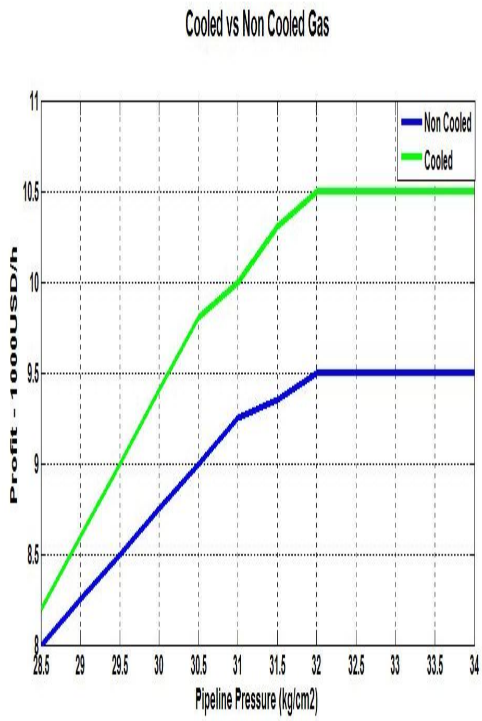

Figure 2.3: Effect of additional cooling capacity on profitability.

The current plant OOS does not allow for high feed rates while trying to achieve high recoveries. If the ROS region required high feed rates the optimisation would try to operate the current plant in a non attainable region. This case study highlights the limitation the IOS region places on the OOS region which could cause the ROS region to lie in a non attainable space. For the current plant using the OOS region developed by the simulated model and the ROS, the DOS can be identified to ensure the plant will operate in a feasible region.

Chemical Industry - Environmental

Plants around the world are also becoming more aware of their impact on the environment. Zhang, Pike & Hertwiget (1995) have implemented optimisation to reduce the emissions of a sulphuric acid plant. The approach selected was to use a process model, an economic model and an optimisation algorithm. The process model was developed using a previously developed kinetic model. The process model included constraint equations such as conservation of mass and energy, reaction kinetics, equilibrium relations and equipment operational bounds. The process model was simulated and the simulation results, the OOS region, was compared with plant data to assess the validity and accuracy of the process model. The economic model of the plant defined the profitability of the plant. The process model, economic model and constraints were solved by the optimisation algorithm. Implementation of the online optimisation resulted in 25% reduction in emissions and a 17% improvement in profit.

Power Industry - OOS Accuracy

The following case study highlights the importance of having a highly accurate OOS region. Thermal power plant with multiple power generating units are commonly used for providing power to the countries they serve and are an integral part of the economy. The economic objective of these plants is to minimise fuel costs corresponding to various generating units (El-Nagger, Alrashidi & Al-Othman, 2009). In multiple power generating units, optimal power flow and operation of each unit is important for planning and operation. The demand for power is inconsistent and is determined by consumer demand which can vary significantly. Producing high outputs at low demands will result in economic losses. The estimation of the power plant heat curve, also known as the fuel cost function curve is a key factor for optimal operation. This curve is derived from each generating unit's input-output characteristic hence is essentially an estimation of the OOS region. Depending on the power demand it would be required to operate each power generating unit at the minimum achievable cost which is based on the fuel cost curve. In the case of the thermal power plant presented by El-Nagger *et al* (2009), correct estimation of the fuel cost curve is vital for the optimisation of the plant., if the estimation is not correct the optimisation algorithm will try and operate in a non attainable region. Several methods were considered to achieve and solve the estimation:

- static estimation techniques e.g. least error square.
- dynamic estimation techniques e.g. Kalman filters.
- methods based on artificial intelligence e.g. artificial neural networks and expert systems .

According to El-Nagger *et al* (2009) different algorithms produce varying levels of accuracy. In this case study the higher the accuracy of the estimated coefficients, the more accurate the results for the economic operation of the power generating units.

Nuclear Industry - Efficiency

In the nuclear industry defining a ROS region without knowing the OOS region can result in highly undesirable outcomes. Increasing profitability or throughput is only valid if safe plant operation and adherence to legislation are achieved. The following case study illustrates identifying the OOS region of the plant can assist in determining the ROS region depending on the plant objective. Sayyaadi & Sabzaligol (2009) considered a pressurised water reactor nuclear power plant for optimisation. Nuclear power plants generally have lower efficiencies than fossil fuel plant such as the case considered by El-Nagger *et al* (2009). Nuclear facilities use fuels such as uranium which are costly and not readily available due to rarity and safety. The objective would therefore be to utilise as much out of the nuclear fuel energy feed to the plant as possible to preserve resources. However, it is also required to produce power in a cost effective manner. Thus there are two different objectives for the operation of the plant. Two analyses were considered to address each objective, the first being an economic and the second thermodynamic. To analyse the economic performance of the plant a thermo economic model of the plant was considered which focused on economical operation and not conservation of resources. The thermodynamic analysis of the plant consisted of modelling based on the energy analysis of the plant. The results showed that the thermodynamic model required more equipment and hence a larger capital outlay but lower operational costs and vice versa for the economic analysis. There is a tradeoff between economic versus thermal efficiency. If the ROS is required to meet both objectives, the DOS region can be used to identify the region which can be part of both the ROS and OOS regions.

Mining Industry - Throughput

In the mining industry, plants that process mined ore are required to be very versatile as mined ore compositions can vary significantly which can cause the OOS region of these plants to vary. Crushing plants are used widely in the mining industry and efficiency of these plants severely affect profitability. The individual performance of production units within a crusher plant affects the efficiency of the entire plant. A change in upstream operations such as a primary crusher unit will affect the downstream production in the plant in such a way that the quality and amount of products produced changes. Svedensten & Evertsson (2005) proposed a novel method for optimisation of a crusher plant which aimed at determining the most profitable settings of the plant that maximised profits as well as production which adhered to customer requirements. The approach of the crusher plant included modelling the plant, feed quality, economic operation and customer requirements. The total production of the plant was described by a plant model such that each production unit in the crushing plant was modelled by a number of mathematical models and constraints related to the specific unit. These individual models were connected to form the crushing plant model. The feed rock material transported between the different production units were also modelled. The rock model included parameters such as the properties of the rock after each production unit. The economic operation of the production costs for each production unit was modelled and the total cost comprised of total operation costs including labour and transportation. In a crushing plant the properties of the products produced by the crushing plant must fulfil customer demands. This naturally places constraints on production and was included in the optimisation process. Using the above approach the crusher plant was modelled and simulated and the OOS region was identified. This was used to calculate the most profitable setting for the plant.

Petrochemical Industry - On-line Optimisation

A petrochemical refinery implemented online optimisation based on a detailed mathematical model of the process and defining all potential constraints (Van Wyk & Pope, 1991) which form the boundaries of the OOS region. The refinery planning and scheduling provides the optimisation system with economic data and quality constraints on a time scale of days to weeks which represents the ROS region. Based on the information received by the planning and scheduling system, the optimisation level decides the operating point for the plant every few hours. These operating points where required to be accepted by plant operators after which targets were downloaded to a number of advanced process controllers. This total cycle takes about three hours. The impact on the operation of the optimisation system was immediate; not only did the system succeed in its primary objective of finding a more profitable operating point, but operation also became steadier as constraints were handled more effectively. However the optimisation assumed the OOS region was convex and the optimisation can request targets which are non feasible which can be rejected by the plant operator. This can be solved by identifying the DOS region and using DOS region boundaries as constraints in the optimisation.

Generalised Optimisation Strategy

The above case studies have shown that in the various applications of power generation, nuclear, chemical, mining, refinery and environmental, optimisation results in more profitable plants whilst still adhering to specified requirements. There is a generalised approach to process optimisation as shown in the Figure 2.4 below.

The generalised approach to optimisation shown in Figure 2.4 is as follows:

Choose Plant Area Choose an area of the plant that requires to be optimised. This will allow input and output boundaries of the process to be defined.

Model the Plant the plant area and associated equipment.

Identify Economic Parameters Identify the various factors which influence the economic operation of the plant.

Define Objective Function defines the objective of the chosen plant area.

Simulate Developed Model using the plant model and IOS constraints.

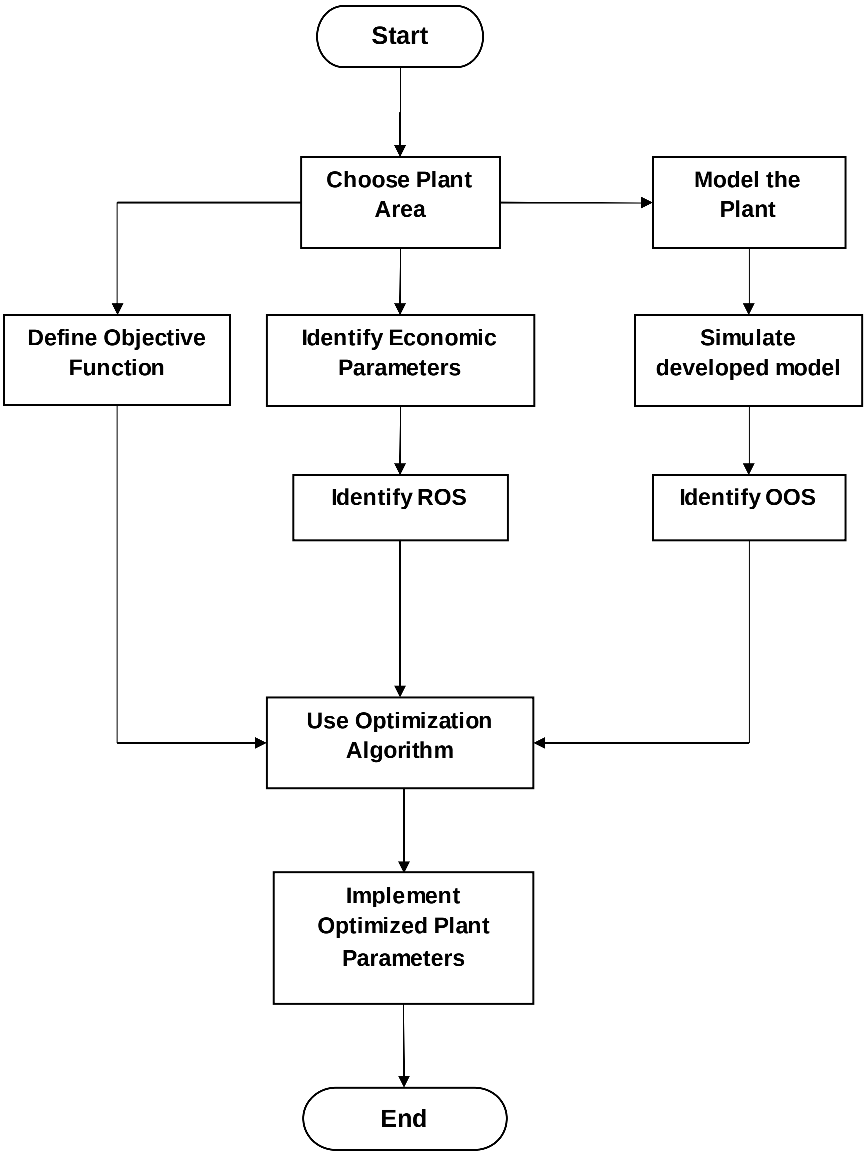

Figure 2.4: Generalised optimisation strategy.

Identify ROS is identified based on the plant requirements and economic considerations.

Identify OOS is identified by the simulated model.

Use Optimisation Algorithm Once the objective function, ROS and OOS bounds are defined, these can be used in the optimisation algorithm to solve the optimal point of operation.

Implement Optimised Plant Parameters The output targets from the optimisation are used as operational parameters for the plant.

The above strategy assumes the region within boundaries of the OOS is convex or feasible. It is also not guaranteed that the ROS bounds lie within the OOS bounds or the optimisation targets to the plant are attainable. This can be solved by determining the DOS region as shown in Figure 2.5

The DOS region is identified by finding the feasible ROS region within the OOS region. This will ensure that the bounds used in the optimisation will result in attainable targets to the plant. To identify the properties the DOS should possess, each step in the generalised optimisation approach will be reviewed in more detail in the following sections. This includes objective functions, optimisation techniques, process modelling and simulation.

2.3 Optimisation

The generalised optimisation approach in Figure 2.4 requires a process objective function and an optimisation algorithm. These two aspects in addition to uncertainties faced during optimisation and the implementation of real time optimisation will be discussed in more detail in this sections.

2.3.1 Objective Functions

As shown in the generalised approach to optimisation in Figure 2.4, a problem statement or objective function is required for the optimiser to solve. In order to solve constrained optimisation objectives, the constraint variables are required (the ROS bounds and/or

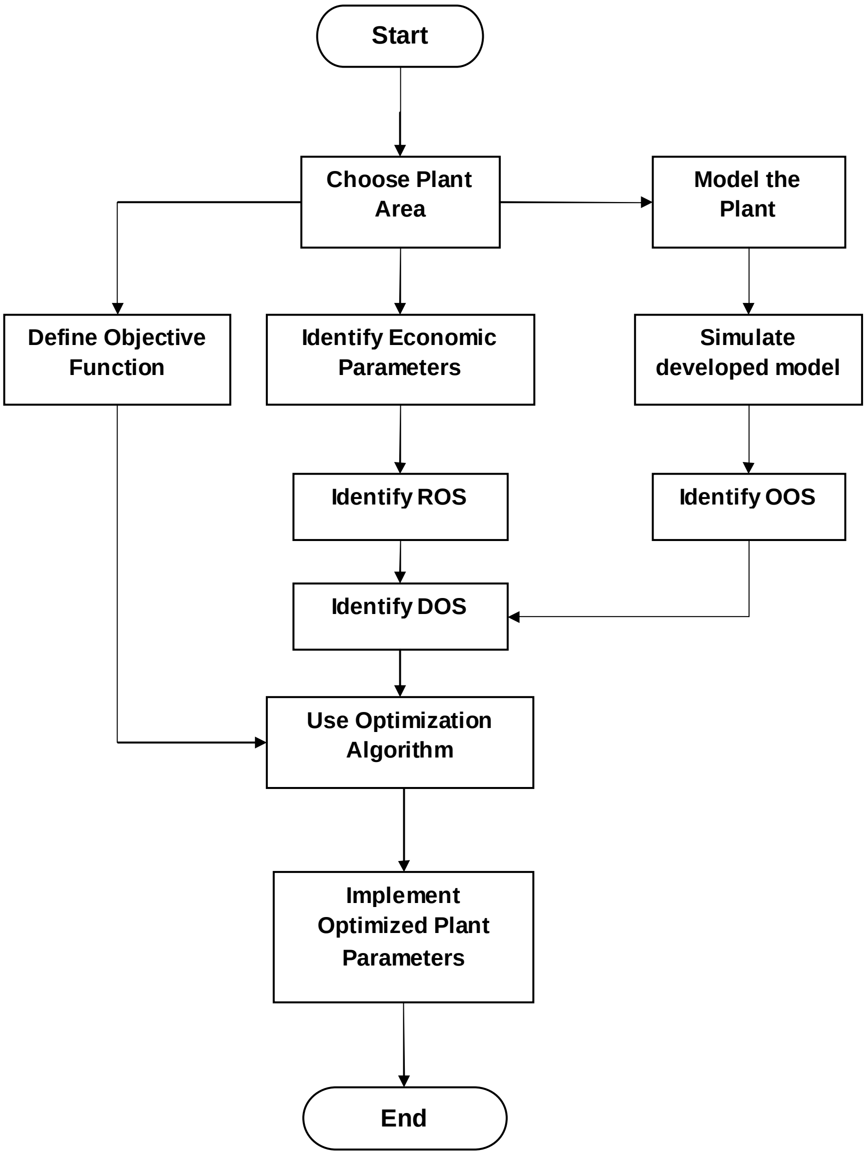

Figure 2.5: Generalised optimisation strategy with DOS region.

the OOS bounds). These constraints are grouped into economic and process constraints. The economic constraints will include factors such as feed costs, operational costs etc., that are either required to be minimised or maximised. These economics are grossly affected by external factors to a plant which include feed and energy costs, market demand, price for end product, etc. The process constraints can originate either from the OOS region that is identified by simulating a steady state process model with design parameters and constraints; or from the ROS which includes customer product specifications, equipment constraints due to maintenance etc. Thereafter the objective function and associated constraints are solved by an optimiser to determine the most profitable region of operation. The optimisation of a process can be described by equation 2.2 (Seborg *et al*, 2004 376-383);

$$\max F(Y_1, Y_2, Y_3) \tag{2.2}$$

subject to constraints

$$G(Y_1, Y_2, Y_3) < 0 \tag{2.3}$$

$$H_i(Y_1, Y_2, Y_3) = 0 \tag{2.4}$$

F(Y) is the objective function of the process and the constraints are defined in equations 2.3 and 2.4, which can be either equality or inequality. The inequality constraint is represented by equation 2.3 and equality constraint represented by equation 2.4. The optimiser is required to solve equation 2.2 whilst adhering to equations 2.3 and 2.4. Correctly defining constraints from the OOS and ROS regions is crucial for optimiser to solve the optimisation problem.

2.3.2 Optimisation Techniques

Optimisation problems can either be constrained or unconstrained. In unconstrained optimisation there are no inequality constraints and all equality constraints can be eliminated by variable substitution in the defined objective function. Hoch & Eliceche (1999) have shown a constrained optimisation problem in a distillation column being formulated as unconstrained. In distillation columns the separation constraints include minimum purity, minimum recovery and maximum impurity in a given product. For conventional columns the operating design variables are the reflux and product flow rates. These are two active constraints at the solution of the optimisation problem. The optimisation is formulated as unconstrained by including the number of stages in each section of the column as continuous optimisation variables. In the case of constrained optimisation, the solution is bounded by specified constraints including both equality and inequality which can either be linear or non linear. Depending on the linearity, different solutions are required to be used to solve the optimisation problem.

Linear objective functions and linear constraints such as equations 2.3 and 2.4 can be solved rapidly using linear programming. In the case where the objective function is quadratic and has linear constraints, the solution can be solved in a similar fashion as linear programming through an iterative technique known as quadratic programming (Marlin, 2000 334-337). When the objective function or constraints are non-linear more advanced optimisation algorithms are required to solve the optimisation problem. Optimisation techniques are mostly based on mathematical or stochastic methods (Beyer & Sendhoff, 2007).

A mathematical approach can involve using modelling or programming. The model-based methods utilise a steady state process model and programming methods include those described above such as linear and quadratic programing. According to a survey conducted by Beyer & Sendhoff (2007) on robust optimisation, model based methods suffer from model mismatch uncertainty due to available measurements and the unavailability of highly accurate models and mathematical optimisation algorithms such as linear programming sometimes fail to reach a local optimum when required to solve problems with large number of variables. A two step process which repeatedly updates uncertain model parameters and use the updated model in the model based optimisation can be used to address some of the drawbacks of model based optimisation (Chachuat, Marchetti & Bonvin, 2007). This two step approach is only valid if the model mismatch is low. Since the constraints of a model would not exactly match the plant constraints Chachuat *et al* (2007) have proposed model based optimisation with a fixed process model and a constraint adaption algorithm that uses process measurements to update constraints. The constraint adaption algorithm was tested on an isothermal continuous stirred reactor. The steady state model of the process was developed from material balance equations. The simulation results proved that the constraint adaption algorithm can also be an alternative in addressing the drawbacks of model based optimisation.

In stochastic optimisation evolutionary algorithms are used to determine steady-state operating periods. Evolutionary algorithms are stochastic search methods based on principles of natural biological evolution and social behaviour of species. These techniques include genetic algorithms, mimetic algorithms, particle swarm optimisation, ant colony systems and shuffled frog leaping. A comparison conducted by Elbeltagi, Hagazy & Grierson (2005) of the evolutionary algorithms yielded that the particle swarm optimisation is the best.

Although most optimisation techniques are based on mathematical or stochastic methods, Li, Gu & Nui (2008) have taken a different approach to optimisation by using the correlation analysis technique to define the operational parameters of a power plant. The approach involved retrieving historical data, validating to remove bad data. Thereafter a correlation analysis was performed on the cleaned operational parameters. Uncorrelated and weakly correlation parameters were eliminated from further analysis. The relationships between strongly correlated parameters were further analysed. Optimal operational parameters settings were determined from these relationships and used as a guideline to optimise operations.

The various optimisation techniques above have associated positive and negative attributes and the technique best suited to the required application will provide the optimisation solution. Correctly defining the objective function and associated constraints or bounds is important for any optimisation technique used.

2.3.3 Uncertainty

Uncertainties in the process will cause these constraints to differ from the original design parameters. Uncertainties can be grouped into two types, aleatory and epistemic (Beyer & Sendhoff, 2007). Aleatory uncertainties are intrinsically irreducible such as noise, humidity, material parameters etc. These uncertainties are probabilistic in nature and can be described mathematically. Epistemic uncertainties result from an uncertain model used to represent the process i.e. approximations, boundary and operating conditions. Typical uncertainties included the following (Beyer & Sendhoff, 2007);

- Changing environmental and operating conditions such as operating temperatures, pressure and changing of material properties.

- Production tolerances and actuator imprecision, the plant production accuracy is limited by the precision of the equipment.
- Uncertainties in the system output, due to measurement errors.
- Feasibility uncertainties that are constraints the design parameters must obey.

In a case study presented by Gao *et al* (2003), two MPC controllers were implemented on the same site but on different processes namely a para-xylene unit and a propylene splitter column. Multivariate controller performance monitoring was implemented for these two MPC controllers and the initial benefit analysis showed improved performance with MPC. The routine performance analysis indicated the performance on the para-xylene unit was sustained however the propylene splitter column performance reduced. The poor performance was largely due to model mismatch during varying load conditions and also poor choice of constraints by operators. This finding highlights that changes in initial plant conditions, a form of uncertainty can result in sub optimal performance and parameters used in optimisation are required to be updated on a regular interval.

2.3.4 Real Time Optimisation

The optimisation techniques discussed can find a solution to the objective function offline or online whilst the process is operational. There are advantages and disadvantages associated with each approach. The implementation and architecture of real time optimisation on the petrochemical refinery has been briefly discussed by Van Wyk & Pope (1991). The following objectives should be met when maximising the economical benefit of an online plant and in order of importance (Tatjewski, 2008);

- Maintain the process in safe operation.
- Meet demands on product quality.
- Maximise the current production profit.

Safety of the control system is most important, once safety is achieved the control system is required to meet demands on product quality. Once these two aims are achieved, the process can be optimised. All the above objectives can be achieved in a multilayer

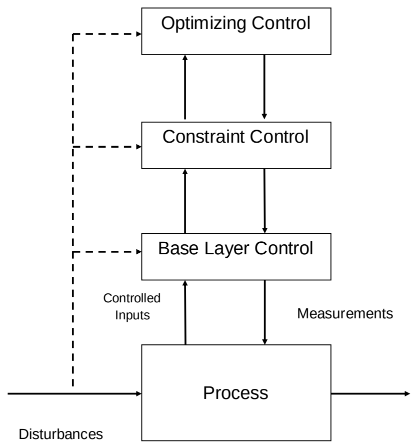

Figure 2.6: Multilayer control structure.

of control which can be broken up into the hierarchy shown in the Figure 2.6 (Tatjewski, 2008);

In the Figure 2.6 above, the base layer control is responsible for the basic safety of the process and achieving sufficient stability to meet product qualities. This layer has direct access to the plant i.e. valves, pumps, etc. The constraint layer is typically advanced control algorithms which is used to optimise the process. The most dominant advanced control technology is model predictive control (MPC) due to the following reasons;

- The predictive ability of MPC, it is very efficient in processes with difficult dynamics.
- MPC has a unique ability to take directly into account constraints imposed on process inputs and outputs which often have an effect on product quality and profitability.

A limitation that occurs in practise is the possible infeasibility of the MPC optimisation problem due to conflicting constraints. This occurs when the ROS region does not form part of the OOS region. The optimisation layer performs economic optimisation related to the controlled process. The aim is to calculate the optimal steady state values for the controllers in subordinate layers. The values of the optimisation result from the optimisation of certain objective functions typically defining profitability. Constraint control is achieved by the use of MPC however it can also be used as an optimiser as it allows handling of static and dynamic constraints on plant variables. Scattloini (2009) has reviewed the architectures for MPC and the results are in agreement with the work of Tatjewski (2008). Scattloini (2009) describes the layers of control as the base layer having faster dynamics than the constraint layer with the optimisation layer having the slowest dynamics. Also in a real time optimiser (RTO) the following must be considered;

- The adopted model must be updated periodically.
- Coherence must be guaranteed between the model used in the optimisation layer and the constraint layer.
- Accurate steady state target optimisation must be done to ensure that the RTO input and output references computed are feasible.

RTO can be defined as the online economic optimisation of a process which is based on a steady state plant model and is only executed when the plant is stabilised and the control problem is solved apart from the optimisation problem (Adetolai & Guay, 2010). Thus these two layers are not necessarily dealing with the same information and the operational point is often sub optimal. The integration of the RTO and control can be solved by the following two techniques (Adetolai & Guay, 2010);

- The one layer approach such that the economic optimisation and control problem are solved simultaneously in a single algorithm. Using MPC the economic objective function can be added to the MPC objective function.
- The two layer approach involves dynamic economic optimisation and non linear MPC. The RTO problem does not solve every sample but based on disturbance dynamics or plant conditions. The dynamic RTO is triggered when disturbances with high sensitivities are detected and feasible set points are recomputed.

Integration of RTO and control is still an open research problem and no theoretical foundation such as stability and performance analysis exists.

There are drawbacks of using RTO as discussed above, however an MPC constraint controller is sufficient to optimise the process under correctly defined constraints. Once the DOS region is correctly identified the constraint layer such as MPC can be used to keep the plant within these bounds.

2.4 Process Modelling and Simulation

The generalised optimisation approach in Figure 2.4 included developing a model of the process and simulating to identify the OOS region. This section will review key concepts regarding process modelling and simulation.

2.4.1 Process Modelling

Modelling a process requires defining the relation between inputs and outputs which can then be used to describe the operation and behaviour of the process. There are several techniques that can be used to model a process. Marlin (2000 426-427) has outlined the following procedure when modelling a process;

1. Define goals of the modelling process to solve the engineering problem and the required accuracy.
2. Identify the process, key variables and defining boundaries and assumptions.
3. Formulate the model by selecting equations based on fundamental principles.
4. Determine the format of the solution such as analytical or numerical.
5. Analyse the results by checking correctness and accuracy.
6. Validate the results by comparing with experimental results.

The first two steps in the process above are general to any modelling exercise. However, in the third step the process model can be formulated either mathematically or by data based techniques. Mathematical models as described above by Marlin (2000 426-427) can be used to develop process models using detailed knowledge of the physics and chemistry of the system. Industrial processes are complex and non linear thus requiring large effort to develop and may be subject to inaccuracies. Thus developing mathematical models of large process can become very costly. Data based modelling techniques are alternatives to develop input-output process descriptions. There are two main categories; the first is based on statistical techniques and the second is based on the use of artificial neural networks (McKay, Willis & Barton, 1997). Simple statistical techniques assume that relationships between input and output variables are linear and normally distributed. There are advanced statistical techniques to establish characteristics of non linear process, however these techniques require a degree of expertise in interpreting these statically based results. Neural networks are black box modelling tools which are based on the learning of input output mappings from experimental data. Appropriate inputs and outputs are required to be selected from the data set for the model. Usually statistical techniques are used to identify the neural network inputs and outputs. Neural networks require large amounts of data for training and verification of the input output mappings.

2.4.2 Simulation

Once the model of the process is developed the OOS region can be identified by simulating the model. There exist various software modelling and simulation tools to support these requirements. Modelling tools and simulators can be classified into two groups, block or equation oriented (Marquardt, 1996). Block oriented approaches compromises of using predefined blocks from a library of function blocks to model the behaviour of a process. The parameters of the predefined blocks model can be configured to represent the process to be modelled. These blocks are thereafter linked in a flow sheet manner to represent the process. Equation oriented approaches involves defining mathematical equations to model the process. Going the route of defining equations requires diverse knowledge of various disciplines such as programming, numerical methods, chemical engineering etc. Depending on the objective of the activity a model in being used in, different degrees of detail in modelling will be required which can be achieved using simulation tools.

2.4.3 Simulation Results

When determining the DOS region, the objective of modelling is to identify OOS region of the plant. In this case the format of the output of the simulated model solution is important. Marlin (2000 426-427) postulated that the format of the output solution of the model can be either analytical or numerical. Analytical solutions are used to determine specific numerical values of the modelling outputs whereas in numerical solutions the output is represented by equations. The OOS region of the plant model can be identified using the analytical solution by varying the inputs of the model.

Rodrigues & Minceva (2005) have also summarised a generalised philosophy in process modelling;

- Start with simple models such that the information from these models should remain valid for complex models.
- Model validity should not be a result of good data fit but rather have the capabilities to predict the system behaviour under operating conditions different from those used to obtain the model.
- Good results can only be obtained if the model represents the system.
- Use the model to obtain useful design parameters and their dependency on operating conditions.

The goal of developing a model is to predict the behaviour of the process being modelled and to interpreting results for applications such as process design, control and optimisation. Erroneous conclusions can be drawn from inadequate models thus building high quality and validated models are important. Models can be validated by plant data or experimental exercises. Collecting large amounts of data for model validation can be resource intensive and poorly designed experiments yield little useful information. Franceshini & Macchietto (2007) have used a technique called design of experiments. The technique aims at obtaining the most information from experiments used to validate models. Experimental design refers to when and how the experimenter will observe phenomena under investigation. These observations are used to validate the model but also to improve model parameters.

Bouchama, Sebastian & Nadeau (2003) considered a two stage flash evaporation circuit which was modelled both theoretically and experimentally. The theoretical model was developed mathematically using fundamental thermodynamic equations. The experimental model was validated by experiments on a pilot scale model. The theoretical model results were compared with the experimental model results. There was a difference in the results with theoretical model being more precise but slightly inaccurate and the resolution led to precise numerical results but was far from experimental results. The theoretical model parameters were fit to the experimental data using a numerical constraint solver. The final model was used for decision support during operation.

In conclusion, modelling and simulating a process can be accomplished by a variety of techniques but it is imperative that the modelling is representative of the process. Developing a process model can be useful in various applications such as process design, troubleshooting etc., however in optimisation it is required for the process model to identify the OOS region. The simulation results of the process model can be used to numerically determine the DOS region via intersection of the OOS and ROS region. The next sections discusses geometric intersection.

2.5 Geometric Intersection

To optimise a process, the optimisation algorithm requires bounds on different variables for constraint optimisation and as highlighted by Gao *et al* (2003), it is important to define these limits as accurately as possible. These bounds can originate from the ROS and or the OOS regions. As identified in the previous section simulation of the process model will result in the identification of the plant OOS region. The output format of the simulated model can either be analytical or numerical. An analytical output will allow the OOS region to be represented geometrically. The ROS bounds as discussed are a function of various factors and can also be represented geometrically. Thus intersection of these two geometric regions would result in the desired region of operation DOS region. This section firstly reviews two dimensional geometric intersection of polygons which includes defining convexity and the use of triangulation. The intersection of higher dimensions are also discussed.

In Figure 2.7, the DOS region is identified by the geometric intersection of the ROS and OOS regions. Intersection of two-dimensional geometric regions is the basis for a higher dimension intersection.

2.5.1 Two-Dimensional Intersection

Various techniques of two-dimensional geometric objects, polygons, intersection have been developed. It is critical before performing any intersection tests to define the type of

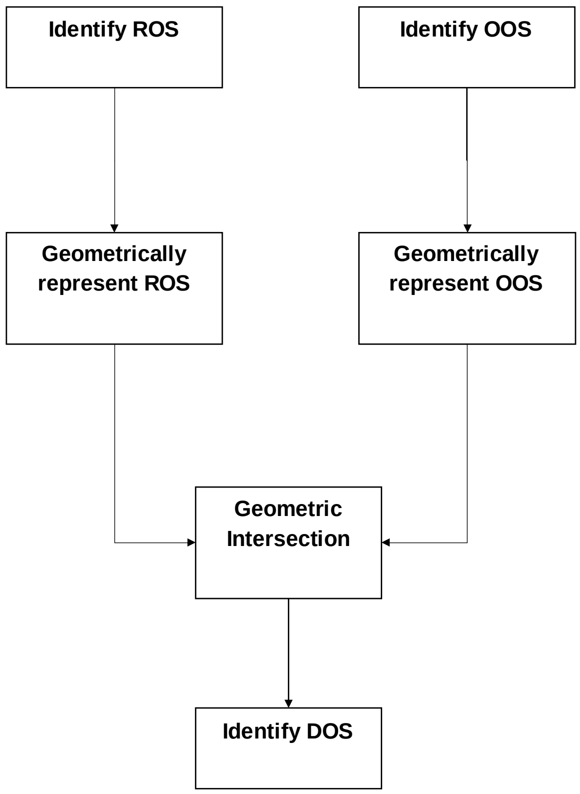

Figure 2.7: Identifying DOS region by geometric intersection.

polygons that are to be used in the intersections. Polygons can grouped as either convex or non convex as shown in Figure 2.8;

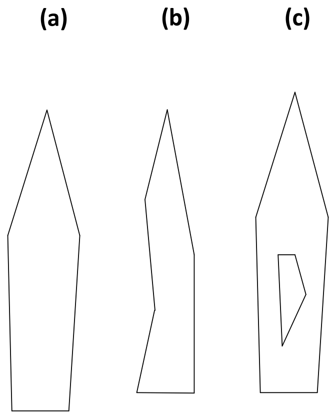

Figure 2.8: Convex(a) and non-convex (b and c) polygons.

In Figure 2.8 (a) a convex polygon has every internal angle less than 180 ° and every line segment of the polygon remains inside the boundary of the polygon. The concave polygon in Figure 2.8 (b) has an interior angle greater than 180 °. The polygon in Figure 2.8 (c) is considered non convex. When a polygon is non convex it is difficult to detect intersection in a reasonable time without pre-processing as large amount of computational effort is required. To improve the efficiency of geometric intersection algorithms when dealing with non convexity, it is required to simplify the geometric shape. The most popular techniques for simplifying geometric shape of a polygon is known as triangulation. Triangulating a polygon requires sub dividing the polygon into triangles without added new vertices.

Figure 2.9 (a) shows a polygon which has been triangulated in Figure 2.9 (b), the dashed lines show the triangles formed. Triangulation can become computational intensive and may take a long time to accomplish, there are techniques such as fast triangulation to shorten the process. Fast triangulation techniques involve inferring global information of the polygon, which can be accomplished by either the top down or left right up approach. The top down approach uses the polygon cutting theorem that states

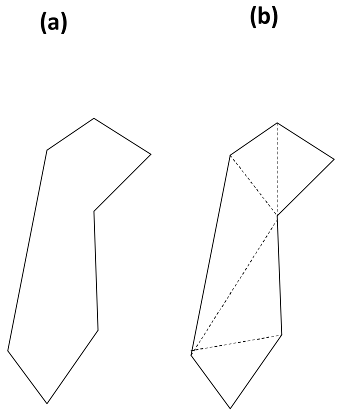

Figure 2.9: Triangulation of a polygon.

that the polygon can be cut along the diagonal into two equal sizes, it is however difficult to find the diagonal. The left right approach involves computing triangulations of the sub pieces of the polygon boundary however this requires the processing of vast amounts of information. The solution presented by Siedel (1991) uses horizontal decomposition, the left right approach whereby the polygon is firstly decomposed into trapezoids. This trapezoidalization algorithm relies on the plane sweep line technique. The vertices of the polygon P must be sorted with respect to their x-coordinates.

A vertical line, V, as shown in Figure 2.10 scans the sorted vertices and the polygon is decomposed into trapezoids with vertical parallel edges. Once the polygon is partitioned into simpler polygons, these polygons can easily be split into triangles by using the greedy algorithm technique presented by O'Rouke (Narkhede & Manocha, 2010). A greedy algorithm makes locally optimal choices with the hope of finding the global optimum. It makes a greedy choices to reduce the problem. It is not exhaustive and does not reconsider choices made and this can lead to a sub optimal solution.

Chazelle (1991) proposed a similar technique by using the left right approach to build a rough approximation of the triangulation then simultaneously use the information obtained left right approach in a top down manner to refine the triangulation.

A survey of the overview of triangulation algorithms of polygons (Lamot & Zalik,

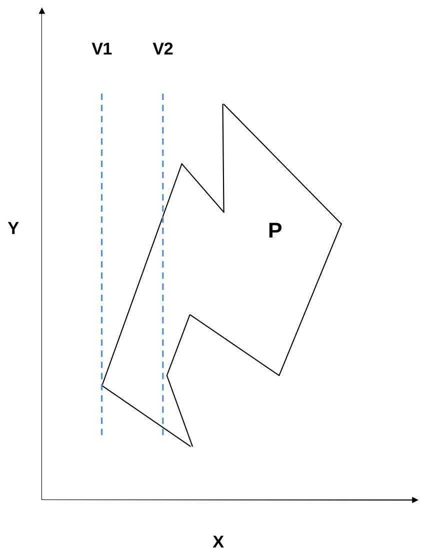

Figure 2.10: Horizontal plane sweep of polygon P.

1999) included various other techniques such as;

- Garey, Johnson, Preparata and Tarjan proposed a divide and conquer algorithm which is completed in two steps. The first step decomposes simple polygon into monotone sub-polygons and the second step triangulates these monotone sub-polygons.
- Kong, Everett and Toussaint developed an algorithm which is based on the Graham scan. The Graham scan is a fundamental backtracking technique in computational geometry.
- The Delaunay triangulation technique for a set P of points in the plane is a triangulation such that no point in P is inside the circumcircle of any triangle. Delaunay triangulations maximize the minimum angle of all the angles of the triangles in the triangulation.

The above survey compared the various algorithms and concluded that the Delaunay technique provided the highest quality and that the Siedel algorithm is the fastest. The Siedel algorithm can also be easily modified to handle non convex polygons and is thus the recommended algorithm for efficient triangulation.

Once the polygons are reduced either to simple polygons or triangles, the intersection can be determined. Shamos and Hoey (O'Rouke *et al*, 1982) developed a technique which determines the intersection of a pair of objects that is based on plane sweep. Each object is bounded by an aligned box, the objects only intersect if their bounding boxes intersect. The boxes intersect by comparing their projections on each coordinate axis. The alternate method of determining whether the intersection exists between the triangulated objects is to compare the vertices of the objects.

Determining the geometric intersection of polygons would involve the following;

- Identify the convexity of polygons.
- Choose a technique to simplify the polygons.
- Triangulate the simplified polygons.
- Perform an intersection test of the above triangles.

The final parameters from the intersection test will result in the DOS parameters required in Figure 2.7. The number of output parameters in the OOS regions determines the dimensions of the intersection, thus higher dimension intersection is discussed in the following section.

2.5.2 Three-Dimensional Intersection

Intersection of geometric objects in a three-dimensional space is more involved than two dimensions. Three-dimensional geometric intersection is frequently used in computer graphics for which it is required to determine collision detection of volumes. These real time three-dimensional intersections require efficient algorithms and a survey conducted by Jimenez, Thomas & Torras (2001) provided an overview of various techniques developed. Most of these real time intersection techniques of three-dimensional objects eventually require applying a static interference test between the three-dimensional polyhedron and similar to the intersection of polygons, convexity of the polyhedron is very important.

Jimenez *et al* (2001) deduced that there are two basic contacts between two polyhedra which reduces the interference problem in detecting edges piercing convex faces. The first type of contact takes place when a face of one polyhedron is in contact with a vertex of the other polyhedron and the other contact type is when an edge of one polyhedron is in contact with an edge of the other polyhedron. Thus, most techniques decompose the polyhedron or their boundaries into convex polyhedra. The aim is to determine the closest points of two polyhedra, and then compute the euclidean distance between them by using techniques such as Dobkin and Kirkpatrick's hierarchical polyhedral representation or the Minkowski difference of two polytopes. An alternative technique in identifying intersection is to navigate along the boundaries of the involved polyhedra in the direction of decreasing distance. Spherical representations are also appealing due to the simplicity of calculating the distance between two spheres, thus ellipsoids are used to approximate convex polyhedra. The sphere-box algorithm presented by Ratschek & Rokn (1994) incorporates the sphere-box test as used in spatial subdivision techniques and ray tracing. The midpoint m and the radius r are the sphere parameters. The tests determine the smallest or largest distance from m to the box, and compare it with r. This determines if the sphere is inside, outside or partially inside the box.

All the intersection tests for polyhedral above, similar to polygon intersection, are dependent on the convexity of the polyhedra. A comparative study was presented by B Chazelle *et al* (1997) on the techniques used to decompose the surfaces of complex polyhedras into simpler convex surfaces. The techniques include space partitioning, space sweeping and flooding.

- The space partitioning technique uses binary space partitioning to split up the surface into convex patches. The method builds a tree by recursively dividing space by a cutting plane. Each node v of the tree is associated with a convex polyhedron Pv. The aim is to explore the two children of v if and only if the portion of the surface within Pv is not convex.

- In the space sweep technique the cross-section of a surface consists of simple polygonal curves which are decomposed into convex pieces. This technique attempts to maintain each curve as long as possible while moving the plane, thus producing convex patches in the process. Each time a convexity violation is found a new convex curve is started.

- In flooding, let H be the dual graph of the surface, where nodes represent facets and arcs join nodes associated with adjacent facets. The class of flooding heuristics refers to the incremental strategy of starting from some node and traversing the graph H, collecting facets along the way as long as they form a convex patch.

For the above study flooding was concluded to be the method of choice. Although it is possible to triangulate all convex polyhedral it has been proven that it is impossible to triangulate non convex polyhedral and little research on convex decomposition of polyhedra has extended beyond the theoretical stage. This has proven to be a limitation on the intersection of geometric objects in dimensions higher than two.

The literature review addressed previous controllability and optimisation methods developed and highlighted the gap for improvement. The various industry approaches to optimisation was reviewed and a generalised approach to optimisation was formulated. Key concepts around optimisation such as objective functions, uncertainty and real time optimisation was discussed. The generalised approach to optimisation required the process to be modelled and simulated to identify the OOS region. The key factors for modelling and simulation were reviewed. Identification of the DOS region requires the intersection of the ROS and OOS feasible regions and concepts of geometric intersection were also reviewed. The information analysed in the literature review can be used to develop the intersection algorithm.

CHAPTER 3

EXPERIMENTAL

It has been established that optimisation algorithms require feasible constraints on plant parameters to operate the plant within the desired regions. Incorrect definition of these constraint parameters could result in the optimisation requiring the control system to operate the plant in an unattainable region. This problem is addressed by the determining the DOS region which is the common region between the ROS and the OOS region. The parameters of the DOS region will provide constraints for the optimisation techniques which will result in a feasible solution. This section reviews the case study that will be used to evaluate the algorithm, the modelling and simulation of the case study, the intersection algorithm and the key performance metrics required for evaluation.

There are various process plants that do not have optimisation techniques, the approach in defining plant parameters is shown in Figure 3.1;

Figure 3.1 is a simplification of the generalised optimisation approach using the DOS region shown in Figure 2.5. The parameters for the plant are only a function of the ROS region. The ROS region is a result of decisions that are defined by the economical operational of the plant, factors influencing production such costs, customer requirements, maintenance, in addition to others. These decisions are typically taken on a daily basis by plant personnel. The bounds of the ROS region must lie within the feasible region. Correctly defining these bounds are important as Gao *et al* (2003) have found that poor choice of constraints by operators led to poor control performance. The same problem of defining feasible operating regions is faced when using and not using optimisation. Thus identifying the DOS region is also valid for processes that do not use optimisation as shown in Figure 3.2;

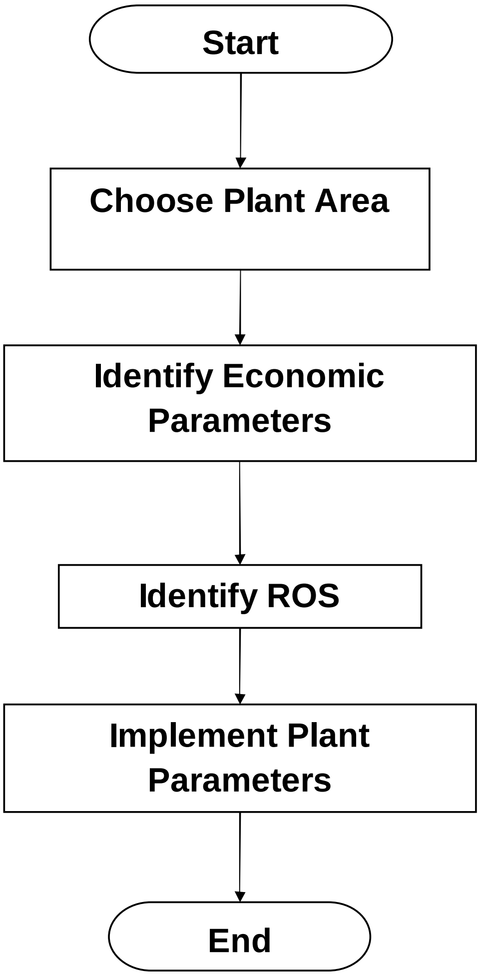

Figure 3.1: Generalised approach when defining plant operational parameters.

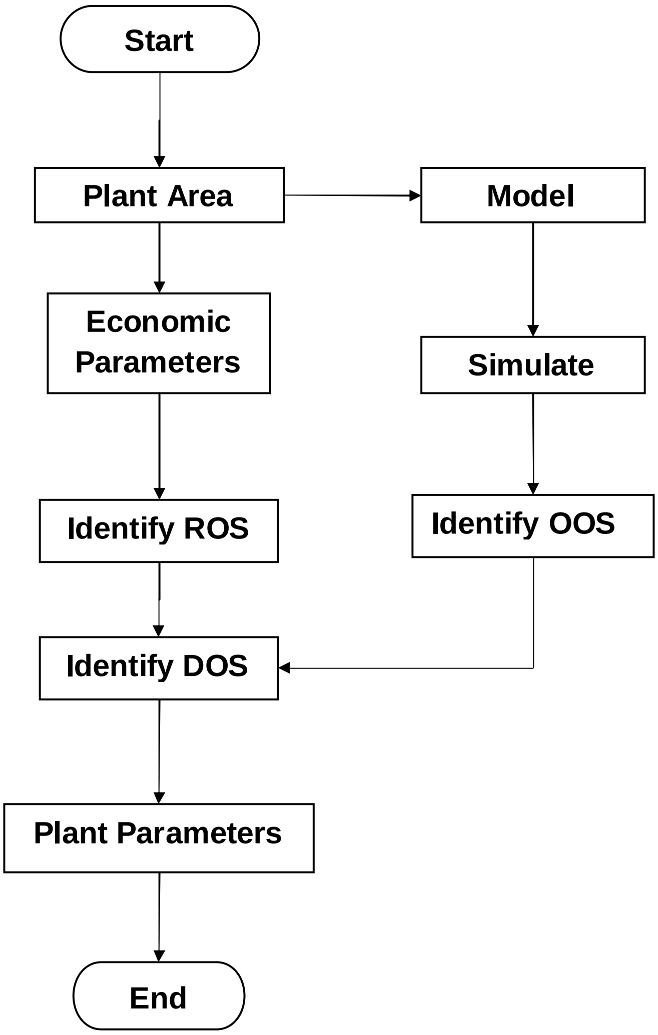

Figure 3.2: Generalised approach when defining plant operational parameters using the DOS region.

Based on the literature and the approach shown in Figure 3.2, automatic constraint propagation to identify the DOS region via numerical methods will involve the following during the experimental procedure;

Identify Plant Area Identification of plants to be used as a case study.

Identify ROS region required for the above identified plant.

Model the above chosen process.

Simulate the above model.

Identify OOS from the output of the simulation.

Identify DOS by determining the intersection of the ROS and OOS regions identified.

Evaluate Results based on key performance metrics.

3.1 Case Study

An HCl flash circuit was chosen as the case study to identify the DOS region via the proposed algorithm.

3.1.1 HCl Flash

The following process uses a flash column to flash off HCl from the available 10N HCl feed. The feed includes the solvent, water.

The plant is designed to operate on a maximum re-boiler duty with an abundance of feed. The feed includes a mixture of fresh 10N HCl and recycled HCl. The acid normality and solvent content of the recycle can vary. Thus the process input variables are;

- Feed rate - kg/h.
- Feed solvent composition - mol/l.

The flash product is required to be within required specifications as determined by down-stream processes and the bottom product is disposed as waste. The output variables of interest are;

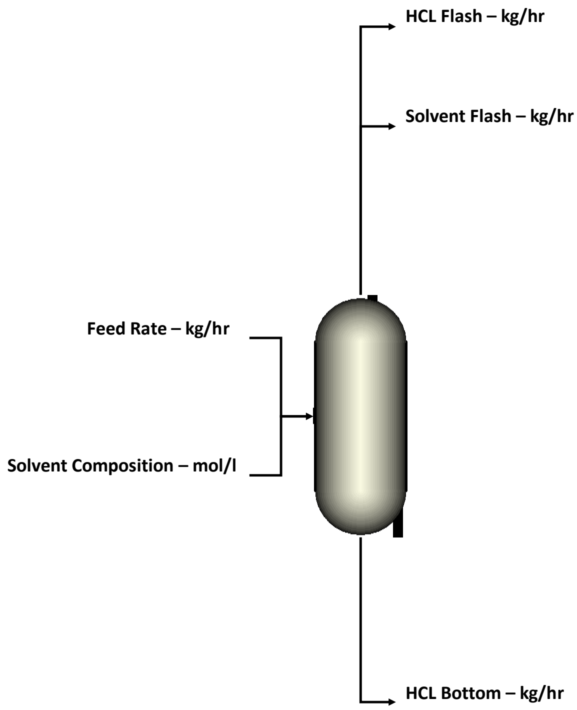

Figure 3.3: HCl FLASH circuit.

- HCl flash product rate - kg/h .
- Solvent flash product rate - kg/h.
- HCl bottom product rate - kg/h.

The typical operating specifications of the plant are shown in Table 3.1.

Table 3.1: HCL flash process operational specifications.

Parameter	Value	Unit
Feed Rate	5	kg/hr
Feed Temperature	330.7	K
Feed Composition	10	NHCL
Flash Temperature	340.7	K
Bottom Temperature	401.7	K
Bottom Composition	6	NHCL
Operating Pressure	117.2	kPa
Re-boiler heat duty	22.4	MW

It would be required to maximise the feed rate particularly the use of recycled acid, which would imply higher solvent composition in the feed. At the same it would also be required to minimise HCl bottom flow rate while still being within the solvent flash product specification.

3.2 Modelling and Simulation

In the literature survey the guideline based on Marlin (2000 334-337) when modelling a process was discussed. The first step in modelling any process is to define the goal of modelling, in the chosen case studies the goal is to develop a model that can be simulated to identify the OOS region. The second step involves identifying all key process variables, that were been identified in the detailed description of each process. The third step requires selecting a modelling technique. There are several methods to model a process which include modelling based on fundamental chemistry and physics or using data driven methods. The modelling technique adopted is based on the approach illustrated by Marquardt (1996) which incorporates block modelling tools in a simulator. The fourth step requires determining the format of the output solution, in order to represent the OOS region geometrically the output was numerical. The Aspen Plus Modelling toolkit was used to model and simulate the chosen process. The following process was followed when modelling each process in the chosen toolkit;

- The appropriate equipment was selected to best represent the system. The process was built in a flow sheet manner by connecting various pieces of equipment to represent the chosen process. The specifications defined in the detail description of the process was used.
- Operational parameters defined in the detailed description of each process were used as inputs for the various equipment and connections that made up the model.
- Key input variables were simulated by selecting variables on a rectangular mesh to identify the effect on key output variables creating the required OOS region. Each input variable was incremented by a fixed step size between its high and low limits.
- The simulation of the input variables via the model resulted in corresponding values for the output variables which represented the OOS region.

Each input variable was incremented by a total number of steps, t_s, between the low and high limits. When two input variable exist, input variable one is incremented through its entire range for each increment of the second variable. The same will apply for systems with larger than two variables. Each increment in an input variable will result in a value for an output variable thus the total number of data points per output variable, d_o, are as follows;

$$d_o = t_s^{x_i} \tag{3.1}$$

where x_i is the number of input variables incremented. Increasing the number of steps or the number of input variables will exponentially increase the number of output values. These increases require a more computational effort and have an impact on the simulation time required. The converse will result in quicker simulation time however there is a risk of losing process information due to low resolution. There is a tradeoff between computational effort and loss of information.

The flow of data is shown in Figure 3.4, the input variables, X, are simulated which results in output variables, Y. The output matrix Y comprises of vectors for each output variable, i.e. the columns of Y. The matrix Y is the OOS.

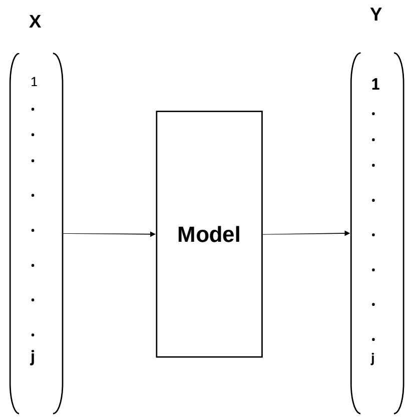

Figure 3.4: Data flow of simulating the process model.

3.3 Intersection

3.3.1 Data Pre-processing

Each output of the simulation namely is the columns of matrix Y, Y_i, of the OOS region was normalised, Y_N, to a range between 0 to 1. The normalised data, Y_N, was meshed into an n-dimensional data structure thus the dimensionality of the data structure is based on the number of output variables. Each dimension of the data structure are the same size i.e. a matrix data structure will be a square. It is therefore required to specify the size of data structure Y_N. Once the size of the data structure is defined the normalised data can be meshed in the data structure, this implies that each element in Y_N will be meshed into bins. Using the size of the data structure the meshing bin size, B_S, can be calculated as follows;

$$B_S = R^{-1} \tag{3.2}$$

where R is the size of the data structure. Similarly to equation 3.1 the larger the size of the data structure the higher the resolution of the data however more computational effort is required. If a normalised output value lies within a bin, the corresponding element is set to 1. The end result is a data structure, Y_N such that the ones represent the OOS region. Figure 3.5 below is an example of two output variables generated from the simulation of the model.

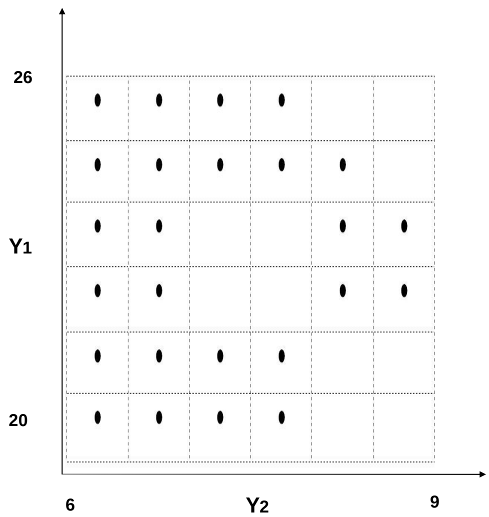

Figure 3.5: OOS data from simulating a model.

In Figure 3.5 variable Y_1 and Y_2 range between 20 and 26, 6 and 9 respectively. The OOS region in Figure 3.5 is represented by the dots. If the size, R, of the normalised matrix Y_N was chosen to be 6, the resolution according to equation 3.2, B_S is 0.166. The meshed normalised meshed data is shown in Figure 3.6;

In Figure 3.6 the ones represent a point that is part of the OOS region. Choosing a large size of the data structure will result in higher resolution however this is limited to the resolution of the simulated output Y. A summary of the data pre-processing is shown in Figure 3.7;

The normalisation of data generated by the simulation is summarised in Figure 3.7, whereby the simulation output matrix Y is normalised and mapped to form Y_{OOS}. Similarly the ROS bounds, Y_R can be represented as matrix Y and by following the same steps, Y_{ROS} can be found such that the 1's represent the ROS. The approach shown in Figure 3.7 can be adopted as follows;

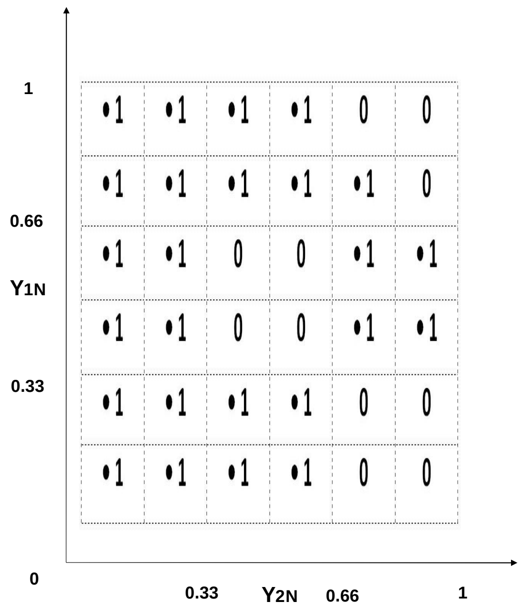

Figure 3.6: Normalised meshed OOS data.

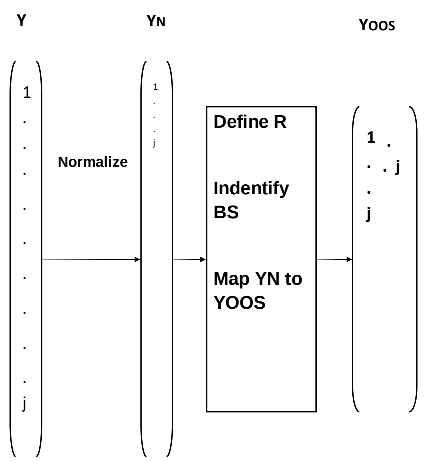

Figure 3.7: Simulation OOS data normalisation flow.

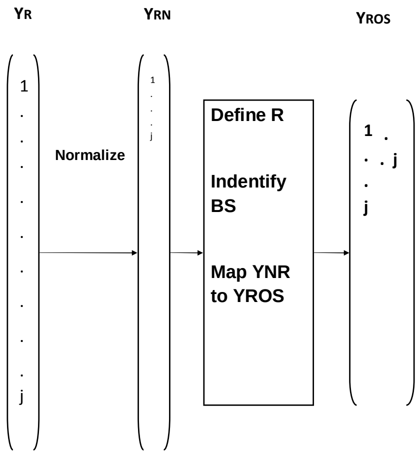

Figure 3.8: ROS data normalisation flow.

Using the approach in Figure 3.8, Y_{ROS} can be determined.

3.3.2 Intersection Test

The OOS and ROS regions after pre-processing are represented by two data structures Y_{OOS} and Y_{ROS} respectively. In the case of a two output variable system, the data structures will be in the form of matrices. Identifying the DOS region involves determining the intersection of Y_{OOS} and Y_{ROS}. The literature survey has shown the most suitable geometric intersection technique is presented by Chazelle (1991) which involves representing Y_{OOS} and Y_{ROS} as polygons, triangulating these polygons and finding the intersection of these triangles. The horizontal decomposition technique presented by Siedel (1991) can be used represent Y_{OOS} and Y_{ROS} as polygons. This technique involves using plane sweep to determine the vertices of the polygon. An alternative technique to identify the intersection of Y_{OOS} and Y_{ROS} involves finding the sum, Y_S of the two matrices as follows;

$$Y_S = Y_{OOS} + Y_{ROS} \tag{3.3}$$

The elements in Y_{OOS} and Y_{ROS} are matrices consisting of 0's and 1's, therefore a summation will result in intersection elements in Y_S having the value of 2. The DOS will become the bounds of elements with the value of 2. This is shown in Figure 3.9;

$$\overset{Y_{OOS}}{\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}} + \overset{Y_{ROS}}{\begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}} = \overset{Y_{S}}{\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 2 & 2 & 1 \\ 0 & 2 & 2 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}}$$

Figure 3.9: Summation of OOS and ROS matrices.

The region of intersection in Figure 3.9 is circled in red on the Y_S matrix. The bounds of the region of intersection can be reconstructed by post data processing.

3.3.3 Data Post Processing

Reconstructing the region of intersection found in Y_S will firstly involve determining the vertices of the intersection region boundaries. These vertices can be represented as rectangles, therefore the horizontal decomposition technique presented by Siedel (1991) will be used. This technique performs a left right plane sweep of the matrix. Along each x-axis coordinate the maximum and minimum y coordinates are stored for consecutive values of 2. This is shown by the red boxes in Figure 3.10;

Using the plane sweep technique produces rectangles, a set of y coordinates for every sweep on each x coordinate, which can result in a large set of DOS values. In Figure 3.10 there are six rectangles and these six rectangles can be optimised and reduced. This is accomplished by identifying larger optimised rectangles within the set of coordinates provided by the plane sweep technique. The optimised rectangles are determined by finding the rate of change of the x and y coordinates. If the rate of change is zero for both the axises then those coordinates form part of the trapezoid. This is shown in Figure 3.11;

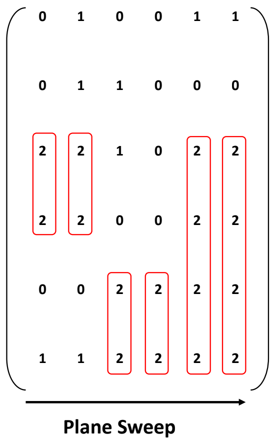

Figure 3.10: Left right plane sweep of intersected matrix.

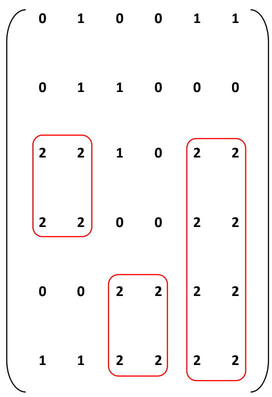

Figure 3.11: Identifying optimised rectangles from plane sweep matrix.

The coordinates of the optimised rectangles become the DOS, Y_{DOS} in the form shown in Table 3.2;

Table 3.2: Final DOS parameters.

Y_{DOSXMN}	Y_{DOSXMX}	Y_{DOSYMN}	Y_{DOSYMX}
1	2	3	4
3	4	1	2
5	6	1	4

The parameters Y_{DOSXMN} is the x axis lower bound, Y_{DOSXMX} is the x axis upper bound, Y_{DOSYMN} is the y axis lower bound and Y_{DOSYMX} is the y axis upper bound. A summary of the data post-processing is shown in Figure 3.12;

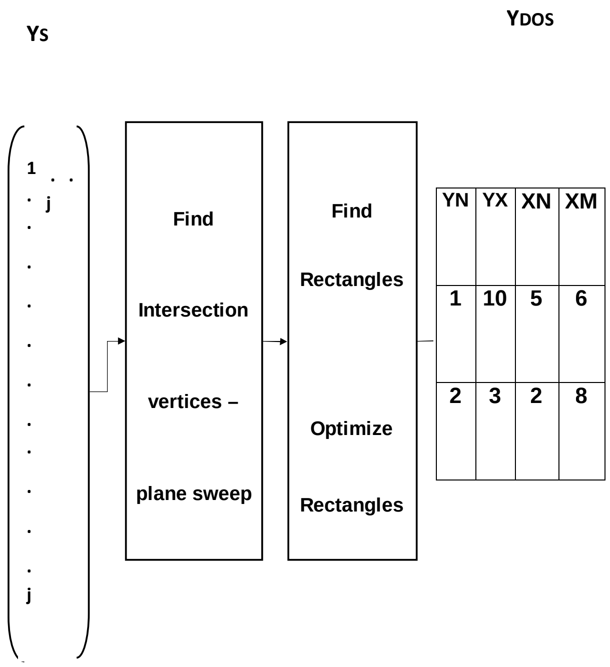

Figure 3.12: Post processing data flow.

A summary of the approach of determining DOS from OOS and ROS region is shown in Figure 3.13;

In Figure 3.13 the procedure is used to determine the DOS region is shown and can be summarised as follows;

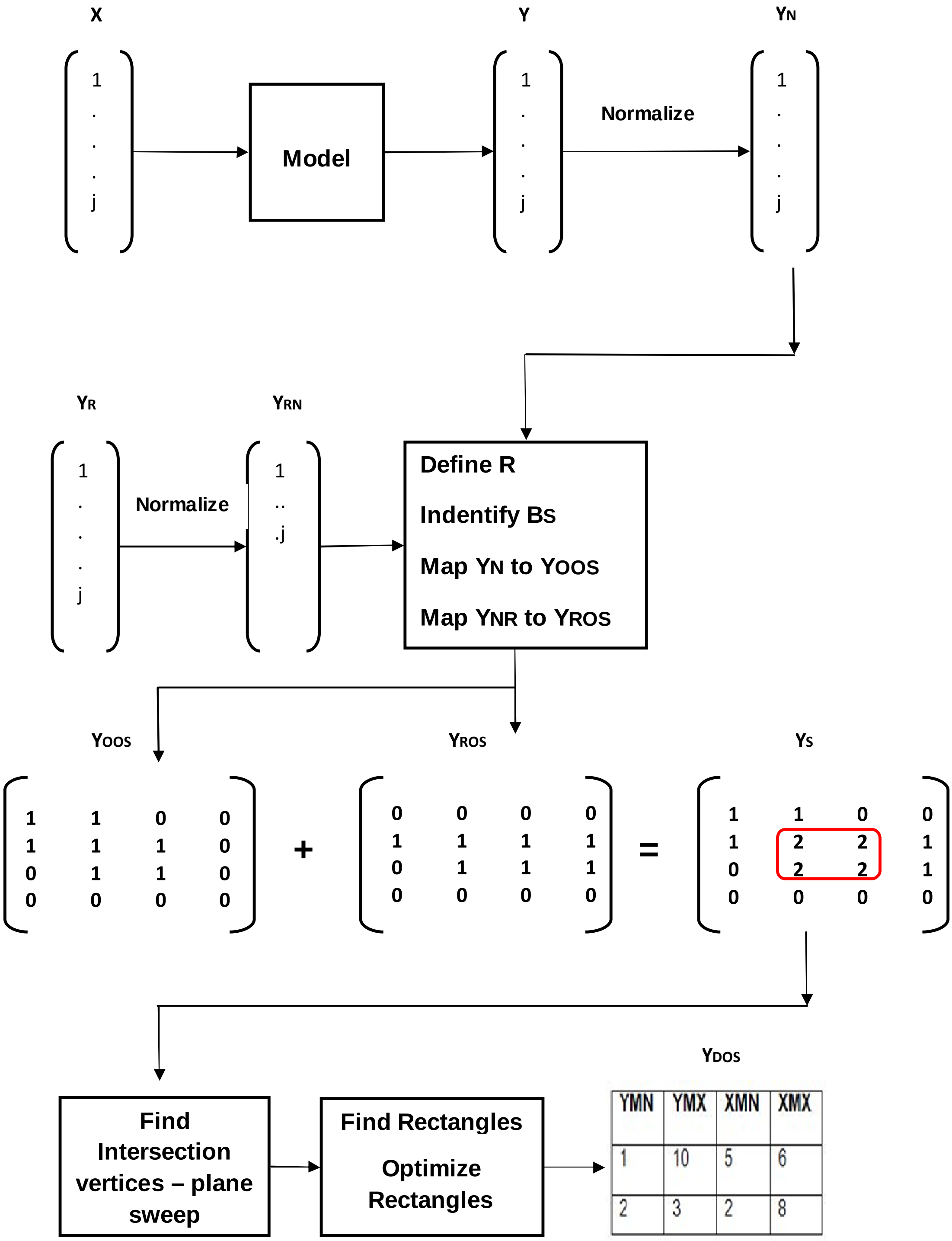

Figure 3.13: Summary data flow to identify DOS region.

- Model the process in the Aspen Plus software.
- Simulate the model by varying the input variables where the number of output data points is determined by equation 3.1.
- This will result in the OOS region, Y, for the output variables of interest.
- Normalise Y resulting in Y_N.
- Define ROS region, Y_R, for the output variables of interest.
- Normalise Y_R resulting in Y_{RN}.
- Group Y_N into Y_{OOS} by defining the matrix resolution ,R,and bin size B_S.
- Similarly re-sample Y_{RN} into Y_{ROS}.
- Find intersection Y_S by the sum of Y_{OOS} and Y_{ROS}.
- Find vertices of Y_S by using the plane sweep technique.
- Find the rectangles from vertices found in plane sweep above.
- Find optimised rectangle that represent the largest feasible region.
- The coordinates of the optimal rectangle is reported as the DOS region Y_{DOS}.

Once the DOS region is identified optimisation and constraint controllers such as MPC can be used to effectively drive the process to the optimal operation point.

3.4 Key Performance Metrics (KPM)

Various applications of optimisation in literature across various industries have proven beneficial. It has also been identified there are different approaches in optimising a process but the end goal remains the same which is operating as efficiently as possible, yielding the largest achievable profit margin while adhering to safety as outlined by Tatjewski (2008). In online optimisation the optimisation model is required to provide feasible solutions to plant output within an acceptable time frame. Optimisation solutions will prove to be of little benefit if the solution takes excessively long due to highly intensive computational effort. The first KPM to be evaluated will be time, τ, required to implement the optimisation solution. Identifying the most feasible region of operation is extremely dependent on the constraints the solutions can be optimised within. Gao *et al* (2003) have shown that poor choice of constraints lead to a poorly performing plant. Literature provided that constraints can be determined by either plant personnel or process modelling methods. Determining constraints using process modelling can be accomplished by determining the boundaries of operation from a model or the technique of geometric intersection. The following KPM would be to determine the maximum achievable feasible space attained by each technique. The feasible region, η will be calculated similarly to the OI developed by Vinson & Georgakis (2000). The feasible region defined by the ROS region will be calculated as follows;

$$\eta_{ROS} = \mu(ROS \cap OOS)/\mu(OOS) \tag{3.4}$$

where μ represents a function calculating the size of the space. If the η_{ROS} is less than 1, this implies the ROS is non attainable. Thus the non attainable fractions will be defined as follows;

$$\eta_{\tilde{ROS}} = 1 - \eta_{ROS} \tag{3.5}$$

The feasible region defined by the DOS region will be calculated as follows;

$$\eta_{DOS} = \mu(DOS \cap OOS)/\mu(OOS) \tag{3.6}$$

If the η_{DOS} is equal to 1, it would also be required to check if the entire OOS region was utilised. The utilisation of the DOS region, ϵ_{DOS}, is calculated as follows;

$$\epsilon_{DOS} = \mu(DOS)/\mu(OOS) \tag{3.7}$$

Thus the KPM are as follows;

- Computational time required to calculate constraints, τ.
- Feasible area due to ROS region, η_{ROS}.
- Non feasible area due to ROS region, $\eta_{\tilde{ROS}}$.
- Feasible area due to DOS region, η_{DOS}.

- Utilisation of OOS region by DOS region, ϵ_{DOS}.

The KPM's above will be evaluated in the next section of results.

CHAPTER 4

RESULTS

In this section, the intersection algorithm was tested on the chosen case study and results were observed. This includes the method used to obtain the results, the analysis of the OOS region, requirements of the ROS region and the DOS region identified by the proposed algorithm. The results of the DOS region were evaluated according to the defined KPM's.

4.1 Method

The methods for determining the DOS have been outlined in the previous section. The following results were observed for the model system discussed in Section 3.1;

- The IOS and the output variables of interest were specified in the detailed description of the case study.
- The OOS region of the case study was identified by using the process model and simulation by varying the IOS between the above specified upper and lower bounds. The OOS region was then represented graphically.
- Thereafter the ROS region was defined whereby these parameters were tabulated and superimposed on the graph representing the OOS region. Three sets of ROS operational parameters were defined and are as follows;
  - The first set of parameters lie within a feasible region.
  - The second set of operational parameters lie in a region that is partially feasible.

  - The third set of parameters lie in a non convex region of the OOS region.

- The intersection algorithm will be used to identify the DOS region parameters. The DOS region will be represented graphically and the bounds will be tabulated.

- The above DOS parameters found above will be evaluated according to the kpm defined.

4.2 OOS region

The inputs of the HCL Flash were defined in section 3.1.1 as the feed rate and the feed solvent composition. The bounds of this IOS space is as follows;

Table 4.1: HCl process Input Operational Space.

Parameter	*LowerBound*	*UpperBound*	*Unit*
Feed Rate	1	10	kg/h
Feed Solvent Composition	0.1	3.0	mol/l

The Feed Rate was incremented in steps of 0.1 and the Feed Solvent Composition was incremented in steps of 0.03. Each variable was incremented by 100 steps and according resulting output of 10 000 data points. The output variables of the HCl Flash were defined in section 3.1.1 as the HCl Flash Flow, Solvent Flash Flow and the HCl Bottom Flow. Based on the simulation of the AIS the range of operation of the output variables are shown in Table 4.2.

Table 4.2: HCl process Available Output Space.

Parameter	*LowerBound*	*UpperBound*	*Unit*
HCL Flash Flow	0.056	9.33	kg/h
Solvent Flash Flow	0.0006	0.109	kg/h
HCL Bottom Flow	0.0015	0.26	kg/h

The normalised OOS region generated in Figure 4.1 shows the achievable solvent flash flow, Fs, versus the bottom HCl, Fb, flow. The objective function of this process is shown in the equation 4.1;

$$\min(Fs) \& \min(Fb) \tag{4.1}$$

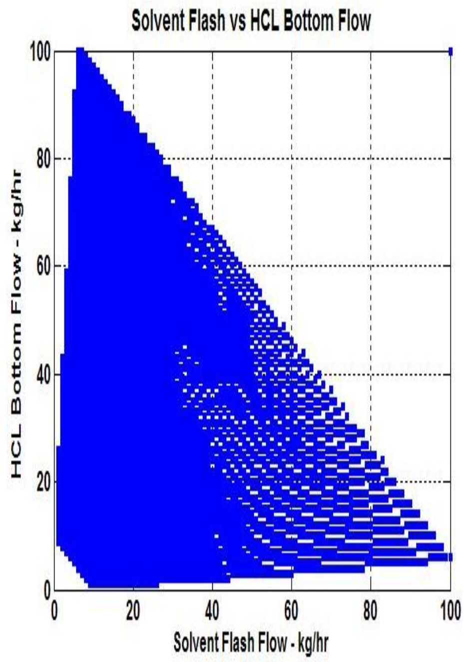

Figure 4.1: OOS region for Flash Solvent Flow versus Bottom HCL Flow.

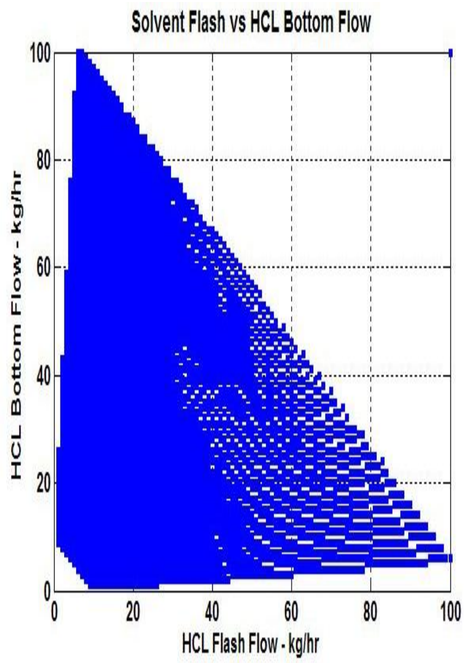

Figure 4.2: OOS region for Flash HCL Flow versus Bottom HCL Flow.

Minimising solvent flash flow will result in a more concentrated product being produced and minimising bottom HCl flow will result in less waste acid. The OOS region generated in Figure 4.2, shows the achievable flash HCl flow versus the bottom HCl flow. It would be required to maximise flash HCl flow and minimise flow bottom HCl flow. The upper bound on the flash HCl flow would be the amount of solvent flow, D_S, the circuits downstream can accommodate. Since the amount of solvent flash flow is directly proportional to flash HCl flow, the objective defined in equation 4.1 will be as follows;

$$\max(Fs)\&\min(Fb) \tag{4.2}$$

Equations 4.1 and 4.2 are only valid if there are no upstream constraints which could include insufficient storage space for recycled acid. It would then be required to achieve a minimum plant throughput, P_R, this will result in a lower bound on the bottom HCl flow. Normal plant, P_N, throughput is calculated as follows;

$$\mathrm{P_N} = \mathrm{BottomHClFlow} + \mathrm{FlashHClFlow} \tag{4.3}$$

thus equation 4.2 is subject to the following constraints;

$$\mathrm{P_N} > \mathrm{P_R} \tag{4.4}$$

and

$$\mathrm{SolventFlashFlow} < \mathrm{D_N} \tag{4.5}$$

The objective function in equation 4.2 will maximise solvent flash flow constrained by downstream capacity that forms the upper bound constraint. The objective function is required to achieve a minimum production rate which forms the lower bound constraint. An optimiser or a constraint controller such as MPC will require these upper and lower bounds of the ROS region for the flash solvent flow and the bottom HCl flow.

4.3 ROS region

Three scenarios, based on normalised operational parameters, have been defined for evaluation and are listed in the tables below. For all three parameter sets above the lower bound on flash solvent and bottom HCl flow are defined by production requirements. The upper bound on flash solvent flow is determined by the capacity of downstream processes. The upper bound on bottom HCl flow is determined by financial constraints. The ROS parameters are listed in Table 4.3;

Table 4.3: ROS parameters Set 1.

Parameter	$Lower Bound$	$Upper Bound$
Set1		
Flash Solvent Flow	10	30
Bottom HCL Flow	10	25
Set2		
Flash Solvent Flow	20	30
Bottom HCL Flow	70	90
Set3		
Flash Solvent Flow	20	40
Bottom HCL Flow	20	30

4.4 DOS region

The ROS regions in Table 4.3 are represented by the green boxes are resulting DOS regions is represented by the red boxes as shown in Figure 4.3;

DOS Parameter Set 1

The DOS region in Figure 4.3 is superimposed on the ROS region and is represented by the red box. The DOS region parameters are shown in Table 4.4;

Table 4.4: DOS parameters Set 1

Fsmin	Fsmax	Fbmin	Fbmax
10	30	10	30
η_{ROS}	$\eta_{\tilde{ROS}}$	η_{DOS}	ϵ_{DOS}
100	0	100	100

The η_{ROS} is 1 which implies the ROS region falls directly within the OOS region and the plant is not required to operate in a non feasible region. Thus the DOS region operational parameters are the same as the ROS region operational parameters. As expected the η_{ROS} and ϵ_{ROS} values are 1.

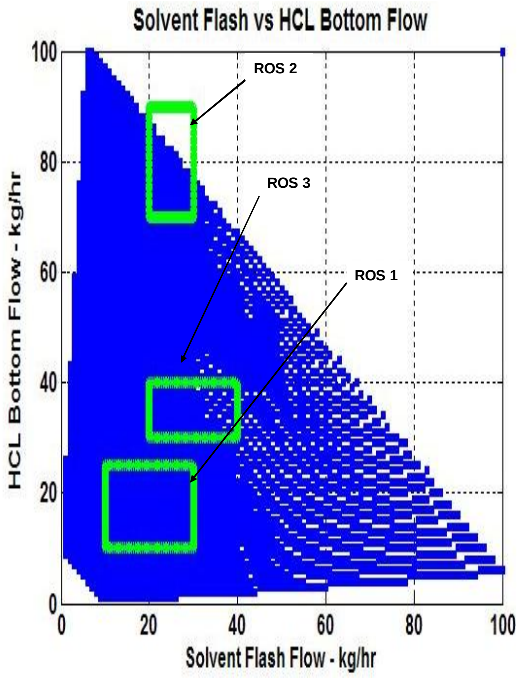

Figure 4.3: DOS regions for Flash HCL Flow versus Bottom HCL Flow ROS.

DOS Parameter Set 2

The DOS region in Figure 4.3 is superimposed on the ROS region and is represented by the red box. The ROS region lies partially outside the OOS region, only 59.7% of the ROS region lies inside the OOS region. The intersection algorithm first identifies rectangles of operation and there are 9 different operational rectangles defined for the DOS region. This is largely due to the fact that the upper boundary of the HCl Flash flow in the OOS region is not a straight line. These rectangles are shown in Figure 4.4;

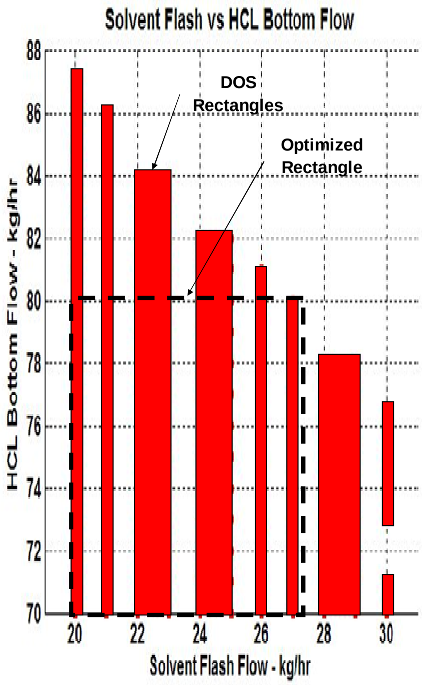

Figure 4.4: DOS rectangles for ROS parameter Set 2.

In Figure 4.4 the DOS regions lie 100 % within the OOS region. The DOS region operational parameters does not cause the plant to operate in a non feasible region as opposed to the parameters defined by the ROS region. The largest rectangle in Figure 4.4 only utilises 19.5 % of the OOS region. Thus it is possible that there exists set of DOS region operational parameters which utilise more than 19.5% of the OOS region. The optimised DOS region parameters based on the rectangles Figure 4.4 are shown in Table 4.5;

There is a much larger utilisation of the OOS region with the optimised DOS region

Table 4.5: DOS optimised parameters Set 2.

Fsmin	Fsmax	Fbmin	Fbmax
20	27	70	80
η_{ROS}	$\tilde{\eta}_{ROS}$	η_{DOS}	ϵ_{DOS}
59.7	40.3	100	38.1

parameters. The optimised DOS rectangle now represents 38.1 % of the OOS region and the boundaries shown in Table 4.5 can be used as upper and lower bounds for control systems and optimisers. These bounds are guaranteed to lie within attainable regions of operations.

DOS Parameter Set 3

The DOS region in Figure 4.3 is superimposed on the ROS region and is represented by the red box. The ROS region lies inside the OOS region however only 91.3% of the ROS region is attainable inside the OOS region. This is a result of the OOS region being non convex within the ROS region, this is seen by the white spaces in Figure 4.3. The intersection algorithm first identifies rectangles of operation and there are 28 different operational rectangles defined for the DOS region. These rectangles are shown in Figure 4.5;

In Figure 4.5 all the DOS regions lie 100 % within the OOS region. The DOS region operational parameters does not cause the plant to operate in a non feasible region as opposed to the parameters defined by the ROS region. The largest rectangle in Figure 4.5 only utilises 52.3% of the OOS region defined within the ROS region. This largest rectangle is the optimised DOS region and is shown in Table 4.6;

Table 4.6: DOS parameters Set 2.

Fsmin	Fsmax	Fbmin	Fbmax
20	30	30	40
η_{ROS}	$\tilde{\eta}_{ROS}$	η_{DOS}	ϵ_{DOS}
91.3	8.7	100	52.3

In Table 4.6 only 91.3% of the ROS region is feasible inside the OOS region, the remainder 8.7% is non attainable. This non attainable region is seen by the spaces between the rectangles is Figure 4.5. The DOS region lies 100% within the OOS region and the DOS region operational parameters does not cause the plant to operate in a non feasible region as opposed to the parameters defined by the ROS region. By using the

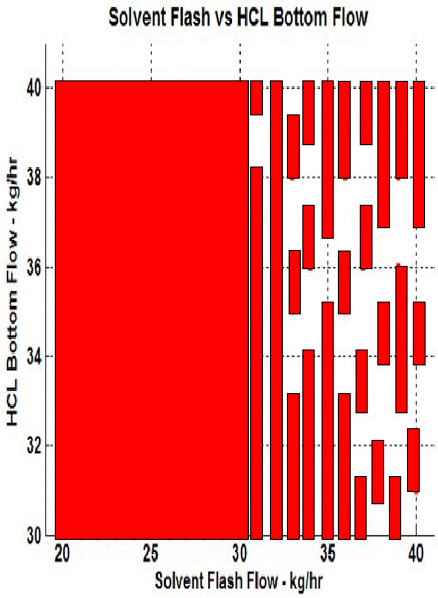

Figure 4.5: DOS rectangles for ROS parameter Set 3.

DOS parameters in Table 4.6 only 52.3% of the OOS region is utilised, however the DOS parameters are guaranteed to lie within a feasible region.

CHAPTER 5

DISCUSSION

The literature review depicts different industries around the world that are continually optimising processes. There is a generalised approach with the main objective of identifying the optimal operational parameters. Defining constraints is crucial when being used as boundaries for optimisation and these boundaries are specified in the form of the ROS region. In order for the optimisation to provide feasible solutions the ROS region must lie within the OOS region. If the ROS region does not lie within the OOS region, the plant may be required to operate in a non attainable region. There are two general scenarios whereby the ROS region will not lie within the feasible OOS region:

- Part or the entire ROS region lies outside the boundaries of the OOS region.
- The ROS region lies within the boundaries of the OOS region however the OOS region is non convex.

In the initial scenario the vertices of the boundaries of the OOS region can be used to solve for parameters which can results in a feasible ROS region. The second scenario is not as straight forward and was successfully addressed by this study. The objective of the study was to develop a method to identify the DOS region via numerical methods. The following approach was developed to deal with plants having non convex OOS regions;

- Identify the ROS region required for the identified plant.
- Model the above chosen process.
- Simulate the model within the boundaries of the AIS.

- Identify the OOS from the output of the simulation.
- Identify the DOS of the ROS and OOS regions by using the intersection algorithm developed.
- Simplify the DOS to one rectangular constraint region.

The above methodology is not limited to processes that are utilising optimisation techniques. Defining a ROS region that is feasible is also required for normal operation.

The method developed to determine the DOS region was evaluated on a HCl flash circuit. The case study chosen had an OOS which was non convex. Three scenarios where evaluated which were;

- Scenario 1: ROS parameters within a convex space of the OOS region.
- Scenario 2: ROS parameters partially within a convex space of the OOS region.
- Scenario 3: ROS parameters within a non convex space of the OOS region.

In scenario 1, the DOS region having the same parameters as the ROS region was expected when the ROS parameters lie within a convex space of the OOS region. In scenario 1, the plant was required to operate with ROS parameters partially within a convex space of the OOS region, would result in the control system trying to operate the plant in a non attainable region. The proposed intersection algorithm found DOS parameters that will ensure the DOS region lies within the feasible OOS region. In this scenario the intersection algorithm is similar to a technique that solves the boundaries of the OOS and ROS region. In the final scenario, the ROS parameters fall within a non convex space of the OOS region the control system might require the plant to operate in a non attainable region. However, solving for the feasible region will require using the intersection algorithm proposed and the resultant DOS region parameters will lie within the feasible OOS region. The numerical technique developed will guarantee that the DOS region is feasible. The DOS boundaries can be used in optimisation and general operations by delivering realistic expectations for throughput and quality to customers and as shown by Makkonen & Lahdelma (2003) proper definition of these factors will affect plant profitability.

Recommendations for Future Work

The DOS parameters generated are in the form of rectangular regions with upper and lower bound. If general linear constraints are allowed the utilisation of the DOS region on the OOS region will be higher. This however should be in alignment with the practical use of linear equations as operational boundaries on real time control systems. The current intersection algorithm was applied to a two dimensional DOS region. This should be extended to a multi-dimensional output space. The computational effort will be significantly increased as the solution will involve dealing with n-dimension data structures. The results will be beneficial to large multi-variable systems.

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