ENHANCING SUSTAINABILITY OF CHEMICAL PLANT OPERATIONS THROUGH DUAL OBJECTIVE HOLISTIC OPTIMISATION – THE CASE OF AN INTEGRATED AMMONIA AND NITROGEN-DERIVATIVES PRODUCTION FACILITY

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Declaration

I, Barrie Michael Cole, do hereby declare that this dissertation is my own unaided work. It is being submitted to the degree of Master of Science in Engineering in the University of the Witwatersrand, Johannesburg. It has not been submitted before for any degree in any other university.

Signed: _______________

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On this the _____ day of ___________________ 2007

Abstract

In recent years, there has been much improvement in the theory and application of mathematical optimisation. Optimisation techniques have now been developed for conditions of uncertainty (fuzzy) and probability (stochastic) and together with existing methodologies, such as linear programming and multiple objectivity, a very powerful set of tools is now available to enable the determination of the 'best' solution for most operational scenarios under a variety of uncertain operating conditions.

Optimisation techniques are currently available for most scenarios involving conditions of uncertainty, e.g. Fuzzy Optimisation, Stochastic Optimisation and Multi-Objective Optimisation. However, very few techniques exist for combinatorial optimisation scenarios, e.g. Stochastic Fuzzy Optimisation and Multi-Objective Fuzzy Optimisation and only one optimisation technique was discovered that covered three different conditions of uncertainty, i.e. Multi-sub-objective Stochastic Fuzzy Optimisation.

However, in the chemical industry, quite a few production operations exist that would greatly benefit if an optimisation methodology existed that covered four different simultaneous conditions of uncertainty, i.e. Multiple Objectivity, Fuzziness, Stochastics and Minmax (simultaneous maximum and minimum solution). A case in point is the interrelated production of ammonia (NH_3) and its downstream nitrogen-derivatives such as nitric acid (HNO_3), ammonium nitrate solution ($NH_4NO_3.H_2O$), ammonium nitrate (NH_4NO_3) and limestone ammonium nitrate. Such an operation is characterised by conditions of Fuzziness (uncertainty in product demand), Stochastics (probability distribution of hydrogen in coal, one of the ammonia production raw materials), Multi-objectives (e.g. the need to simultaneously maximise production in a number of different plants) and Minmax (e.g. the need to maximise production while simultaneously minimising effluent discharge)

In this research project, a 4 – Way (Multi-sub-objective, Stochastic, Fuzzy, and Minmax) Optimisation methodology was successfully derived, based on existing singular optimisation methodologies, and successfully applied to the interrelated ammonia and downstream nitrogen-derivatives production facility.

The Holistic Optimisation methodology derived could be easily applied to a wide variety of chemical and operational scenarios.

Dedication

This dissertation is dedicated to my two daughters, Michelle and Stephanie Cole, to my mother Freda Cole and especially to my girlfriend, Debby Lapidos, for all their help and support

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1. INTRODUCTION

1.1. General Background

The concept and mathematical application of optimisation has always been a fascinating topic and after some fairly recent advancement in this field, this has become even more the case. This is because optimisation in standard equality relationship mathematics has recently (> 1995) been extended to include:

a) '*Multiple Objectives*': - Finding the '*best*' solution for a situation involving multiple objective functions with some common variables..
b) '*Uncertainty*' or '*Fuzziness*': - represented by inequality relationships ($<$, $>$, $\leq$, $\geq$), which definitely exist in real-life, mathematical modeling situations.
c) '*Stochastics*' or '*Probability*': - typically represented by probability distribution functions in real-life situations
d) '*Minmax*': - Finding simultaneous minimum and maximum solutions.

All the above are extremely beneficial in determining '*best*' solution(s) for scenarios under a wide variety of (uncertain) conditions that typically exist in many industries and plants.

It became apparent that a 'Holistic' (combination of Multi-objective, Fuzzy, Stochastic and Minmax) optimisation methodology could be applied to many Chemical Engineering Production applications with great operational and financial advantage.

Of great interest was an inter-related ammonia and nitrogen derivative (Nitric Acid – HNO_3, Ammonium Nitrate Solution – $NH_4NO_3.H_2O$, Ammonium Nitrate - NH_4NO_3 and Limestone Ammonium Nitrate – $Ca/MgO.NH_4NO_3$) production facility, situated at Modderfontein in Gauteng. Holistic conditions of uncertainty exist in this environment with *multi-objectivity* potentially representing any one of a wide variety of conditions, *fuzziness* representing uncertainty in product demand, *stochastics* representing the probability distribution of hydrogen (H) in the raw material, coal and *Minmax* representing the simultaneous achievement of, for example, maximum production and minimal effluent discharge. The holistic operational/financial optimisation of such a scenario would be tremendously beneficial.

Initial research revealed that while independent and certain combinational optimisation methodologies certainly exist, no comprehensively holistic optimisation methodology could be found. The purpose, therefore, of this research project was to find and/or derive a methodology that would enable the Holistic Optimisation of Ammonia and downstream Nitrogen-derivatives production.

1.2. Problem Statement

From a Chemical Engineering standpoint, optimisation techniques are normally applied to individual design initiatives but seldom to overall plant operational requirements. This is mainly because such techniques are not common in published literature. The optimisation technique called Linear Programming is occasionally applied to determine optimal flow scenarios but the technology simply does not exist to extend the scope to include conditions of uncertainty and probability.

Therefore it would be tremendously beneficial both from an operational and financial perspective if the techniques of optimisation could be extended to include conditions of Multiple objectivity, Uncertainty (fuzzy), Probability (stochastic) and Minmax (conditions of simultaneous maxima and minima), in other words, a 'Holistic Optimisation' methodology that could be applied to plant operations. It could be a most powerful tool to enhance the sustainability of a chemical plant.

1.3. Hypothesis

It should be possible to derive and apply a holistic optimisation methodology in a complex, inter-related Ammonia and Nitrogen-derivatives production environment that involves conditions of multiple objectivity, uncertainty (fuzzy), probability (stochastics) and Minmax (simultaneous maxima and minima).

Such derivation will involve the compatibility analysis of individual optimisation methodologies and combining the best of these into a Holistic Optimisation methodology.

1.4. Purpose and Aim of the Investigation

The application of a holistic optimisation methodology will involve the complex, inter-related chemical production environment based on the Ammonia and Nitrogen-derivatives (nitric acid, ammonium nitrate solution, ammonium nitrate and limestone ammonium nitrate) production facility situated in Modderfontein, Gauteng

Therefore, the principal aim of this research project is to derive the methodology and then use it to holistically optimise (multi-sub-objective, fuzzy, stochastic, Minmax), both from a financial and an operational perspective, the combined production of the inter-related ammonia and nitrogen-derivatives (nitric acid, ammonium nitrate solution, ammonium nitrate and limestone ammonium nitrate) production facility with regard to two key objectives:

a) Maximum Gross Profit of Production Rate

…whilst simultaneously determining…

b) Minimum Effluent Discharge Rate

The decision to select the two Objective Functions, Gross Production Profit and Effluent Discharge, was purely based on business and environmental considerations. These are probably the two most important considerations facing a large chemical commercial operation. However, any two or more Objective Functions could have been selected but an increasing number of Objective Functions dilutes the impact of individual Objective Functions, therefore practicality was the key. Naturally, there would be a requirement of Maximising Gross Production Profit whilst simultaneously Minimising Effluent Discharge Rate.

Solution of both objectives will include the determination of the flow rates of all raw material, intermediary and production streams within the capabilities of the production infrastructure.

Therefore, the principal aims of this research are twofold:

1) Derivation of a Dual Objective Holistic (Multi-sub-Objective Stochastic Fuzzy Minmax) Optimisation methodology
2) The successful application of the methodology on an Ammonia and Nitrogen-Derivatives integrated production facility

Such an exercise, if successful, will provide a powerful template for conducting holistic optimisation exercises on most other chemical or appropriate operations (e.g. retail, distribution and inventory operations etc. etc.), thereby facilitating the most sustainable way, from both an operational and financial perspective, of running the chosen facility.

1.5. Presentation of the Dissertation

This dissertation has been arranged in a logical fashion, starting with a literature review that initially explains the methodology used to search the literature, which is then followed by summaries of the selected material under key category (e.g. Fuzzy Optimisation, Stochastic Optimisation) headings. These categories may be further subdivided depending on the nature of the content.

After the 'Literature Survey' section, there is an 'Application Methodology' section that, initially, attempts to enhance existing inadequate methodologies. This is followed by a brief evaluation of all existing and the one derived methodology. The section is concluded with the derivation and presentation of the desired 'Dual Objective Holistic (Multi-sub-Objective, Stochastic, Fuzzy, and Minmax) Optimisation methodology.

The 'Application Methodology' section is followed by the core 'Application' section that involves the Holistic Optimisation of a complex, interrelated Ammonia and Nitrogen-derivatives (HNO_3, $NH_4NO_3.H_2O$, NH_4NO_3 and Ca/MgO, NH_4NO_3) production facility. Dual Objective Holistic Optimisation is conducted with regard to two key Minmax objectives, i.e. maximum Gross Profit of Production and minimum Total Effluent Discharge. Apart from the optimum values of these objectives, the solution subsection also includes a list of all determined optimal flow variables.

The 'Application' section is followed by the 'Conclusion and Recommendations' section, which presents the conclusions from the research and then makes some recommendations with regard to potential follow-up action.

2. LITERATURE SURVEY

2.1. Introduction

The standard practise with postgraduate literature reviews is to critically review the current state of knowledge in the area of research by identifying and highlighting gaps in the current state of knowledge and development. This is normally followed by a motivation and indication of how this research work would address these gaps and contribute new knowledge to the research area. This review technique is mainly applicable in instances where the research objective(s) is known. In certain cases, the overall research objective could be generic and consist of a number of independent or semi-independent, subordinate objectives. In this case, the literature review could cover a number of independent or semi-independent literature topics that all pertain to the same core theme, which is exactly applicable in the case of this research project, 'Multi-sub-objective Dual Objective Holistic (Stochastic Fuzzy) Optimisation', where the central theme is 'Optimisation'.

Dual Objective Holistic (Multi-sub-objective Stochastic Fuzzy) Optimisation is essentially a mathematical methodology that seeks the 'best' solution (minimum or maximum) for most mathematically-modeled operational scenarios that are characterized by conditions of uncertainty (fuzzy) and/or probability (stochastic) and also involve multiple objectives. This concept is only a recently emerging (mainly 21st century) paradigm that is currently receiving much worldwide research and commercial attention, probably because of the huge potential benefits that can be derived and also because of recent advances in Applied Mathematics and Computing,

Multi-sub-objective Stochastic Fuzzy Optimisation is a 'best' solution methodology that can be applied to operational situations involving multiple objectives associated with conditions of uncertainty and probability. It is referred to as holistic optimisation because the 'best' solution is sought under conditions of multiple objectives <u>and</u> uncertainty <u>and</u> probability. It is, of course, possible to find optimum solutions for subordinate subset combinations, e.g. multi-objective stochastic optimisation, fuzzy optimisation or stochastic fuzzy optimisation, which is why it is important to conduct the research effort along the lines of independent/semi-independent subordinate objectives, (*For the sake of clarity, the term, 'Optimisation' is used in this report instead of the term, 'Programming', which is used in many of the journals surveyed for the same application*) as itemised below. These three scenarios plus an additional semi-derived one, Minmax Fuzzy Optimisation (combination of objectives to be minimised *and* maximised), jointly constitute an effective platform for demonstrating the combinational variety of some subordinate optimisation characteristics.

i) Single Objective Fuzzy Optimisation.
ii) Single Objective Stochastic Fuzzy Optimisation
iii) Multiple Objectives Fuzzy Optimisation
iv) Minmax Fuzzy Optimisation

The literature review will therefore critically analyse all selected publications and journals with regard to these three scenarios with a view to identifying and selecting the better procedures and/or methodologies that can be logically combined to create the ultimate, desired objective: Multi-sub-objective Dual Objective Holistic (Stochastic Fuzzy) Optimisation.

Since this research project is only concerned with the operational aspects of chemical production, there will be no need to investigate and research the mathematical differential aspects of Optimisation that is usually required for most Chemical Engineering design work.

A number of articles have been reported in literature dealing with the various aspects of optimisation, which are (i) single objective stochastic (ii) single objective fuzzy and (iii) single objective stochastic fuzzy and multi-objective techniques such as (iv) multi-objective fuzzy (v) multi-objective stochastic and (vi) multi-objective stochastic fuzzy. The complete list of categorized reference material is given in the appendix

However, of these, very few were pertinent to the current study, and they will be dealt with in more detail in the following sections of the literature review. The literature mentioned in tables 2.1 and 2.2 often deals with single objective optimisation, and also sometimes with multi-objective optimisation. Furthermore, it is clear from the list of recent literature summarised in table 2.1 that most of the cited articles deal with the non-chemical industry problems e.g. transportation systems (BIT et al, 1993, SINHA, 2003), portfolio selection (ABDELAZIZ *et al* 2005), a reservoir system (AZAIEZ *et al* 2005), supply networks (CHEN and LEE, 2004), inventory models (DAS *et al* 2004) and project selection (GABRIEL *et al* 2005). The only one closely related to a production plant describes nuclear fuel cycle optimisation using multi-objective stochastic linear programming (KUNSCH and TEGHEM, 1987). Although this and all the other examples tested here have a common multi-objective optimisation goal, usually obtained by either a fuzzy programming or a stochastic programming approach, none of them utilises a combinational holistic approach to achieve their optimisation objectives. As such, no single literature report on the holistic approach adopted in this research could be found, and therefore the remainder of this chapter will describe the bases of methods adopted in previous investigations listed above in tables 2.1 and 2.2 to provide a foundation for the explanation on how the combined holistic algorithm was derived and successfully applied to the case study investigated in this work. This will be done by providing a description of the principles involved in each case, and illustrating the application with a relevant example to demonstrate the advantages and limitations of each particular methodology.

2.2. Optimisation Model Building

2.2.1. An Introduction to Optimisation Modelling

According to WINSTON (2004), the scientific approach to optimisation and decision-making usually involves the use of one or more mathematical models. A mathematical model is a representation of an actual situation that may be used to make better decisions or simply to improve the understanding of those situations.

2.2.2. Optimisation Models

In simple terms, an optimisation model prescribes the behaviour of a system in order that the system objectives can be achieved. The components of an optimisation model are:

i) Objective Function

The objective function mathematically describes the desired objective(s) of the system in terms of some of the decision variables defined further below. The intention, in an optimisation model, would be to optimise (either maximise or minimise) the objective function(s), which in turn would determine the optimum values of the decision variables and also satisfy the given constraints.

ii) The Decision Variables

The variables whose values are controllable and influence the performance of the system are called decision variables and both the objective function(s) and the constraints are defined in terms of the decision variables. An optimum solution determines a set of values of the decision variables.

iii) Constraints

In most modelling situations, the values of some of the decision variables may only assume certain values and the set of linear equations that describe the various combinational relationships of decision variables and coefficients are called constraints.

The inequality constraint relationships are termed, ‘fuzzy’ whereas probabilistic constraint relationships are termed, ‘stochastic’ e.g.:

- Normal Constraint: - $a_1x_1 + a_2x_2 + a_3x_3 + \ldots + a_nx_n = b_1$
- Fuzzy Constraint: - $a_1x_1 + a_2x_2 + a_3x_3 + \ldots + a_nx_n \leq b_1$
- Stochastic Fuzzy Constraint: - Prob $[\sum_{j=1}^{n}(a_{ij}x_j \leq b_i] \geq 1 - \alpha_i$

2.2.3. Optimisation Model Types

i) Static and Dynamic Models

A **static** model is one in which the decision variables do not involve sequences of decisions over multiple periods. A **dynamic** model is a model in which the decision variables do involve sequences of decisions over multiple periods. In static models, a ‘one-shot’ problem is defined as one in which the current optimal solution prescribes the optimal values of all decision variables for all points in time. However, with dynamic models, optimal solutions must be simultaneously determined for all points in time.

ii) Linear and Non-linear Models

A **linear model** is one in which each constraint consists of the summation of relevant decision variables multiplied by corresponding coefficients. Alternatively, a **non-linear model** could consist of constraints with a variety of different mathematical relationships e.g.:

- Linear Constraint: - $a_1x_1 + a_2x_2 + a_3x_3 + \ldots + a_nx_n \leq b_1$
- Non-linear Constraint: - $a_1x_1^2 - a_2x_1x_2 + a_3x_2^2$

iii) Integer and non-Integer Models

If one or more decision variables are integers then the optimisation model is regarded as an **integer model**. If, however, the decision variables assume fractional values, the optimisation model is called a **non-integer model**.

iv) Deterministic and Stochastic Models

If the values of the decision variables, the value of the objective function and the satisfaction of the constraints is known with certainty then the optimisation model is called a **deterministic optimisation model**. If these variables and functions are not known with certainty then the optimisation model is called a **stochastic optimisation model**.

2.2.4. The Optimisation Model-Building Process

In applying the optimisation model-building process, the following procedure is often adopted:

<u>Step 1</u>: Formulate the Problem

Definition of the problem involves specification of the system objectives, *k*.:

$$Z_k = \sum c_{ij}^{k} x_{ij}),\ k = 1, 2 \ldots K$$

Where x_{ij} = decision variable *i, j*
c_{ij} = decision variable coefficient

<u>Step 2</u>: Record the System Parameters

All parameters that affect the performance of the system must be recorded. These parameters are used to develop a mathematical model of the problem and typically include the decision variables, the nature of the constraints and the existence of any probability relationships.

<u>Step 3</u>: Formulate a Mathematical Model of the System

Such a model could encompass a number of independent or dependent component models, with each component model describing the mathematical relationships pertaining to each objective. Typically, each component model would consist of an objective function, some decision variables and a set of constraint equations.

<u>Step 4</u>: Perform Optimisation Calculations

In the case of the System Problem involving only **one objective function**, the optimisation calculation is fairly simple and dependent only on the objective function and constraints of one objective function, e.g.

Objective Functions (*k*): - Max/min ($z_k = \sum c_{ij}^{k} x_{ij}$), $k = 1, 2 \ldots K$

Subject to Constraints: -

$$\begin{aligned} a_{11}x_{11} + a_{12}x_{12} + \ldots + a_{1n}x_{1n} &\leq b_1 \\ a_{21}x_{21} + a_{22}x_{22} + \ldots + a_{2n}x_{2n} &\leq b_2 \\ :: \quad :: \quad :: \quad & :: \\ a_{m1}x_{m1} + a_{m2}x_{m2} + \ldots + a_{mn}x_{mn} &\leq b_m \end{aligned}$$

In the case where there the System Problem involves **several objective functions**, the optimisation procedure is a more complex two-stage process involving the definition and equality of different aspiration functions (λ_k) pertaining to each objective function (k), where $\lambda_k = (U_k - z_k)/(U_k - L_k)$; U_k = Highest objective optimum value of all objectives k with all the other objectives serving as constraints; L_k = Lowest objective optimum value of all objectives k with all the other objectives serving as constraints; z_k = objective function, k. This is done as follows:

Stage 1: Max/min ($z_k = \sum c_{ij\_}k(x_{ij})$, $k = 1, 2 \ldots K$ subject to constraints for each objective function

Stage 2: Max λ_k subject to common objective constraints and equality of aspiration level functions ($\lambda_1 = \lambda_2 = \ldots = \lambda_m$)

Step 5: Record the Optimum Solution

Record the values of all optimum objective functions as well as the values of all decision variables pertaining to the optimum solution set.

2.3. Fuzzy Optimisation: - Decision Making Under Uncertainty

2.3.1 Introduction and Definitions

Fuzzy Optimisation is the process of determining the 'best' solution of an operational process under conditions of uncertainty.

The operational process must first be subject to Optimisation Modeling, which involves the selection of decision variables, the formulation of the Objective Function, the definition of various constraint equations, the mathematical recognition, the assignment of any decision variable limits and the mathematical modeling of the process itself.

The term 'fuzzy' is applied to those constraint equations and limits that are described by uncertain or inequality mathematical relationships, e.g.

$$
\begin{array}{l}
a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n,}x_m \leq b_1 \\
a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n,}x_m \geq b_2 \\
\;::\quad\;\; ::\quad\;\; ::\quad\;\; :: \\
a_{m1}x_1 + a_{m2}x_2 + \ldots + a_{mn}x_m \leq b_m
\end{array}
$$

Additionally, a Fuzzy Optimisation program can involve one or many Objective Functions. The solution of a Multi-objective Fuzzy Optimisation program is more complex than that of a Single Objective Fuzzy Optimisation program and both are covered below.

Traditionally, single or multiple objective(s), multiple constraints, fuzzy optimisation was referred to simplistically as linear programming, where the term, 'fuzzy' refers to the inequality constraints in the linear program. According to WINSTON (2004), linear programming is a tool for solving optimisation problems. An efficient method, called the Simplex Algorithm, was developed for solving these problems. The characteristics of a linear program are:

1) *Decision Variables*: - The decision variables completely describe the decisions to be made (solved) by the linear program.

2) *Objective Function*: - A mathematical relationship involving all or some of the decision variables that describes the main objective of the linear program, e.g. profit or variable cost determination. Typically, this function (z) would be minimized or maximised in a linear program in order to determine an optimum value.

3) *Constraints*: - Various limitations to the linear programming model expressed in terms of different relationships involving the decision variables.

4) *Limitations*: - Certain decision variables may be subject to certain limitation values.

2.3.2. Single Objective Fuzzy Optimisation

The procedure for developing a Single Objective Fuzzy Optimisation Model is done in accordance with the previously defined Optimisation Model Building Process. The process will be further illustrated by means of the accompanying practical example extracted from WINSTON (2004). One such example is illustrated below.

Example: Giapetto's Woodcarving Inc. manufactures two types of wooden toys, soldiers and trains. A soldier is sold for $27 and uses $10 worth of raw materials. Each soldier that is manufactured increases Giapetto's variable labour and overhead costs by $14. A train sells for $21 and uses $9 worth of raw material. Each train built increases Giapetto's variable labour and overhead costs by $10. The manufacture of wooden soldiers and trains requires two types of skilled labour: carpentry and finishing. A soldier requires 2hrs finishing labour and 1hr carpentry labour. Each week, Giapetto can obtain all the needed raw material but only 100 finishing hours and 80 carpentry hours are available for work to be done. Demand for trains is unlimited but at most, 40 soldiers are bought each week. Giapetto wants to maximise weekly profits. Formulate a mathematical model of Giapetto's situation that can be used to maximise weekly profit.

Single Objective Fuzzy Optimisation Methodology:

1) *Identify the Decision Variables*: - The decision variables completely describe the decisions to be made (solved) by the linear program:

   Let x_1 = no. of soldiers
   Let x_2 = no. of trains

2) *Formulate the Objective Function*: - A mathematical relationship involving all or some of the decision variables that describes the main objective of the linear program, e.g. profit or variable cost determination. Typically, this function (z) would be minimized or maximised in a linear program in order to determine an optimum value.

Objective Function (z): Profit = Revenue – Costs
= (Weekly revenue from soldiers and trains) – (Weekly costs from soldiers and trains)
$= (27x_1 + 21x_2) - (10x_1 + 9x_2) - (14x_1 + 10x_2)$
$= 3x_1 + 2x_2$

Therefore the Objective function to be maximised is $z = (3x_1 + 2x_2)$

3) *Define the Constraints*: - Various limitations to the linear programming model expressed in terms of different relationships involving the decision variables.

   i. Finishing hours: $3x_1 + 2x_2 \leq 100$
   ii. Carpentry hours: $x_1 + x_2 \leq 80$

4) *Assign Limitations*: - Certain decision variables may be subject to certain limitations values.

   i. Maximum weekly production: $x_1 \leq 40$
   ii. Sign restriction $x_1 \geq 0$
   iii. Sign restriction $x_2 \geq 0$

5) *Formulate the Model*:

In this example, a Linear Program is formulated as follows:

Objective Function: Max $(3x_1 + 2x_2)$

Subject to Constraints: $3x_1 + 2x_2 \leq 100$
$x_1 + x_2 \leq 80$

Subject to Limitations: $x_1 \leq 40$
$x_1 \geq 0$
$x_2 \geq 0$

6) *Solve the Model*

Most program models can be solved using MS-Excel Solver, shown in Table 2.3

Table 2.3 MS Excel – Solver Optimisation Model Solution

<u>MS-Excel Solver Optimum Solution</u>

		Decision Variables x_1		x_2	Max Obj. z		
		23.07692		15.38462	100		
		Constraints.			Equation Value	Sign	Constraint Limit
Constraints Equations	i)	$3x_1$	+	$2x_2$	100	$\le$	100
	ii)	$1x_1$	+	$1x_2$	38.46154	$\le$	80
	iii)	$1x_1$			23.07692	$\le$	40
	iv)	$1x_1$			23.07692	$\ge$	0
	v)			$1x_2$	15.38462	$\ge$	0

7) *Record the optimum solution*

a) Objective value (z) = 100
b) Decision Variables: x_1 = 23.08; x_2 = 15.38

This extract from WINSTON (2004) basically represents the fundamentals of standard single objective linear optimisation or linear programming as it is more frequently referred to in the relevant literature. The reason it is incorporated in this research project is to provide some background to the concept of 'Multi-sub-objective Stochastic Fuzzy Minmax Optimisation'.

For the sake of clarity, the expression 'Fuzzy' is a term that simply refers to the state of uncertainty represented by the inequalities in the linear/non-linear programming constraint relationships, while the term 'Stochastic' refers to the existence of any probability distribution relationships in the constraint equations.

Linear programming can be relatively easily extended to include non-linear programming, which is typically more appropriate in the Engineering environment. This is also covered in WINSTON (2004). The concept of linear / non-linear programming can also be extended to include any uncertainty (Fuzzy) and/or probability (Stochastic) characteristics, which is demonstrated a little further in this research project. Further examples of this approach can be found in a number of recent / relevant texts and journals such as CHAO-FANG *et al* (2007), SAKAWA *et al* (2004) and SINHA (2003).

2.3.3. Multiple Objectives Fuzzy Optimisation

BIT *et al*, (1993) proposed an additive fuzzy programming model for a multi-objective transportation problem in which weights and priorities are assigned to non-equivalent objectives. This model therefore provides a non-dominated solution, which provides the 'best' compromise solution.

An initial fuzzy model of the multi-objective transportation problem is formulated as follows:

$$\text{Min } z_k = \sum_{i=1}^{m}\sum_{j=1}^{n} c_{ij}^{k}(x_{ij}),\ k = 1\ldots K$$

Subject to:

$$\sum_{j=1}^{n} x_{ij} = a_i,\ i = 1, 2\ldots m$$

$$\sum_{j=1}^{n} x_{ij} = b_j,\ j = 1, 2\ldots n$$

`

$$x_{ij} \geq 0,\ i = 1, 2\ldots m,\ j = 1, 2\ldots n$$

These equations are then transformed into a simple additive fuzzy programming model with the following steps:

<u>Compromise Solution Methodology</u>

<u>Step 1</u>: The multi-objective problem is solved as a single objective problem, using each objective in turn as the single objective function whilst using all the others as criteria.

<u>Step 2</u>: From the results of step 1, the corresponding decision-variable values are determined for each optimum objective.

<u>Step 3</u>: From step 2, a lower and upper bound-value is determined for the set of solutions for each objective function, Z_k. The lower bound is designated L_k, whilst the upper bound is designated U_k.

<u>Note:</u> For a multi-objective problem, the membership function, $u_k(x)$, for the k^{th}-objective function is defined as:

$$u_k(x) = \begin{cases} 1 & ;\text{if } Z_k \leq L_k \\ 1 - (Z_k - L_k)/(U_k - L_k) & ;\text{if } L_k < Z_k < U_k \\ 0 & ;\text{if } Z_k \geq U_k \end{cases}$$

$u_k(x) = 1$ if $U_k = L_k$ for all k and the appropriate values are substituted accordingly for all k.

Step 4: Aspiration Levels (λ_k) are defined for each objective as follows:
$\lambda_k = 1 - (Z_k - L_k)/(U_k - L_k) = (U_k - Z_k)/ U_k - L_k)$ and these are maximized per objective function subject to all corresponding constraints and the additional constraint that λ_k only has one value across all objective functions.

Step 5: Maximise the Aspiration Level Functions and select the Aspiration Level with the highest value ⇒ Optimum Aspiration Level

Step 6: The decision-variables compromising the optimum aspiration level, λ_k, then constitute the optimum solution with the corresponding optimum objective function values (Z_k).

An example of the application of this approach is given below:

Example: In a manufacturing and distribution operation, there are four production sources and five destinations. The three key business objectives are (i) minimum transportation cost (Z_1), (ii) minimum delivery time (Z_2) and (iii) total relative safety (Z_3) per given route.

The Objective functions are given by:

$$\text{Min } Z_1 = \begin{pmatrix} 9 & 12 & 9 & 6 & 9 \\ 7 & 3 & 7 & 7 & 5 \\ 6 & 5 & 9 & 11 & 3 \\ 6 & 9 & 11 & 2 & 2 \end{pmatrix} \qquad \text{Min } Z_2 = \begin{pmatrix} 2 & 9 & 8 & 1 & 4 \\ 1 & 9 & 9 & 5 & 2 \\ 8 & 1 & 8 & 4 & 5 \\ 2 & 8 & 6 & 9 & 8 \end{pmatrix}$$

$$\text{Min } Z_3 = \begin{pmatrix} 2 & 4 & 6 & 3 & 6 \\ 4 & 8 & 4 & 9 & 2 \\ 5 & 3 & 5 & 3 & 6 \\ 6 & 9 & 6 & 3 & 1 \end{pmatrix}$$

Subject to Constraints:

$\sum_{j=1}^{5} x_{1j} = 5$, $\sum_{j=1}^{5} x_{2j} = 4$, $\sum_{j=1}^{5} x_{3j} = 2$,
$\sum_{j=1}^{5} x_{4j} = 9$, $\sum_{i=1}^{4} x_{i1} = 4$, $\sum_{i=1}^{4} x_{i2} = 4$,
$\sum_{j=1}^{4} x_{i3} = 6$, $\sum_{j=1}^{4} x_{i4} = 2$, $\sum_{j=1}^{4} x_{i5} = 4$,
$x_{ij} \geq 0$, $i = 1, 2, 3, 4$, $j = 1, 2, 3, 4$

Implementation of 'Compromise' Solution Methodology:

Step 1: The multi-objective problem is solved as a single objective problem, using each objective in turn as the single objective function whilst using all the others as criteria. The corresponding multi-objective fuzzy linear program that can be compiled is given in Table T2.4.

MULTI-OBJECTIVE FUZZY OPTIMISATION

(Bit *et al*, 1993)

	x_{11}	x_{12}	x_{13}	x_{14}	x_{15}	x_{21}	x_{22}	x_{23}	x_{24}	x_{25}	x_{31}	x_{32}	x_{33}	x_{34}	x_{35}	x_{41}	x_{42}	x_{43}	x_{44}	x_{45}	$Z_1[x_i^{\sim}]$	$Z_2[x_i^{\sim}]$	$Z_3[x_i^{\sim}]$		
Coeffs.	9	12	9	6	9	7	3	7	7	5	6	5	9	11	3	6	8	11	2	2	**102**	**148**	**100**	$Z_i[x_1^{\sim}]$	
c. Var.($x_1^{\sim}$)	0	0	5	0	0	0	4	-0	0	0	1	0	1	-0	0	3	0	0	2	4					
Coeffs.	2	9	8	1	4	1	9	9	5	2	8	1	8	4	5	2	8	6	9	8	**157**	**72**	**86**	$Z_i[x_2^{\sim}]$	
c. Var.($x_2^{\sim}$)	3	0	0	2	0	0	0	0	-0	4	0	2	0	0	0	1	2	6	0	0					
Coeffs.	2	4	6	3	6	4	8	4	9	2	5	3	5	3	6	6	9	6	3	1	**134**	**122**	**64**	$Z_i[x_3^{\sim}]$	
c. Var.($x_3^{\sim}$)	3	2	0	0	0	1	0	3	0	0	0	2	0	0	-0	0	0	3	2	4					
$\Sigma x_{1j} = 5$	1	1	1	1	1																5.00	5.00	5.00	=	5
$\Sigma x_{2j} = 4$						1	1	1	1	1											4.00	4.00	4.00	=	4
$\Sigma x_{3j} = 2$											1	1	1	1	1						2.00	2.00	2.00	=	2
$\Sigma x_{4j} = 9$																1	1	1	1	1	9.00	9.00	9.00	=	9
$\Sigma x_{i1} = 4$	1					1					1					1					4.00	4.00	4.00	=	4
$\Sigma x_{i2} = 4$		1					1					1					1				4.00	4.00	4.00	=	4
$\Sigma x_{i3} = 6$			1					1					1					1			6.00	6.00	6.00	=	6
$\Sigma x_{i4} = 2$				1					1					1					1		2.00	2.00	2.00	=	2
$\Sigma x_{i5} = 4$					1					1					1					1	4.00	4.00	4.00	=	4
$x_{11} \geq 0$	1																				-	3.00	3.00	≥	0
$x_{12} \geq 0$		1																			-	-	2.00	≥	0
$x_{13} \geq 0$			1																		5.00	-	-	≥	0
$x_{14} \geq 0$				1																	-	2.00	-	≥	0
$x_{15} \geq 0$					1																-	-	-	≥	0
$x_{21} \geq 0$						1															0.00	0.00	1.00	≥	0
$x_{22} \geq 0$							1														4.00	-	-	≥	0
$x_{23} \geq 0$								1													(0.00)	-	3.00	≥	0
$x_{24} \geq 0$									1												-	(0.00)	-	≥	0
$x_{25} \geq 0$										1											-	4.00	-	≥	0
$x_{31} \geq 0$											1										1.00	-	-	≥	0
$x_{32} \geq 0$												1									-	2.00	2.00	≥	0
$x_{33} \geq 0$													1								1.00	-	-	≥	0
$x_{34} \geq 0$														1							(0.00)	-	-	≥	0
$x_{35} \geq 0$															1						0.00	-	(0.00)	≥	0
$x_{41} \geq 0$																1					3.00	1.00	-	≥	0
$x_{42} \geq 0$																	1				-	2.00	-	≥	0
$x_{43} \geq 0$																		1			-	6.00	3.00	≥	0
$x_{44} \geq 0$																			1		2.00	-	2.00	≥	0
$x_{45} \geq 0$																				1	4.00	-	4.00	≥	0

Step 2: From the results of step 1, the corresponding optimum decision-variable values are determined for each optimum objective.

$x_1^{/}$ = (0, 0, 5, 0, 0, 0, 4, 0, 0, 0, 1, 0, 1, -0, 0, 3, 0, 0, 2, 4)

$x_2^{/}$ = (3, 0, 0, 2, 0, 0, 0, 0, -0, 4, 0, 2, 0, 0, 0, 1, 2, 6, 0, 0)

$x_3^{/}$ = (3, 2, 0, 0, 0, 1, 0, 3, 0, 0, 0, 2, 0, 0, -0, 0, 0, 3, 2, 4)

Step 3: From step 2, a lower and upper bound-value is determined for the set of solutions for each objective function, Z_k. The lower ('best') bound is designated L_k, whilst the upper ('worst') bound is designated U_k.

Objective Function	U_k('Worst')	L_k('Best')
Min Z_1	157	102
Min Z_2	148	72
Min Z_3	100	64

Step 4: Derive Aspiration Level Functions (λ_k) for each objective as follows:

$\lambda_k = 1 - (Z_k - L_k)/(U_k - L_k) = (U_k - Z_k)/ U_k - L_k)$

$\lambda_1 = [148 - (9x_{11} + 12x_{12} + 9x_{13} + 6x_{14} + 9x_{15} + 7x_{21} + 3x_{22} + 7x_{23} + 7x_{24} + 5x_{25} + 6x_{31} + 5x_{32} + 9x_{33} + 11x_{34} + 3x_{35} + 6x_{41} + 9x_{42}$. $+ 11x_{43} + 2x_{44} + 2x_{45})]/(157 - 102)$

$\lambda_2 = [157 - (2x_{11} + 9x_{12} + 8x_{13} + x_{14} + 4x_{15} + x_{21} + 9x_{22} + 9x_{23} + 5x_{24} + 2x_{25} + 8x_{31} + x_{32} + 8x_{33} + 4x_{34} + 5x_{35} + 2x_{41} + 8x_{42} + 6x_{43}$. $+ 9x_{44} + 8x_{45})]/(148 - 72)$

$\lambda_3 = [134 - (2x_{11} + 4x_{12} + 6x_{13} + 3x_{14} + 6x_{15} + 4x_{21} + 8x_{22} + 4x_{23} + 9x_{24} + 2x_{25} + 5x_{31} + 3x_{32} + 5x_{33} + 3x_{34} + 6x_{35} + 6x_{41} + 9x_{42} + .$
$6x_{43} + 3x_{44} + x_{45})]/(100 - 64)$

Therefore, the aspiration level functions are:

$$\lambda_1 = 3.083 - \begin{pmatrix} 0.188 & 0.250 & 0.188 & 0.125 & 0.188 \\ 0.146 & 0.063 & 0.146 & 0.146 & 0.104 \\ 0.125 & 0.104 & 0.187 & 0.229 & 0.063 \\ 0.125 & 0.188 & 0.229 & 0.042 & 0.042 \end{pmatrix}$$

$$\lambda_2 = 1.847 - \begin{pmatrix} 0.024 & 0.106 & 0.094 & 0.012 & 0.048 \\ 0.012 & 0.106 & 0.106 & 0.059 & 0.024 \\ 0.094 & 0.012 & 0.094 & 0.059 & 0.059 \\ 0.024 & 0.094 & 0.071 & 0.106 & 0.094 \end{pmatrix}$$

$$\lambda_3 = 1.914 - \begin{pmatrix} 0.029 & 0.057 & 0.086 & 0.057 & 0.086 \\ 0.057 & 0.114 & 0.057 & 0.129 & 0.029 \\ 0.071 & 0.043 & 0.071 & 0.043 & 0.086 \\ 0.086 & 0.129 & 0.086 & 0.043 & 0.014 \end{pmatrix}$$

Step 5: Maximise the Aspiration Level Functions subject to the identical set of constraints and limitations that were used in the initial optimisation exercise involving the Objective Functions and select the Aspiration Level with the highest value $\Rightarrow$ Optimum Aspiration Level, which according to BIT *et al* (1993) defines the optimum solution for a Multi-objective Fuzzy Optimisation problem.

Using MS-Excel Solver, the aspiration level is maximized across all objective functions and the optimum decision variables are given in Table 2.5. The first three rows consist of the solution decision variables for the corresponding three objective functions

5 **Maximisation of Aspiration Levels**

	x_{12}	x_{13}	x_{14}	x_{15}	x_{21}	x_{22}	x_{23}	x_{24}	x_{25}	x_{31}	x_{32}	x_{33}	x_{34}	x_{35}	x_{41}	x_{42}	x_{43}	x_{44}	x_{45}	λ_1^{max}	λ_2^{max}	λ_3^{max}		
54	0.218	0.164	0.073	0.073	0.018	0.055	0.127	0.127	0.091	0.109	0.091	0.164	0.200	0.055	0.109	0.164	0.200	0.036	0.036	**1.07**				
0	0	5	0	-0	2	2	1E-07	0	0	0	2	0	0	0	2	0	1	2	4					
6	0.118	0.105	0.013	0.053	0.013	0.118	0.118	0.066	0.026	0.105	0.013	0.105	0.039	0.079	0.026	0.105	0.079	0.118	0.013		**1.06**			
0	2	1	2	0	4	0	-0	0	7E-09	0	2	0	0	0	0	-0	5	0	4					
6	0.111	0.167	0.083	0.086	0.111	0.222	0.111	0.250	0.056	0.139	0.083	0.139	0.083	0.167	0.167	0.250	0.028	0.083	0.028			**0.72**		
	2	0	0	0	1	0	0	0	3	0	2	0	0	0	0	0	6	2	1					
	1	1	1	1																5	5	5	=	5
					1	1	1	1	1											4	4	4	=	4
										1	1	1	1	1						2	2	2	=	2
															1	1	1	1	1	9	9	9	=	9
					1					1					1					4	4	4	=	4
	1					1					1					1				4	4	4	=	4
		1					1					1					1			6	6	6	=	6
			1					1					1					1		2	2	2	=	2
				1					1					1					1	4	4	4	=	4
																				0	0	3	≥	0
	1																			0	2	2	≥	0
		1																		5	1	0	≥	0
			1																	0	2	0	≥	0
				1																-0	0	0	≥	0
					1															2	4	1	≥	0
						1														2	0	0	≥	0
							1													1E-07	-0	0	≥	0
								1												0	0	0	≥	0
									1											0	7E-09	3	≥	0
										1										0	0	0	≥	0
											1									2	2	2	≥	0
												1								0	0	0	≥	0
													1							0	0	0	≥	0
														1						0	0	0	≥	0
															1					2	0	0	≥	0
																1				0	-0	0	≥	0
																	1			1	5	6	≥	0
																		1		2	0	2	≥	0
																			1	4	4	1	≥	0

<u>Step 6</u>: The decision-variables compromising the optimum aspiration level, λ_k, then constitute the optimum solution with the corresponding optimum objective function values (Z_k). This is regarded as the weighted optimum solution.

Therefore optimum solution @ λ_3 = 1.07 and corresponding decision variables are:

$$\begin{pmatrix} 0 & 0 & 5 & 0 & 0 \\ 2 & 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 2 & 0 & 1 & 2 & 4 \end{pmatrix}$$

And the compromise versus respective optimum solutions is:

	Nature	Composite	Optimum
Z_1	Min	110.00	102
Z_2	Min	122.00	72
Z_3	Min	88.00	64

Conclusion

The multi-objective fuzzy programming algorithm proposed in this paper by BIT et al (1993) can be applied in all instances where the weighted additive fuzzy programming model or the preemptive priority model can be applied to determine a non-dominated optimum solution, irrespective of whether the relative importance of objectives are known.

According to these authors, other proposed multi-objective algorithms are only applicable when all objective functions are equally important.

It is therefore a suitable method as the basis for the development of a Multi-objective ***Stochastic*** Fuzzy Optimisation methodology in that only an appropriate stochastic optimisation methodology has to be found and integrated with the above multi-objective fuzzy programming algorithm to create a robust ***Multi-objective Holistic (Stochastic, Fuzzy) Optimisation*** methodology. A few instances reported in literature following this approach include CHAO-FANG *et al* (2007), SAKAWA *et al* (2004) and KAPUR (1970).

2.4. Stochastic Fuzzy Optimisation: - Probability and Uncertainty

2.4.1. Introduction and Definitions

The procedure for developing a Single Objective Stochastic Optimisation Model is also in accordance with the defined Optimisation Model Building Process, as well as taking into account the probabilistic considerations.

According to GAVER and THOMPSON (1973), Stochastic Optimisation/Programming is often referred to as Chance Constrained Programming because some of the constraints, e.g. $ax_1 + bx_2 < c_j$, are subject to probability distribution in that the variable coefficients, *a* and *b*, are known fixed numbers while the right-hand values c_j's are random variables with known probability distributions, F(*z*). In other words $P\ [c_j \leq z] = F_j\ (z)$ where F(z) is the probability distribution of c_j.

It is generally impossible to determine *a's and b's* that are satisfied for all possible outcomes of the random variable, c_j. However, the constraint equations can be replaced with:

$$P\ [\sum_{i=1}^{m} (a_i x_i)] > \alpha_j,$$

Here, $0 \leq \alpha_j \leq 1$ is a number that measures the probability of achieving the j^{th} constraint. Similarly, the probability of not achieving the j^{th} constraint can be defined as $p_j = 1 - \alpha_j$

Therefore the format of a stochastic optimisation or a chance-constrained programming problem may be defined as follows:

$$\text{Min/Max} \sum_{i=1}^{m} (b_i x_i)$$

Subject to: $P\ [\sum_{i=1}^{m} (w_i a_{ij})] > \alpha_j$

Again, the process will be further illustrated by means of the accompanying practical example extracted from BIT et al (1993), below.

2.4.2. Single Objective Stochastic Fuzzy Optimisation

The following example was extracted from BIT *et al* (1993)

Example: *The Critical Path Method*: - Most projects can be subdivided into small tasks or jobs. For instance, in building a house, necessary jobs might include excavating, laying footers, laying the foundation, building walls, framing windows etc. Work on some pairs of tasks can proceed simultaneously, while other jobs must be worked on in series. Thus, in the house-building example, it is possible to do rough plumbing and electrical work simultaneously but it remains necessary to construct the walls before constructing the roof. The various technological preference relationships can be effectively illustrated using project graphs as indicated below:

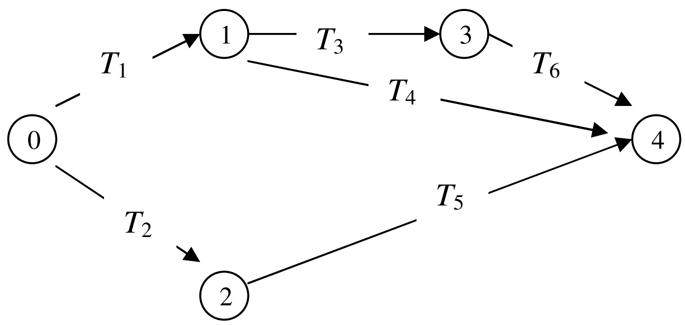

Fig 2.1: Project Graph

The completion times, T_i, for the various tasks are not known exactly but there is a probability distribution for each task. Specifically, it is assumed that each task in the project is characterised by a crash time, $d - l$, and a pessimistic time, $d + l$. and that the actual job times are distributed between these two times according to the probability distribution defined below:

$$F(x) = \begin{cases} 0 & \text{, for } x < d - l \\ \tfrac{1}{2}\sqrt[3]{(x-d)/l} + \tfrac{1}{2} & \text{, for } d - l < x < d + l \\ 1 & \text{, for } d + l < x \end{cases}$$

Actual project-time data and corresponding probability distributions are shown in Table 2.6

T2.6 Project-time data and corresponding probability distribution functions

Job	Crash Time	Pessimistic Time	*d*	*l*	Probability Distribution $F_j(z)$
T_1	9	29	19	10	½ ($^3\sqrt{}$[[(x – 19)/10])
T_2	8	18	13	5	½ ($^3\sqrt{}$[[(x – 13)/5])
T_3	1	3	2	1	½ ($^3\sqrt{}$[[(x – 2)/1])
T_4	19	31	25	6	½ ($^3\sqrt{}$[[(x – 25)/6])
T_5	21	53	37	16	½ ($^3\sqrt{}$[[(x – 37)/16])
T_6	7	27	17	10	½ ($^3\sqrt{}$[[(x – 17)/10])

Stochastic Optimisation Methodology:

1) *Identify the Decision Variables*: - The decision variables completely describe the decisions to be made (solved) by the linear program:

   Decision Variables: - x_0, x_1, x_2, x_3, x_4

2) *Formulate the Objective Function*: - A mathematical relationship involving all or some of the decision variables that describes the main objective of the linear program, e.g. profit or variable cost determination. Typically, this function (*z*) would be minimized or maximised in a linear program in order to determine an optimum value.

   Objective Function: - Min ($-x_0 + x_4$)

3) *Define the Constraints*:

$$
\begin{aligned}
-x_0 + x_1 &\geq t_1 \\
-x_0 + x_2 &\geq t_2 \\
-x_1 + x_3 &\geq t_3 \\
-x_1 + x_4 &\geq t_4 \\
-x_2 + x_4 &\geq t_5 \\
-x_3 + x_4 &\geq t_6
\end{aligned}
$$

4) *Assign Limitations*: - $x_0 = 0$

5) *Convert the program into a Chance Constrained Program with assigned probabilities*

Objective Function: Min x_4

Subject to Constraints:

$$
\begin{aligned}
&P[+x_1 \geq T_1] > 0.8\\
&P[+x_2 \geq T_2] > 0.9\\
&P[-x_1 + x_3 \geq T_3] > 0.7\\
&P[-x_1 + x_4 \geq T_4] > 0.9\\
&P[-x_2 + x_4 \geq T_5] > 0.8\\
&P[-x_3 + x_4 \geq T_6] > 0.7
\end{aligned}
$$

6) *Invert the chance constraints by inverting their probability distributions*
This is done using the inversion function, $x = F^{-1}(y) = d + l\,(2y - 1)^3$; $0 \leq y \leq 1$, and shown in the table 2.7:

T2.7 Inverted Chance Constraints

Job	***d***	***l***	$F^{-1}(z)$	α_i	$F_j^{-1}(\alpha_i)$
T_1	19	10	$19 + 10(2y - 1)^3$	0.8	21.1
T_2	13	5	$13 + 5(2y - 1)^3$	0.9	15.6
T_3	2	1	$2 + (2y - 1)^3$	0.7	2.1
T_4	25	6	$25 + 6(2y - 1)^3$	0.9	28.1
T_5	37	16	$37 + 16(2y - 1)^3$	0.8	40.5
T_6	17	10	$17 + 10(2y - 1)^3$	0.7	17.6

7) *Generate the deterministic equivalent of the chance constrained programming problem.*

Objective Function: Min x_4

Subject to constraints:

$$
\begin{aligned}
&+x_1 \geq 20.1\\
&+x_2 \geq 15.6\\
&-x_1 + x_3 \geq 2.1\\
&-x_1 + x_4 \geq 28.1\\
&-x_2 + x_4 \geq 40.5\\
&-x_3 + x_4 \geq 17.6
\end{aligned}
$$

8) *Solve the model*

This is now an ordinary linear programming problem and the solution, using MS-Excel Solver, is shown in Table 2.8.

T2.8 Chance constrained linear program

x_1	x_2	x_3	x_4	Constraint Equation	Min x_4	Constraint Limit
23.5	15.6	25.6	56.1		56.1	
1				23.50	$\geq$	20.1
	1			15.60	$\geq$	15.6
-1		1		2.10	$\geq$	2.1
-1			1	32.60	$\geq$	28.1
	-1		1	40.50	$\geq$	40.5
		-1	1	30.50	$\geq$	17.6

9) *Record the solution* (Table 2.9)

T2.9 Chance constrained linear programming solution

Job	Job Duration Expression	Optimum Completion Times
T_1	x_1	23.5
T_2	x_2	15.6
T_3	$- x_1 + x_3$	2.1
T_4	$- x_1 + x_4$	32.6
T_5	$- x_2 + x_4$	40.5
T_6	$- x_3 + x_4$	30.5

Chance-constrained or stochastic programming represents a very effective, practical technique for achieving optimisation under conditions of probabilistic uncertainty, providing that appropriate variable probability density functions are available. Apart from the chance-constrained programming methodology, the problem with uncertainty in the coefficients of a linear programming problem may be overcome by applying linear programming with *recourse*, which is not covered in this research project but may be found in GABRIEL (2005).

The linear programming with *recourse* technique involves the initial estimation of the optimum value of a programming problem before all the variable relationship profiles (e.g. constraint equations) are known. If the estimate is either high or low, a penalty cost is incurred. The objective is then to minimise the penalty costs. This technique is a bit more complex than that required for standard chance-constrained programming because in the former case, probability distributions would be required for both high and low deviations.

Therefore, in the researcher's opinion, chance-constrained programming remains the preferred method of Stochastic Optimisation and further examples of this may be found in AZAIEZ *et al* (2005); AY EN APAYDIN *et al* (1997) and LIAO and RUTTSCHER (2006)

3. APPLICATION METHODOLOGY

3.1. Introduction

Since there is definitely no precedent in the chemical industry for the application of a Dual Objective Holistic (Multi-sub-objective Stochastic Fuzzy Minmax Optimisation) methodology (MSFMO) for any aspect of chemical production and since, also, that such a methodology does not appear to exist in the first place, it was decided to derive and then subsequently apply such an approach as a research project.

The first stage of this research is to derive a Dual Objective Holistic (Multi-sub-objective Stochastic Fuzzy Minmax) Optimisation methodology for application in chemical plant environments. This will be based on an analysis of existing methodologies with a view to selecting the required and preferred components and then logically integrating them to create a Dual Objective Holistic (Multi-sub-objective Stochastic Fuzzy Minmax) Optimisation Methodology.

3.2. Methodology Derivation: - Minmax Fuzzy Optimisation

The concept of Minmax Programming / Optimisation is fairly frequently encountered / mentioned in the Research Literature, and involves the combination of objective functions, some of which must be maximised, while others simultaneously minimised. Unfortunately, the proof and application thereof in Literature is often too vague and theoretical ***and not really appropriate for engineering applications*****.**

The existence of an easily implementable Minmax Optimisation methodology would be extremely beneficial in practice because there are many instances where simultaneous maximum and minimum solutions would be ideally required, e.g. in a Chemical Plant production environment requiring the maximisation of production whilst also requiring the minimisation of effluent discharge. For these reasons it was decided to derive a straight-forward, implementable Minmax optimisation methodology based on proven, integrable component methodologies / technologies, i.e. in this case, Single and Multi-objective Fuzzy Optimisation.

The derivation of a Minmax Fuzzy Optimisation methodology will be based on the Multi-objective Fuzzy Optimisation example covered in 2.3.3. The example will be slightly modified to accommodate *Minmax* Fuzzy Optimisation. As before, a methodology will be proposed in concert with the presentation of the solution.

Example: In a manufacturing and distribution operation, there are four production sources and five destinations. The three key business objectives are (i) minimum transportation cost (Z_1), (ii) maximise delivery time (Z_2) and (iii) total relative safety (Z_3) per given route.

The Objective functions are given by:

$$\text{Min } Z_1 = \begin{pmatrix} 9 & 12 & 9 & 6 & 9 \\ 7 & 3 & 7 & 7 & 5 \\ 6 & 5 & 9 & 11 & 3 \\ 6 & 9 & 11 & 2 & 2 \end{pmatrix} \qquad \text{Max } Z_2 = \begin{pmatrix} 2 & 9 & 8 & 1 & 4 \\ 1 & 9 & 9 & 5 & 2 \\ 8 & 1 & 8 & 4 & 5 \\ 2 & 8 & 6 & 9 & 8 \end{pmatrix}$$

$$\text{Min } Z_3 = \begin{pmatrix} 2 & 4 & 6 & 3 & 6 \\ 4 & 8 & 4 & 9 & 2 \\ 5 & 3 & 5 & 3 & 6 \\ 6 & 9 & 6 & 3 & 1 \end{pmatrix}$$

Subject to Constraints:

$\sum_{j=1}^{5} x_{1j} = 5$, $\sum_{j=1}^{5} x_{2j} = 4$, $\sum_{j=1}^{5} x_{3j} = 2$,
$\sum_{j=1}^{5} x_{4j} = 9$, $\sum_{i=1}^{4} x_{i1} = 4$, $\sum_{i=1}^{4} x_{i2} = 4$,
$\sum_{j=1}^{4} x_{i3} = 6$, $\sum_{j=1}^{4} x_{i4} = 2$, $\sum_{j=1}^{4} x_{i5} = 4$,
$x_{ij} \geq 0$, $i = 1, 2, 3, 4$, $j = 1, 2, 3, 4$

Note: *The difference to the original example is that, in this case, the second (ii) objective function is now a maximum function instead of a minimum function.*

Solution Methodology:

1) *Identify the Decision Variables*: - In this case the decision variables represent all the source and destination possibilities, i.e. x_{11}, x_{12}, x_{13}, x_{14}, x_{15}, x_{21}, $3x_{22}$, x_{23}, x_{24}, x_{25}, x_{31}, x_{32}, x_{33}, x_{34}, x_{35}, x_{41}, x_{42}, x_{43}, x_{44} and x_{45}

2) *Formulate the Objective Functions*: - A mathematical relationship involving all or some of the decision variables that describes the main objective of the linear program, e.g. profit or variable cost determination. Typically, this function (z) would be minimized or maximised in a linear program in order to determine an optimum value.

The Objective functions are given by:

$$\text{Min } Z_1 = \begin{pmatrix} 9 & 12 & 9 & 6 & 9 \\ 7 & 3 & 7 & 7 & 5 \\ 6 & 5 & 9 & 11 & 3 \\ 6 & 9 & 11 & 2 & 2 \end{pmatrix} \qquad \text{Max } Z_2 = \begin{pmatrix} 2 & 9 & 8 & 1 & 4 \\ 1 & 9 & 9 & 5 & 2 \\ 8 & 1 & 8 & 4 & 5 \\ 2 & 8 & 6 & 9 & 8 \end{pmatrix}$$

$$\text{Min } Z_3 = \begin{pmatrix} 2 & 4 & 6 & 3 & 6 \\ 4 & 8 & 4 & 9 & 2 \\ 5 & 3 & 5 & 3 & 6 \\ 6 & 9 & 6 & 3 & 1 \end{pmatrix}$$

3) *Define the Constraints*: - Various limitations to the linear programming model expressed in terms of different relationships involving the decision variables.

Subject to Constraints:

$\sum_{j=1}^{5} x_{1j} = 5$, $\sum_{j=1}^{5} x_{2j} = 4$, $\sum_{j=1}^{5} x_{3j} = 2$,
$\sum_{j=1}^{5} x_{4j} = 9$, $\sum_{i=1}^{4} x_{i1} = 4$, $\sum_{i=1}^{4} x_{i2} = 4$,
$\sum_{j=1}^{4} x_{i3} = 6$, $\sum_{j=1}^{4} x_{i4} = 2$, $\sum_{j=1}^{4} x_{i5} = 4$,

3) *Assign Limitations*: - Certain decision variables may be subject to certain limitation values.
$x_{ij} \geq 0$, $i = 1, 2, 3, 4$, $j = 1, 2, 3, 4$

4) *Formulate the Model*:
In this example, a Multi-objective Linear Program is formulated as follows:

<u>Objective functions</u>:

$$\text{Min } Z_1 = \begin{pmatrix} 9 & 12 & 9 & 6 & 9 \\ 7 & 3 & 7 & 7 & 5 \\ 6 & 5 & 9 & 11 & 3 \\ 6 & 9 & 11 & 2 & 2 \end{pmatrix} \qquad \text{Max } Z_2 = \begin{pmatrix} 2 & 9 & 8 & 1 & 4 \\ 1 & 9 & 9 & 5 & 2 \\ 8 & 1 & 8 & 4 & 5 \\ 2 & 8 & 6 & 9 & 8 \end{pmatrix}$$

$$\text{Min } Z_3 = \begin{pmatrix} 2 & 4 & 6 & 3 & 6 \\ 4 & 8 & 4 & 9 & 2 \\ 5 & 3 & 5 & 3 & 6 \\ 6 & 9 & 6 & 3 & 1 \end{pmatrix}$$

<u>Subject to Constraints and Limitations</u>:

$\sum_{j=1}^{5} x_{1j} = 5$, $\sum_{j=1}^{5} x_{2j} = 4$, $\sum_{j=1}^{5} x_{3j} = 2$,
$\sum_{j=1}^{5} x_{4j} = 9$, $\sum_{i=1}^{4} x_{i1} = 4$, $\sum_{i=1}^{4} x_{i2} = 4$,
$\sum_{j=1}^{4} x_{i3} = 6$, $\sum_{j=1}^{4} x_{i4} = 2$, $\sum_{j=1}^{4} x_{i5} = 4$,

$x_{ij} \geq 0$, $i = 1, 2, 3, 4$, $j = 1, 2, 3, 4$

5) *Independently optimise each objective function subject to respective optimisation requirements (Max or Min) and the pertinent constraints and limitations (Table 3.1)*

T3.1 Minmax	x_{11}	x_{12}	x_{13}	x_{14}	x_{15}	x_{21}	x_{22}	x_{23}	x_{24}	x_{25}	x_{31}	x_{32}	x_{33}	x_{34}	x_{35}	x_{41}	x_{42}	x_{43}	x_{44}	x_{45}	$Z_1(\tilde{x}_i)$	$Z_2(\tilde{x}_i)$	$Z_3(\tilde{x}_i)$		
Coefficients	9	12	9	6	9	7	3	7	7	5	6	5	9	11	3	6	8	11	2	2	102	148	100	$Z_i(\tilde{x}_1)$	
Variables ($\tilde{x}_1$)	-	-	5.00	-	-	0.00	4.00	-	-	-	1.00	-	1.00	-	0.00	3.00	-	-	2.00	4.00					
Coefficients	2	9	8	1	4	1	9	9	5	2	8	1	8	4	5	2	8	6	9	8	126	157	81	$Z_i(\tilde{x}_2)$	
Variables ($x\sim_2$)	-	3.00	2.00	-	-	-	-	4.00	-	-	2.00	-	-	-	-	2.00	1.00	-	2.00	4.00					
Coefficients	2	4	6	3	6	4	8	4	9	2	5	3	5	3	6	6	9	6	3	1	134	122	64	$Z_i(\tilde{x}_3)$	
Variables ($\tilde{x}_3$)	3.00	2.00	-	-	-	1.00	-	3.00	-	-	-	2.00	-	-	-	-	-	3.00	2.00	4.00					
$\sum_{j=1}^{5} x_{1j} = 5$	1	1	1	1	1																5.00	5.00	5.00	=	5
$\sum_{j=1}^{5} x_{4j} = 9$						1	1	1	1	1											4.00	4.00	4.00	=	4
$\sum_{j=1}^{4} x_{i3} = 6$											1	1	1	1	1						2.00	2.00	2.00	=	2
$\sum_{j=1}^{5} x_{2j} = 4$																1	1	1	1	1	9.00	9.00	9.00	=	9
$\sum_{i=1}^{4} x_{i1} = 4$	1					1					1					1					4.00	4.00	4.00	=	4
$\sum_{j=1}^{4} x_{i4} = 2$		1					1					1					1				4.00	4.00	4.00	=	4
$\sum_{j=1}^{5} x_{3j} = 2$			1					1					1					1			6.00	6.00	6.00	=	6
$\sum_{i=1}^{4} x_{i2} = 4$				1					1					1					1		2.00	2.00	2.00	=	2
$\sum_{j=1}^{4} x_{i5} = 4$					1					1					1					1	4.00	4.00	4.00	=	4
$x_{11} \geq 0$	1																				-	-	3.00	≥	0
$x_{12} \geq 0$		1																			-	3.00	2.00	≥	0
$x_{13} \geq 0$			1																		5.00	2.00	-	≥	0
$x_{14} \geq 0$				1																	-	-	-	≥	0
$x_{15} \geq 0$					1																-	-	-	≥	0
$x_{21} \geq 0$						1															0.00	-	1.00	≥	0
$x_{22} \geq 0$							1														4.00	-	-	≥	0
$x_{23} \geq 0$								1													-	4.00	3.00	≥	0
$x_{24} \geq 0$									1												-	-	-	≥	0
$x_{25} \geq 0$										1											-	-	-	≥	0
$x_{31} \geq 0$											1										1.00	2.00	-	≥	0
$x_{32} \geq 0$												1									-	-	2.00	≥	0
$x_{33} \geq 0$													1								1.00	-	-	≥	0
$x_{34} \geq 0$														1							-	-	-	≥	0
$x_{35} \geq 0$															1						0.00	-	-	≥	0
$x_{41} \geq 0$																1					3.00	2.00	-	≥	0
$x_{42} \geq 0$																	1				-	1.00	-	≥	0
$x_{43} \geq 0$																		1			-	-	3.00	≥	0
$x_{44} \geq 0$																			1		2.00	2.00	2.00	≥	0
$x_{45} \geq 0$																				1	4.00	4.00	4.00	≥	0

6) *Calculate the optimum value of each objective function (Z_k) based on the corresponding optimum set of variable values (x_{ij}). (Table 3.2/3.3)*

T3.2/3.3 Optimum DV	x_{11}	x_{12}	x_{13}	x_{14}	x_{15}	x_{21}	x_{22}	x_{23}	x_{24}	x_{25}	x_{31}	x_{32}	x_{33}	x_{34}	x_{35}	x_{41}	x_{42}	x_{43}	x_{44}	x_{45}	$Z_1(\tilde{x}_i)$	$Z_2(\tilde{x}_i)$	$Z_3(\tilde{x}_i)$	
Coefficients	9	12	9	6	9	7	3	7	7	5	6	5	9	11	3	6	8	11	2	2	102	148	100	**$Z_i(\tilde{x}_1)$**
Variables ($\tilde{x}_1$)	-	-	5.00	-	-	0.00	4.00	-	-	-	1.00	-	1.00	-	0.00	3.00	-	-	2.00	4.00				
Coefficients	2	9	8	1	4	1	9	9	5	2	8	1	8	4	5	2	8	6	9	8	126	157	81	**$Z_i(\tilde{x}_2)$**
Variables ($\tilde{x}_2$)	-	3.00	2.00	-	-	-	-	4.00	-	-	2.00	-	-	-	-	2.00	1.00	-	2.00	4.00				
Coefficients	2	4	6	3	6	4	8	4	9	2	5	3	5	3	6	6	9	6	3	1	134	122	64	**$Z_i(\tilde{x}_3)$**
Variables ($\tilde{x}_3$)	3.00	2.00	-	-	-	1.00	-	3.00	-	-	-	2.00	-	-	-	-	-	3.00	2.00	4.00				

7) *Determine the lower – 'best' (L_k) and the upper – 'worst' (U_k) bound values for each objective function calculated – Table 3.4*

T3.4 *'Worst' (U_k) and 'Best' (L_k) Bound Optimum* Values

Objective Function	**Nature**	**U_k ('Worst')**	**L_k ('Best')**
1	Min	148	100
2	Max	81	157
3	Min	134	64

8) *Formulate Aspiration Level relationships (λ_k) for each Objective Function where:*

$$\lambda_k = (U_k - Z_k)/(U_k - L_k)$$

Therefore:

1) $\lambda_1 = (129 - Z_1)/(129 - 125)$

$= [129 - (9x_{11} + 12x_{12} + 9x_{13} + 6x_{14} + 9x_{15} + 7x_{21} + 3x_{22} + 7x_{23} + 7x_{24} + 5x_{25} + 6x_{31} + 5x_{32} + 9x_{33} + 11x_{34} + 3x_{35} + 6x_{41} + 9x_{42} + 11x_{43} + 2x_{44} + 2x_{45})]/4$

$$\therefore \lambda_1 = 32.25 - \begin{pmatrix} 2.25 & 3.00 & 2.25 & 1.25 & 2.25 \\ 1.75 & 0.75 & 1.75 & 1.75 & 1.25 \\ 1.50 & 1.25 & 2.25 & 2.75 & 0.75 \\ 1.50 & 2.25 & 2.75 & 0.50 & 0.50 \end{pmatrix}$$

2) $\lambda_2 = (118 - Z_2)/(118 - 157)$

$[118 - (2x_{11} + 9x_{12} + 8x_{13} + x_{14} + 4x_{15} + x_{21} + 9x_{22} + 9x_{23} + 5x_{24} + 2x_{25} + 8x_{31} + x_{32} + 8x_{33} + 4x_{34} + 5x_{35} + 2x_{41} + 8x_{42} + 6x_{43} + 9x_{44} + 8x_{45})]/(-39)$

$$\therefore \lambda_2 = -3.026 + \begin{pmatrix} 0.051 & 0.231 & 0.211 & 0.026 & 0.103 \\ 0.026 & 0.154 & 0.154 & 0.132 & 0.055 \\ 0.205 & 0.026 & 0.205 & 0.103 & 0.128 \\ 0.051 & 0.205 & 0.154 & 0.231 & 0.205 \end{pmatrix}$$

3) $\lambda_3 = (81 - Z_3)/(81 - 64)$

$= [81 - (2x_{11} + 4x_{12} + 6x_{13} + 3x_{14} + 6x_{15} + 4x_{21} + 8x_{22} + 4x_{23} + 9x_{24} + 2x_{25} + 5x_{31} + 3x_{32} + 5x_{33} + 3x_{34} + 6x_{35} + 6x_{41} + 9x_{42} + 6x_{43} + 3x_{44} + x_{45})]/(17)$

$$\lambda_3 = 4.765 - \begin{pmatrix} 0.118 & 0.059 & 0.353 & 0.176 & 0.353 \\ 0.235 & 0.471 & 0.235 & 0.529 & 0.118 \\ 0.294 & 0.176 & 0.294 & 0.176 & 0.353 \\ 0.353 & 0.529 & 0.353 & 0.176 & 0.059 \end{pmatrix}$$

9) *Formulate an Aspiration Level optimisation program consisting of all Aspiration Level Functions (λ_k) and all pertinent constraints*

Objective Functions:

$$\lambda_1 = 32.25 - \begin{pmatrix} 2.25 & 3.00 & 2.25 & 1.25 & 2.25 \\ 1.75 & 0.75 & 1.75 & 1.75 & 1.25 \\ 1.50 & 1.25 & 2.25 & 2.75 & 0.75 \\ 1.50 & 2.25 & 2.75 & 0.50 & 0.50 \end{pmatrix}$$

$$\therefore \lambda_2 = -3.026 + \begin{pmatrix} 0.051 & 0.231 & 0.211 & 0.026 & 0.103 \\ 0.026 & 0.154 & 0.154 & 0.132 & 0.055 \\ 0.205 & 0.026 & 0.205 & 0.103 & 0.128 \\ 0.051 & 0.205 & 0.154 & 0.231 & 0.205 \end{pmatrix}$$

$$\lambda_3 = 4.765 - \begin{pmatrix} 0.118 & 0.059 & 0.353 & 0.176 & 0.353 \\ 0.235 & 0.471 & 0.235 & 0.529 & 0.118 \\ 0.294 & 0.176 & 0.294 & 0.176 & 0.353 \\ 0.353 & 0.529 & 0.353 & 0.176 & 0.059 \end{pmatrix}$$

<u>Subject to Constraints and Limitations</u>:

$\sum_{j=1}^{5} x_{1j} = 5$, $\sum_{j=1}^{5} x_{2j} = 4$, $\sum_{j=1}^{5} x_{3j} = 2$,
$\sum_{j=1}^{5} x_{4j} = 9$, $\sum_{i=1}^{4} x_{i1} = 4$, $\sum_{i=1}^{4} x_{i2} = 4$,
$\sum_{j=1}^{4} x_{i3} = 6$, $\sum_{j=1}^{4} x_{i4} = 2$, $\sum_{j=1}^{4} x_{i5} = 4$,

$x_{ij} \geq 0$, $i = 1, 2, 3, 4$, $j = 1, 2, 3, 4$

10) *Solve the Aspiration Level Optimisation program by maximising each Aspiration Level Function (Table 3.5) and selecting the highest one to represent the optimum solution.*

Highest Aspiration Level = λ_3 = 3.85

Corresponding Optimum Decision Variables:

T3.6 – Overall Optimum Solution

x_{11}	x_{12}	x_{13}	x_{14}	x_{15}	x_{21}	x_{22}	x_{23}	x_{24}	x_{25}
3.00	2.00	- 0.00	-	-	-	-	4.00	0.00	-
x_{31}	x_{32}	x_{33}	x_{34}	x_{35}	x_{41}	x_{42}	x_{43}	x_{44}	x_{45}
-	2.00	-	-	-	1.00	-	2.00	2.00	4.00

'Compromised' Objective Function Values

T3.6 – Overall Optimum Solution

Objective	Nature	Compromise Value	Optimum Value
1	Min	129.00	102
2	Max	126.00	157
3	Min	64.00	64

Minmax Multi-Objective Fuzzy Optimisation

T3.5	x_{11}	x_{12}	x_{13}	x_{14}	x_{15}	x_{21}	x_{22}	x_{23}	x_{24}	x_{25}	x_{31}	x_{32}	x_{33}	x_{34}	x_{35}	x_{41}	x_{42}	x_{43}	x_{44}	x_{45}	λ_1^{max}	λ_2^{max}	λ_3^{max}		
Coeffs.	0.19	0.25	0.19	0.13	0.19	0.15	0.06	0.15	0.15	0.10	0.13	0.10	0.19	0.23	0.06	0.13	0.19	0.23	0.04	0.04	1.0				
Variables	0.00	-	5.00	-	0.00	-0.00	3.00	1.00	-	-	1.00	1.00	-	-	-	3.00	-	-0.00	2.00	4.00					
Coeffs.	0.03	0.12	0.11	0.05	0.05	0.01	0.12	0.12	0.07	0.03	0.11	0.01	0.11	0.05	0.07	0.03	0.11	0.08	0.12	0.11		0.99			
Variables	0.00	3.00	2.00	-	-	-	-	4.00	-	-	2.00	-	-	-	-	2.00	1.00	-	2.00	4.00					
Coeffs	0.03	0.06	0.09	0.04	0.09	0.06	0.11	0.06	0.13	0.03	0.07	0.04	0.07	0.04	0.09	0.09	0.13	0.09	0.04	0.01			3.85		
Variables	3.00	2.00	-0.00	-	-	-	-	4.00	0.00	-	-	2.00	-	-	-	1.00	-	2.00	2.00	4.00					
$\sum_{j=1}^{5} x_{1j} = 5,$	1	1	1	1	1																5	5	5	=	5
$\sum_{j=1}^{5} x_{2j} = 4,$						1	1	1	1	1											4	4	4	=	4
$\sum_{j=1}^{5} x_{3j} = 2,$											1	1	1	1	1						2	2	2	=	2
$\sum_{j=1}^{5} x_{4j} = 9,$																1	1	1	1	1	9	9	9	=	9
$\sum_{i=1}^{4} x_{i1} = 4,$	1					1					1					1					4	4	4	=	4
$\sum_{i=1}^{4} x_{i2} = 4,$		1					1					1					1				4	4	4	=	4
$\sum_{j=1}^{4} x_{i3} = 6,$			1					1					1					1			6	6	6	=	6
$\sum_{j=1}^{4} x_{i4} = 2,$				1					1					1					1		2	2	2	=	2
$\sum_{j=1}^{4} x_{i5} = 4,$					1					1					1					1	4	4	4	=	4
$x_{11} \geq 0$	1																				1E-11	4E-07	3	≥	0
$x_{12} \geq 0$		1																			0	3	2	≥	0
$x_{13} \geq 0$			1																		5	2	-0	≥	0
$x_{14} \geq 0$				1																	0	0	0	≥	0
$x_{15} \geq 0$					1																1E-12	0	0	≥	0
$x_{21} \geq 0$						1															-0	0	0	≥	0
$x_{22} \geq 0$							1														3	0	0	≥	0
$x_{23} \geq 0$								1													1	4	4	≥	0
$x_{24} \geq 0$									1												0	0	3E-11	≥	0
$x_{25} \geq 0$										1											0	0	0	≥	0
$x_{31} \geq 0$											1										1	2	0	≥	0
$x_{32} \geq 0$												1									1	0	2	≥	0
$x_{31} \geq 3$													1								0	0	0	≥	0
$x_{34} \geq 0$														1							0	0	0	≥	0
$x_{35} \geq 0$															1						0	0	0	≥	0
$x_{41} \geq 0$																1					3	2	1	≥	0
$x_{42} \geq 0$																	1				0	1	0	≥	0
$x_{43} \geq 0$																		1			-0	0	2	≥	0
$x_{44} \geq 0$																			1		2	2	2	≥	0
$x_{45} \geq 0$																				1	4	4	4	≥	0

3.2. Evaluation of the Various Optimisation Models

The literature research process was quite successful in that <u>all</u> components constituting the development of the desired Multi-objective Dual Objective Holistic (Stochastic Fuzzy Minmax) Optimisation Methodology were discussed and analysed. In particular, the model derivation methodology pertaining to the last three optimisation scenarios researched, namely

i) Optimisation Model Building
ii) Single and Multi-Objective Fuzzy Optimisation
iii) Single Objective Stochastic Fuzzy Optimisation
iv) Multi-Objective Minmax Fuzzy Optimisation

These were investigated through various examples.

It was subsequently decided that these three optimisation approaches could combinatorially constitute a workable Dual Objective Holistic optimisation methodology.

The research effort in the following section is involved with the derivation of a robust, workable multi-objective Dual Objective Holistic optimisation methodology based on these proven independent/combinational methodologies. This is followed by a comprehensive application example involving the production of ammonia and its nitrogen-derivatives in a chemical plant

3.3. Multi-Objective Stochastic Fuzzy Minmax Optimisation (MSFMO)

3.3.1. Introduction

The first and key objective of this research is to find, derive and/or formulate a robust, reliable, operable and integrable methodology to accomplish the multi-objective, stochastic, fuzzy Minmax optimisation of an ammonia and nitrogen derivatives (e.g. nitric acid, ammonium nitrate and limestone ammonium nitrate) production facility.

Multi-objective Stochastic Fuzzy Optimisation is an expression that was originally derived for application in the Operations Research (specifically decision-making) or Management Science arena. The expression describes the quest for a 'best' solution, be it a maximum or a minimum, in a system characterised by the need for multiple independent goals or objectives, while the terms 'Fuzzy' and 'Stochastic' respectively refer to any conditions of uncertainty and probability that may exist in the system.

The production of ammonia and its nitrogen derivatives may be accomplished in an integrated production facility including ammonia (NH_3), nitric acid (HNO_3), ammonium nitrate solution (ANS), ammonium nitrate (AN) and limestone ammonium nitrate (LAN) plants. This is shown simplistically in Fig.3.1 below:

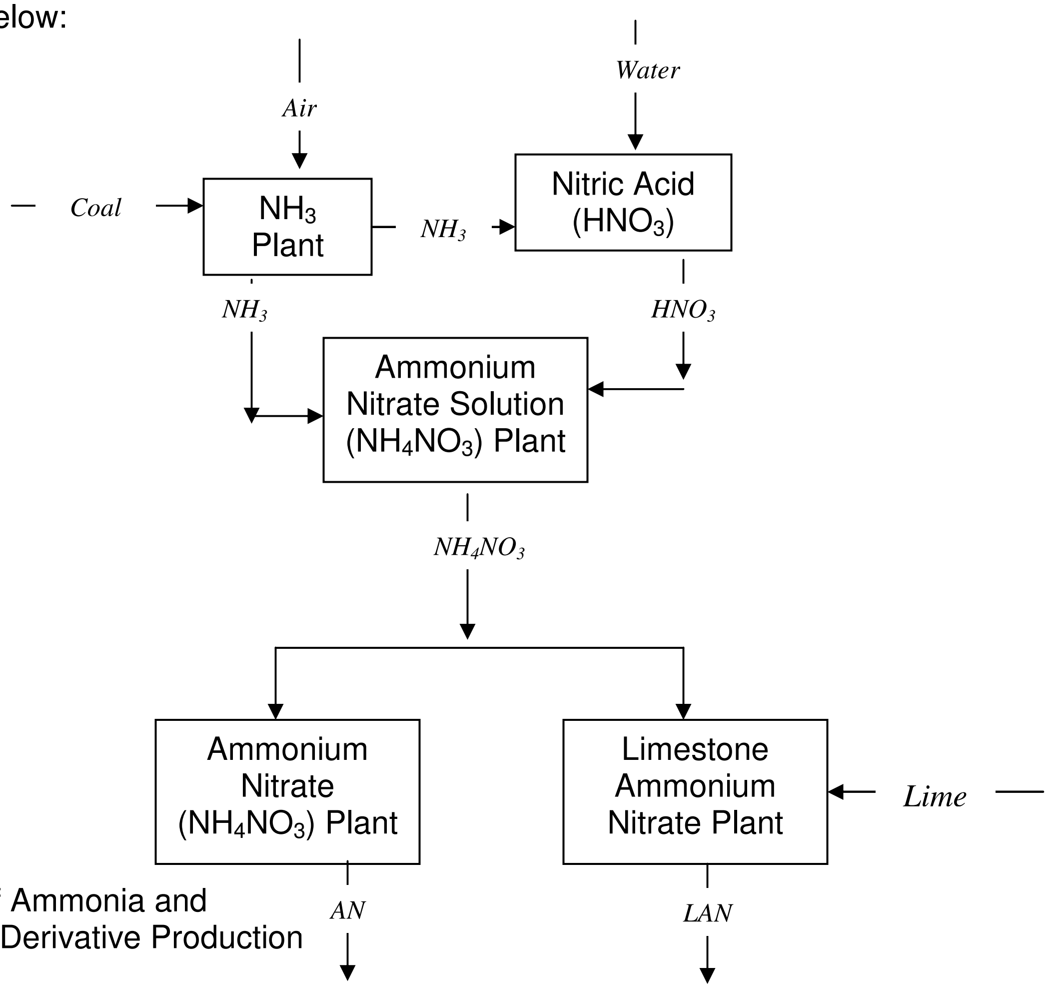

Fig. 3.1: Sketch of Ammonia and Nitrogen-Derivative Production

Now the requirement is to determine the optimum production flows both from an operational perspective whilst minimising the various effluent discharge rates. This will be a fairly challenging task because there are multiple objectives such as **maximising** the many, various production flows both from an operational and commercial perspective whilst **minimising** the various effluent streams. Each of these requirements constitutes a different objective. The difficulty is exacerbated by the fact that certain objectives must be maximised while others have to be simultaneously minimised. The scenario in which one objective is to be maximised whilst the other is minimised is referred to as '**Minmax**'.

The intention, therefore, is to develop a Multi-objective Stochastic Fuzzy Minmax Optimisation methodology based on the detection and extraction of independent or combinational robust, reliable and integrable technologies and methodologies that were discussed in the previous chapter.

a) *The actual procedure that will be followed in deriving an application methodology for 'Multi-objective Stochastic Fuzzy Minmax Optimisation' will involve an analysis and breakdown of procedures in an initial scenario, namely 'Single Objective Fuzzy Optimisation'. A scenario application methodology will be derived by scrutinising and sequentially analysing the various steps taken with a view to compiling an appropriate procedural methodology. This will be followed by a similar analysis, breakdown and compilation of methodologies for the second and third scenarios, 'Single Objective Stochastic Optimisation' and 'Single Objective Stochastic Fuzzy Optimisation'. Based on the analyses of the various combinational scenarios above, an application methodology will be derived for the holistic concept, 'Multi-objective Stochastic Fuzzy Minmax Optimisation'.*

b) This methodology will then be applied to an Ammonia and Nitrogen-derivatives (Nitric Acid, Ammonium Nitrate Solution (ANS), Ammonium Nitrate (AN), and Limestone Ammonium Nitrate (LAN)) production facility in order to determine the optimum production flows from an operational and commercial perspective.

These two statements jointly represent the core of this research.

3.3.2. Methodology

A methodology for the Multi-Objective Stochastic Fuzzy Minmax Optimisation of an operational process will best be derived by initially discovering and identifying the preferred, integrable subcomponent methodologies from the literature and then rationally integrating these to create an overall Multi-Objective Stochastic Fuzzy Optimisation methodology.

The creation of a Multi-sub-objective Stochastic Fuzzy Minmax Optimisation methodology will be achieved by initially identifying the required, preferred and integrable subcomponent process steps from the various Optimisation methodologies available and then allocating the chosen steps to the desired methodology shown in Table 3.7.

T3.7 Multi-Objective Stochastic Fuzzy Minmax Optimisation Methodology

Operational Process Step	**Multi-Objective Fuzzy Optimisation**	**Single Objective Stochastic Fuzzy Optimisation**	**Minmax Fuzzy Optimisation**	**Multi-Objective Stochastic Fuzzy Minmax Optimisation**
1) Develop a process flow diagram, identifying all process flow components and process flow relationships	Y	Y	Y	**Y**
2) Identify all Decision Variables (x_{ij})	Y	Y	Y	**Y**
3) Derive Objective Function(s) ($Z_i = c_1x_1 + c_2x_2 + c_3x_3 + \ldots + c_nx_n$)	Y	Y	Y	**Y**
4) Define Constraints (e.g. $a_1x_1 + a_2x_2 + \ldots + a_nx_n \leq b_1$)	Y	Y	Y	**Y**
5) Assign all Limitations (e.g. $x_1 \leq L_1$)	Y	Y	Y	**Y**
6) Convert the program into a Chance Constrained Program with assigned probabilities	N	Y	N	**Y**
7) Invert the chance constraints by inverting their probability distributions	N	Y	N	**Y**
8) Generate the (deterministic equivalent) fuzzy program	Y	Y	Y	**Y**
9) Solve the model a number of times according to the number of objective functions	Y	N	Y	**Y**
10) For each objective optimum solution derived, determine the corresponding values for all the other objective functions	Y	N	Y	**Y**
11) Determine the upper (U_k) Lower bounds (L_k)	Y	N	Y	**Y**

for each objective function, based on all the objective function values and whether they are Maximum or Minimum Functions				
12) Generate Aspiration Level Functions, $\lambda_k = (U_k - Z_k) \backslash (U_k - L_k)$ per the number of . . Objective Functions	Y	N	Y	**Y**
13) Maximise each one of the Aspiration Level Functions subject to the pertinent constraints and limitations	Y	N	Y	**Y**
14) Select the highest value Aspiration Level	N	N	Y	**Y**
15) Record the corresponding Solution (Z_i, x_{ij})	Y	Y	Y	**Y**

Based on the above analysis, the compilation of the Multi-Objective Stochastic Fuzzy Optimisation methodology can be done as follows:

1) Develop an *operational process flow diagram*, identifying all process flow components and process flow relationships

2) Identify all Decision Variables (x_{ij}) that affect the performance of the operation.

3) Formulate the required number of Objective Function(s) for the operation - A mathematical relationship ($Z_i = c_1x_1 + c_2x_2 + c_3x_3 + \ldots + c_nx_n$) involving all or some of the decision variables that describes the main objective of the linear program, e.g. profit or variable cost determination. Typically, this function (z) would be minimized or maximised in a linear program in order to determine an optimum value.

4) Define all the Constraint Equations (e.g. $a_1x_1 + a_2x_2 + \ldots + a_nx_n \leq b_1$) for the operation.

5) Assign Limitations, if any, (e.g. $x_1 \leq L_1$) to the Decision Variables and append to the list of constraints.

6) Convert the Constraint Equations into a Chance Constrained Program with assigned probabilities to each probabilistic constraint.

7) Invert the chance constraints by inverting their probability distributions

8) Generate the (deterministic equivalent) stochastic fuzzy program model.

9) Solve the model a number of times according to the number of objective functions, with each objective, in turn, serving as the program Objective Function while the other objectives are treated simply as constraints.

10) For each objective function optimum solution, determine the values for all the other objective functions based on the same set of decision variables.

11) Determine the upper (U_k) and lower bounds (L_k) for each objective function, based on all the objective function values determined in 10) above and based on whether they are Maximum or Minimum Functions

12) Generate Aspiration Level Functions, $\lambda_k = (U_k - Z_k)\backslash(U_k - L_k)$ according to the number of Objective Functions

13) Maximise each one of the Aspiration Level Functions subject to the pertinent constraints and limitations

14) Select the highest value Aspiration Level with its associated variables and calculate all the Objective Function values accordingly.

15) Record the Optimum Solution (Z_i, x_{ij})

4. APPLICATION: - MSFMO OF A AMMONIA AND NITROGEN-DERIVATIVES PLANT

4.1. Introduction

The main intention of this research project is to successfully derive and apply an appropriate Optimisation Methodology to a complex, multi-faceted and integrated chemical production facility in order to determine the most favourable operating conditions, principally from a financial maximisation perspective, but also from an effluent minimisation perspective.

This complex, multi-faceted and integrated chemical production facility was entirely based upon the Ammonia and Nitrogen-derivatives (i.e. Nitric Acid – HNO_3, Ammonium Nitrate Solution – $NH_4NO_3.H_2O$, Ammonium Nitrate - NH_4NO_3 and Limestone Ammonium Nitrate – $Ca/MgCO_3.NH_4NO_3$) production plant at the Modderfontein site in Gauteng.

This plant is an ideal candidate for Multi-Objective, Stochastic, Fuzzy and Minmax Optimisation of production because of the following conditions:

a) The probabilistic (stochastic) nature of the carbon (C) and associated hydrogen (H) content in the chief ammonia production raw material, coal. This difficulty can be overcome through the successful application of stochastic programming/optimisation techniques.

b) In a complex, integrated production environment, there are typically quite a few production objectives that *should* be optimised, e.g. maximisation of production, minimisation of effluent discharge and the minimisation of water and power usage. Therefore a multi-objective optimisation capability is important.

c) As mentioned above, there is often a need to maximise certain production objectives whist simultaneously minimising others. This can be achieved through effective Minmax optimisation

d) The uncertainty in product demand and supply and any other inequality relationships must be accommodated for effective production management. This can be achieved through effective fuzzy programming/optimisation.

Since there are four different aspects of Dual Objective Holistic optimisation (Multi-sub-objective Stochastic Fuzzy Minmax), the term '*holistic*' is applied to accommodate a total combinational and integrated optimisation methodology. The application of this methodology follows the derived procedure for MSFMO optimisation as follows:

a) Production of an Operational Process Flow diagram
b) Identification and selection of Decision Variables
c) Choice and derivation of Objective Functions
d) Specification/Definition of Constraints and Limitations
e) Population of the MSFMO model
f) Solution of the MSFMO model

4.2. *Application of MSFMO Methodology*

4.2.1. Operational Process Flow Diagram

The flowchart (Fig.4.1) accurately represents the main production processes and their interrelation in an Ammonia (NH_3) and Nitrogen-Derivatives (i.e. Nitric Acid, Ammonium Nitrate and Limestone Ammonium Nitrate) production facility.

HOLISTIC OPTIMISATION OF AMMONIA AND NITROGEN-DERIVATIVES PRODUCTION

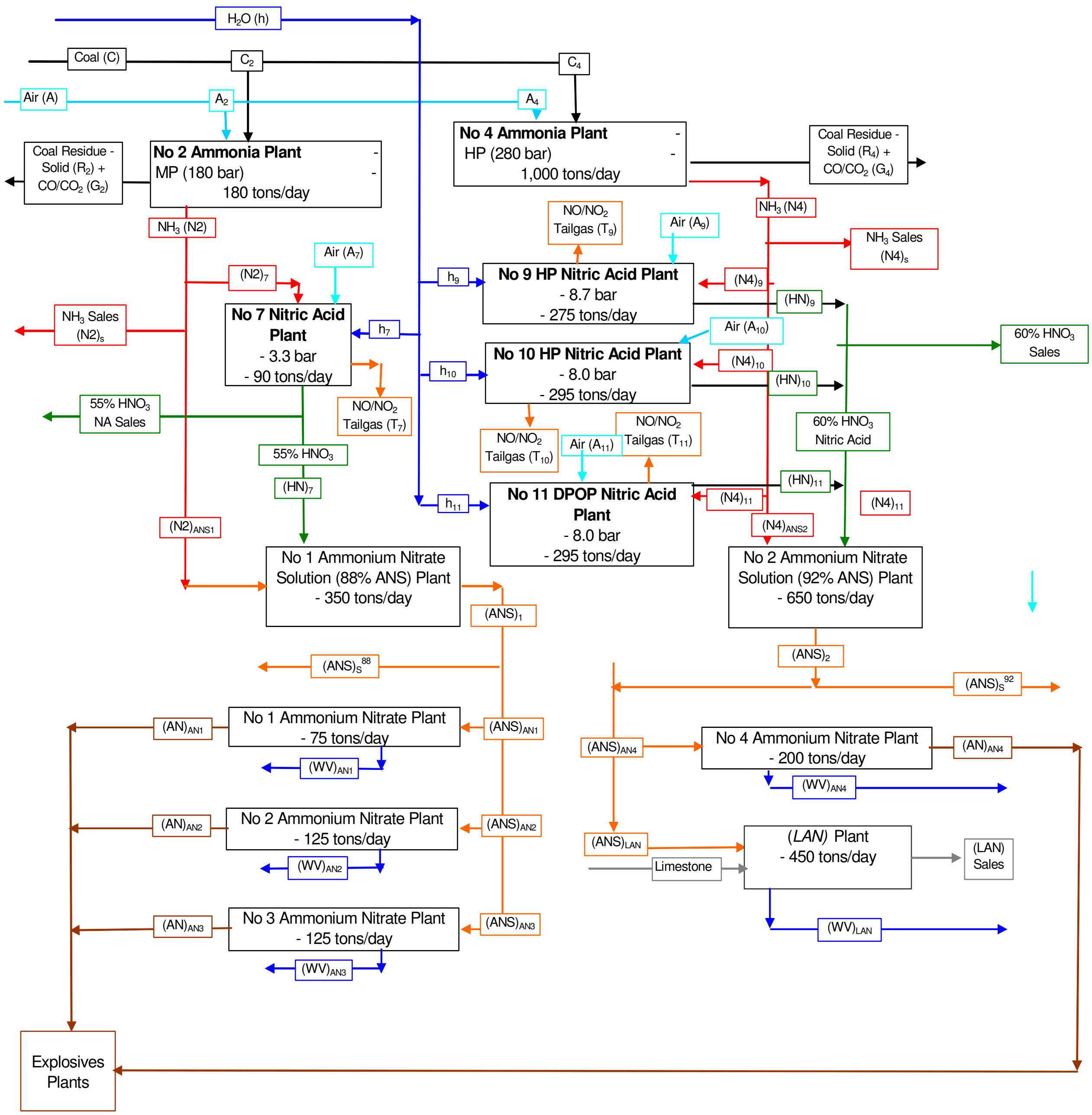

Fig 4.1

4.2.2. Definition of the Decision Variables

Table 4.1 defines all the decision variables to be used in the Multi-sub-objective Stochastic Fuzzy Minmax Optimisation program for the plant utilised in this investigation.

T4.1 Multi-sub-objective Stochastic Fuzzy Minmax Optimisation Decision Variables

Decision Variable	Description
Overall Definitions	
h	Total input distilled water for all process requirements, *tons/day*
C	Total coal input for NH_3 Plants, *tons/day*
A	Total input air for NH_3 Plants, *tons/day*
R	Total coal residue and gas discharge from NH_3 Plants, *tons/d*ay
Ammonia (NH_3) Production and Sales	
P_{NH3}	Selling Price per ton of NH_3 , *SA Rands*
No 2 Ammonia Production Plant	
C_2	Input Coal for No 2 NH_3, *tons/day*
$N2$	Total NH_3 produced from No. 2 NH_3 Plant, *tons/day*
$(N2)_s$	Total NH_3 external sales from No 2 NH_3 , *tons/day*
A_2	Supply of air to No 2 NH_3, *tons/day*
R_2	Coal residue from No 2 NH_3, *tons/day*
G_2	CO/CO_2 discharge from No 2 NH_3, *tons/day*
No 4 Ammonia Production Plant	
C_4	Input Coal for No 4 NH_3, *tons/day*
$N4$	Total NH_3 produced from No. 4 NH_3 Plant, *tons/day*
$(N4)_s$	Total NH_3 external sales from No 4 NH_3, *tons/day*
A_4	Supply of air to No 4 NH_3, *tons/day*
R_4	Coal residue from No 4 NH_3, *tons/day*
G_4	CO/CO_2 discharge from No 4 NH_3, *tons/day*
Nitric Acid Production and Sales	
P^{55}_{HNO3}	Selling price per ton 55% HNO_3, *SA Rands*
P^{60}_{HNO3}	Selling price per ton 60% HNO_3, *SA Rands*
$(HN)_S^{60}$	Sales of 55% HNO_3 from 7 *NA*, *tons/day*
$(HN)_S^{55}$	Sales of 60% HNO_3 from 9, 10 & 11 *NA, tons/day*

No 7 Nitric Acid Production Plant	
h_7	Distilled water for No 7 Nitric Acid Plant (7 *NA*), *tons/day*
A_7	Air for reactor, *tons/day*
$(N2)_7$	NH_3 produced from No 2 NH_3 going to No 7 *NA*, *tons/day*
$(HN)_7$	Total 55% HNO_3 produced on No 7 *NA*, *tons/day*
T_7	NO/NO_2 Tailgas discharge from No 7 *NA*, *tons/day*
No 9 Nitric Acid Production Plant	
h_9	Distilled water for No 9 *NA*, *tons/day*
A_9	Air for reactor, *tons/day*
$(N4)_9$	NH_3 produced from No 4 NH_3 going to No 9 *NA*, *tons/day*
$(HN)_9$	Total 60% HNO_3 produced on No 9 *NA*, *tons/day*
T_9	NO/NO_2 Tailgas discharge from No 9 *NA*, *tons/day*
No 10 Nitric Acid Production Plant	
h_{10}	Distilled water for No 10 *NA*, *tons/day*
A_{10}	Air for reactor, *tons/day*
$(N4)_{10}$	NH_3 produced from No 4 NH_3 going to No 10 *NA, tons/day*
$(HN)_{10}$	Total 60% HNO_3 produced on No 10 *NA, tons/day*
T_{10}	NO/NO_2 Tailgas discharge from No 10 *NA, tons/day*
No 11 Nitric Acid Production Plant	
h_{11}	Distilled water for No 11 *NA, tons/day*
A_{11}	Air for reactor, *tons/day*
$(N4)_{11}$	NH_3 produced from No 4 NH_3 going to No 11 *NA, tons/day*
$(HN)_{11}$	Total 60% HNO_3 produced on No 11 *NA, tons/day*
T_{11}	NO/NO_2 Tailgas discharge from No 11 *NA, tons/day*
Ammonium Nitrate Solution (ANS) Production and Sales	
$(ANS)_S$	Total external *ANS* sales, *tons/day*
P_{ANS}	Selling price of *ANS* per ton
No 1 ANS Production Plant	
$(N2)_{ANS1}$	NH_3 produced from No 2 NH_3 going to No 1 *ANS, tons/day*
$(HN)_{ANS1}$	55% HNO_3 produced from No 7 *NA* going to No. 1 *ANS, tons/day*
$(ANS)_1$	ANS produced on No 1 *ANS, tons/day*
No 2 ANS Production Plant	
$(N4)_{ANS2}$	NH_3 produced from No 4 NH_3 to No 2 *ANS, tons/day*
$(HN)_{ANS2}$	60% HNO_3 produced from 9, 10 & 11 *NA* going to No 2 *ANS, tons/day*
$(ANS)_2$	ANS produced on No 2 *ANS, tons/day*

Ammonium Nitrate (AN) Production and Sales	
$(AN)_S$	Total external sales of ammonium nitrate, *tons/day*
P_{AN}	Selling price of *AN* per ton, *SA Rands*
No I Ammonium Nitrate (AN) Production	
$(ANS)_{AN1}$	ANS transferred to No 1 *AN, tons/day*
$(AN)_{AN1}$	AN produced on No. 1 *AN, tons/day*
$(WV)_{AN1}$	Water Vapour released from No 1 *AN, tons/day*
No 2 Ammonium Nitrate (AN) Production	
$(ANS)_{AN2}$	ANS transferred to No 2 *AN, tons/day*
$(AN)_{AN2}$	AN produced on No. 2 *AN, tons/day*
$(WV)_{AN2}$	Water Vapour released from No 2 *AN, tons/day*
No 3 Ammonium Nitrate (AN) Production	
$(ANS)_{AN3}$	ANS transferred to No 3 *AN, tons/day*
$(AN)_{AN3}$	AN produced on No. 3 *AN, tons/day*
$(WV)_{AN3}$	Water Vapour released from No 3 *AN, tons/day*
No 4 Ammonium Nitrate (AN) Production	
$(ANS)_{AN4}$	ANS transferred to No 4 *AN, tons/day*
$(AN)_{AN4}$	AN produced on No. 4 *AN, tons/day*
$(WV)_{AN4}$	Water Vapour released from No 4 *AN, tons/day*
Limestone Ammonium Nitrate (LAN) Production and Sales	
P_{LAN}	Selling price of *LAN* per ton, *SA Rands*
$(ANS)_{LAN}$	ANS transferred to *LAN, tons/day*
$(LAN)_S$	*LAN* produced and sold on *LAN, tons/day*
$(WV)_{LAN}$	Water Vapour released from *LAN, tons/day*
(L)	Limestone required for the production of *LAN, tons/day*

4.2.3. Formulation of the Objective Function(s)

4.2.3.1 Objective 1: Maximise Gross Profit of Production

An accurately modelled optimised financial performance, i.e. *Gross Profit*, of a complex and integrated chemical production facility, like that above, would give an excellent indication of which production related factors should be concentrated on to ensure optimum production performance, which is the major component of optimum financial performance.

Another reason that the financial performance indicator, *Gross Profit*, is an ideal production performance indicator is that *Gross Profit* is only concerned with the sales revenues less direct operating costs on the production plants and not concerned with ancillary non-production expenses as accounted for in *Net Profits*. A certain aspect of chemical production, which became increasingly important in the late 20th century and is most certainly a key consideration in the 21st century, is the issue of effluent control. It would therefore be extremely beneficial if production performance could be optimised while, at the same time, minimising effluent discharge. Therefore, the intention in this research is to optimise production from a financial standpoint (Gross Profit), which can be mathematically represented as follows:

<u>Objective 1</u>:- Max $[(GP)_{NH3}((N2)_s + (N4)_s) + (GP)^{55}_{HNO3}(HN)_S^{55} + (GP)^{60}_{HNO3}(HN)_S^{60} + (GP)_{ANS}(ANS)_S + (GP)_{AN}(AN)_S + P_{LAN}(LAN)_{PS}]$

Substituting for prevailing unit prices from Table 4.2 that were obtained from arbitrary financial data.

T4.2: Arbitrary Plant Financial Data

Chemical	Plant	Cost (R/ton)	Production Cost (R/ton)	Transfer Price (R/ton)	Selling Price (R/ton)	Gross Profit (R/ton)
NH_3	No 2	-	305	305	350	45
NH_3	No 4	-	275	275	350	75
55% HNO_3	No 7	305	350	655	750	95
60% HNO_3	No. 9, 10 & 11	275	350	625	775	125
Limestone	-	75	-	-	-	-
92% & 88% NH_4NO_3	No. 1 & 2	900	325	1225	1350	125
100% NH_4NO_3	No. 1, 2, 3 & 4	1225	275	1500	1575	175
LAN	*LAN*	1300	150	1450	1545	95

Therefore Objective 1 will be:

Max $[45(N2)_s + 75(N4)_s + 95(HN)_S^{55} + 125(HN)_S^{60} + 125(ANS)_S + 175(AN)_S + 95(LAN)_S]$

4.2.3.2 Objective 2: Minimise Effluent Discharge

Now, the other somewhat conflicting objective is to minimise total effluent discharge. It is conflicting because maximisation of production would typically maximise effluent discharge but since only certain production streams incur effluent, an overall financial production and sales optimisation exercise would be extremely valuable because less profitable (e.g. effluent incurring) production streams should be minimised, whilst more profitable production streams should be maximised.

In the production of ammonia and its nitrogen derivatives, the chief effluent sources are:

a) NOx (NO/NO_2) tailgas from the Nitric Acid Plants (T_7, T_9, T_{10}, T_{11}).
b) Nitrogenous liquid effluent from the Ammonia and Nitrogen Plants [Nitric Acid (*NA*), Ammonium Nitrate Solution (*ANS*) plants and the Ammonium Nitrate (*AN*) Plants.
c) CO/CO_2 tailgas from the Ammonia plants (G_2, G_4).

Since the CO/CO_2 gas discharge from the Ammonia plants is neither particularly hazardous nor visually unappealing and because the nitrogenous liquid effluent is well managed by the Modderfontein dam system (in fact people used to fish barbel at both Modderfontein dams!), the focus of this research will only be on the minimisation of the NOx (NO/NO_2) tailgas from the Nitric Acid Plants.

Examination of the performance of the Nitric Acid Plants based on detailed plant operational data yielded the following trends:

1) NOx concentration, [NOx], in the tailgas increased with an increase in the production rate $\Rightarrow$ [NOx] $\propto P$ (production rate)

2) [NOx] in the tailgas also increased with a corresponding decrease in reactor (Au/Pd) efficiency (calculated by comparing the nitrogen (N) content in [NOx] exiting the reactor with the (N) content in the incoming Ammonia (NH_3) stream). This trend was detected after analysis of plant operating data before and after plant shutdowns when the Au/Pd catalyst was exchanged for a new or refurbished one and reductions in the [NOx} levels were observed $\Rightarrow$ [NOx] $\propto R_e$ (reaction efficiency)

The reactions occurring in the Nitric Acid reactors are shown in Table 4.3.

T4.3 Nitric Acid Reactor reactions

Reactions in the Reactor	**Nature of Reaction**
$5O_2 + 4NH_3 \leftrightarrow 4NO + 6H_2O$	Primary
$O_2 + 2NO \leftrightarrow 2NO_2$	Secondary

> *Note: the* $O_2 + 2NO \leftrightarrow 2NO_2$ *reaction, necessary for* HNO_3 (*Nitric Acid*) *formation, subsequently and substantially takes place in the downstream Absorption Columns.*

Since reaction efficiency and [NOx] in the tailgas are interrelated and are both dependent on production rate (*P*), it was decided to create a new variable, the product of Reaction Efficiency with [NOx] in the tailgas –

EEP (efficiency/effluent product) = R_e x [NOx]

, and calculate and graphically represent this relationship versus daily production for each of the four Nitric Acid plants in order to determine and assess the relationship(s).

Such an all encompassing variable would be extremely beneficial in the various optimisation procedures because such a single variable could accommodate the chief technical and environmental concerns related to commercial Nitric Acid production.

The EEP data from each Nitric Acid plant was calculated and plotted against the corresponding flowrates for each plant. In each case the plot yielded almost a perfect binomial profile from which MS-Excel could easily and automatically determine the equations corresponding to each plant binomial profile. The average degree of fit for each binomial curve to the corresponding plant data exceeded 80%. The graph for Nos. 7, 9, 10 & 11 Nitric Acid along with the corresponding polynomial regression relationship is shown in Figs. 4.2, 4.3 and 4.4

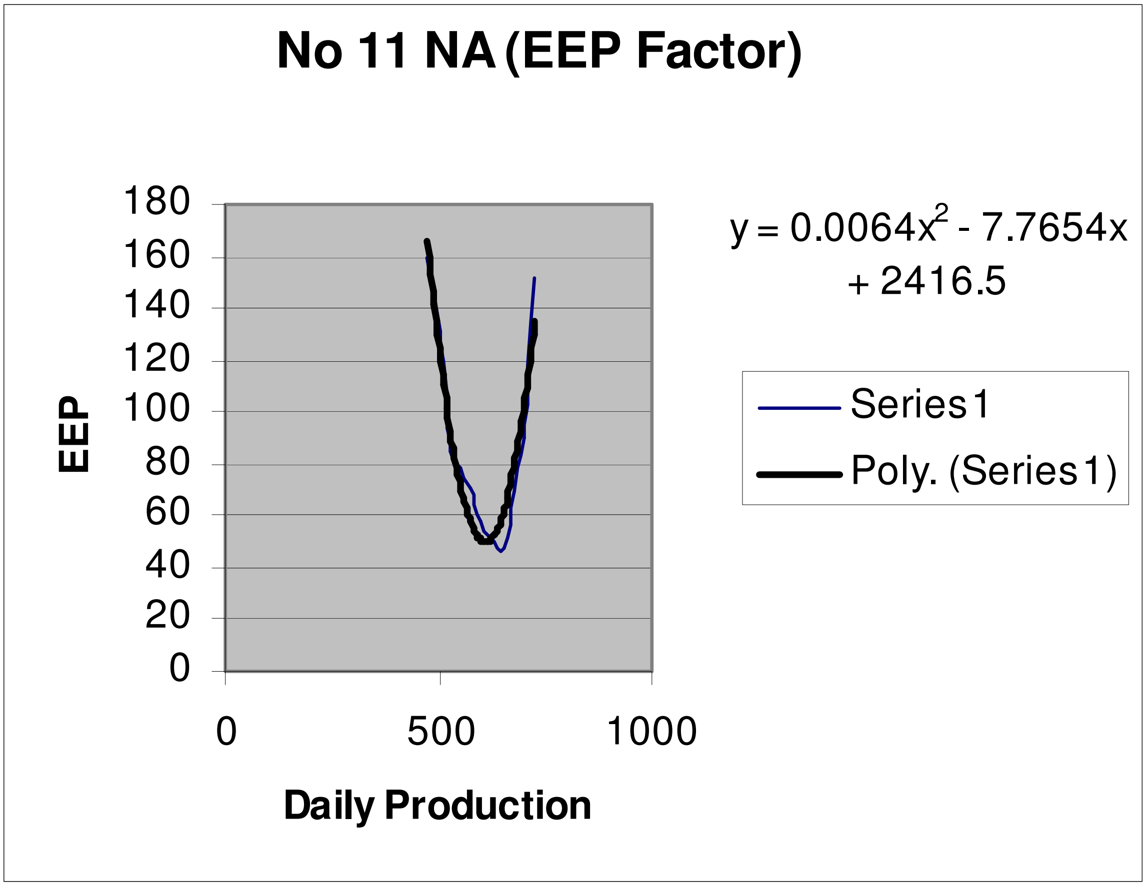

Fig 4.2 *EEP* vs. Daily Production Graph – No 11 *NA*

Quite clearly there is an excellent relationship between the *EEP* factor and the daily production figures for No. 11 Nitric Acid and the fact that it is a concave quadratic curve makes it ideal for *EEP*, and hence effluent, minimisation purposes. Similar trends can be seen in Figs 4.3 and 4.4 for No's 9 & 10 Nitric Acid Plants.

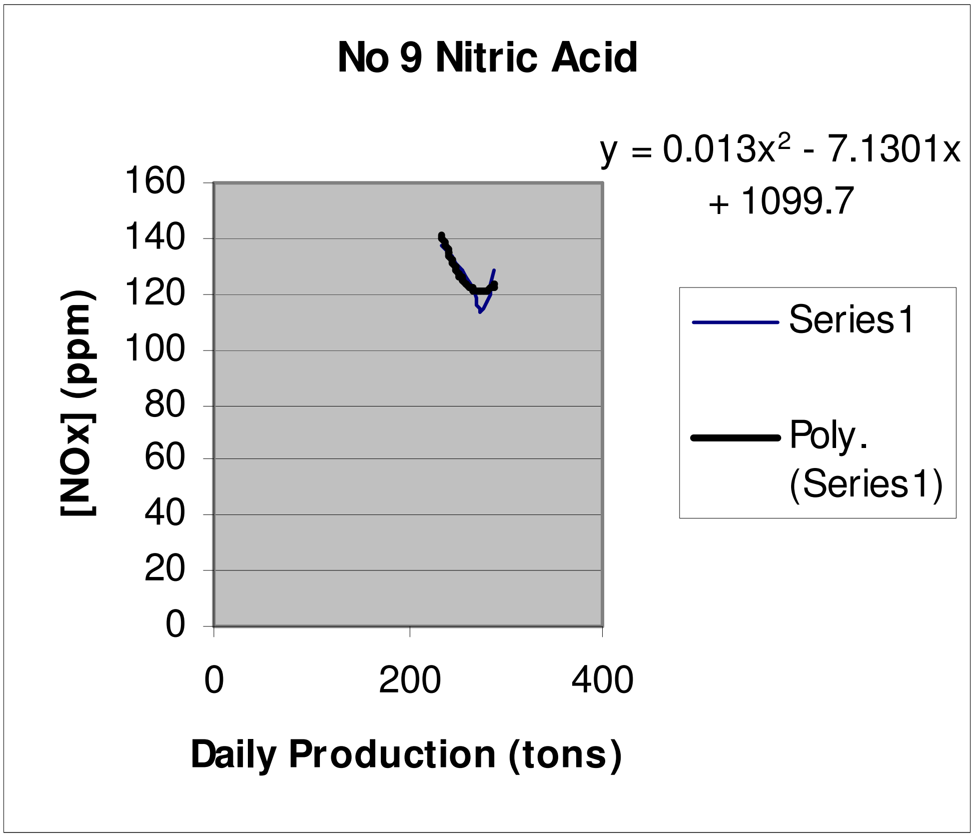

Fig. 4.3: NOx vs. Production – No 9 Nitric Acid

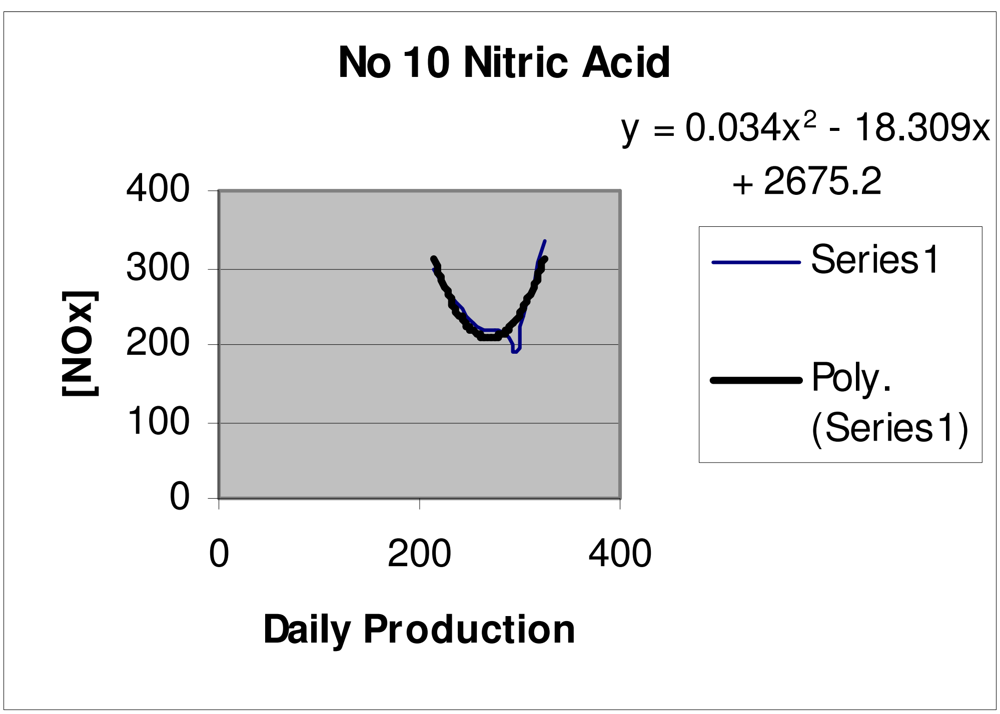

Fig. 4.4 NOx vs. Production – No 10 Nitric Acid

As can be seen, all plants show a very good relationship between their daily production and their *EEP* factors and Table 4.4 demonstrates their correspondingly derived polynomial curves:

T4.4 *EEP* Polynomial Regression Curves

Plant	***EEP* Polynomial Regression Equations**
No 7 NA	$EEP_7 = 0.0746(HN)_7^2 - 11.16(HN)_7 + 461.39$
No 9 NA	$EEP_9 = 0.013(HN)_9^2 - 7.130(HN)_9 + 1099.7$
No 10 NA	$EEP_{10} = 0.034(HN)_{10}^2 - 18.309(HN)_{10} + 2675.2$
No 11 NA	$EEP_{11} = 0.0064(HN)_{11}^2 - 7.765(HN)_{11} + 2416.5$

Therefore Objective 2 is:

<u>Objective 2</u>: - Min $[(EEP)_7 + (EEP)_9 + (EEP)_{10} + (EEP)_{11}]$

Or more mathematically:

$$\text{Min}[0.0746(HN)_7^2 - 11.16(HN)_7 + 461.39 + 0.013(HN)_9^2 - 7.130(HN)_9 + 1099.7 + 0.034(HN)_{10}^2 - 18.309(HN)_{10} + 2675.2 + 0.0064(HN)_{11}^2 - 7.765(HN)_{11} + 2416.6]$$

$$= \text{Min}[0.0746(HN)_7^2 - 11.16(HN)_7 + 0.013(HN)_9^2 - 7.130(HN)_9 + 0.034(HN)_{10}^2 - 18.309(HN)_{10} + 0.0064(HN)_{11}^2 - 7.765(HN)_{11} + 6652.89]$$

4.2.4 Definition of the Constraint Equations and Limitations

Before constraints and limitations can be formulated for the ammonia and nitrogen derivatives production program, the probabilistic concentration of hydrogen in the raw material coal must be defined and determined.

4.2.4.1 Stochastics - Probability Distribution of Hydrogen in Coal

There is a requirement to define a constraint pertaining to the concentration and availability of hydrogen in coal. Some work has been done in Australia in this regard: SMITH and SMITH, (2006), and it is realistically assumed that South African and Australian coals have similar carbon profiles. In order to derive an empirical relationship between the carbon and hydrogen contents of coals and their measured vitrinite reflectances, SMITH and SMITH, (2006) had to initially measure the carbon and hydrogen contents of coal in Australia where the tests were conducted. Hydrogen concentration measurements for a large number of coal samples are given in Table 4.5

T4.5 Hydrogen concentration in coal

[H]	[H]	[H]	[H]
4.0	6.1	6	6.1
5.9	5.4	4.8	5.7
6.1	5.7	6.2	4.2
4.7	4.7	4.9	5
5.1	5.5	4.9	5.1
5.6	5.2	5.3	5.5
5.1	5.7	5.5	4.8
5.1	5.3	5.3	5.4
5.7	5.5	5.4	5.2
4.6	6.6	5	5.5
5.5	5.4	4.1	5.3
5.3	5.3	5.4	5.3
5.1	5	5.2	5.6
6.9	6.6	6.4	5.1
4.7	4.5	4.5	6.3
5.3	5	5.3	5.3
5	4.5	4.9	4.4
5.3	4.6	4.3	5.2
4.9	4.3	4.6	4.1
5.3	4.7	4.4	4.7
4	4.1	4.2	4.1
4	4	3.9	4.6
4.5	4.8	4.4	5.4
4.9	5.7	5.7	5.6
214.4	215.8	210.8	213.8

Although the data above is based on Australian coal, a similar measurement methodology can be applied to South African coal and it is realistically assumed that South African (Modderfontein) coal has a similar content composition.

The [H] data profile strongly suggests a Normal Probability Distribution of hydrogen (*x*) in coal, and if this assumption is made, the following normal probability parameters and graph can be determined:

Probability Parameters:

1) Normal Probability Distribution Function: $f(x, \mu, \sigma) = 1/\sqrt{(2\pi\sigma)}\exp\text{-}\{(x - x^m)^2/2\sigma^2$ where:

   a) Standard Deviation (σ): $\sigma = \sqrt{[\sum(x - x^m)^2/(n - 1)}$; $\Rightarrow \sigma = \sqrt{(17.2 + 17 + 15.6 + 11.9)/(41 - 1)} = 1.241$ (from the table above)
   b) Mean (μ) = $\sum x_i /n = (214.4 + 215.8 + 210.8 + 213.8)/41 = 5.21$ (from the table above)

2) Required probability: - It is required to determine the mean or average [H] (*x*) concentration in coal. This can be achieved by determining the *x*-value corresponding to a cumulative probability of 50%, indicated in Table 4.6.

T4.6 Cumulative Probability of Hydrogen in Coal

x = [H^+] (%)	**Probability (%)**
9.00	0.3%
8.50	1.0%
8.00	2.6%
7.50	5.8%
7.25	8.3%
6.80	14.2%
6.25	22.6%
5.86	28.0%
5.52	31.2%
5.21	32.2%
4.90	31.2%
4.56	28.0%
4.00	20.0%
3.00	6.6%
2.00	1.1%
1.00	0.1%

and shown in the corresponding probability graph in Fig. 4.5

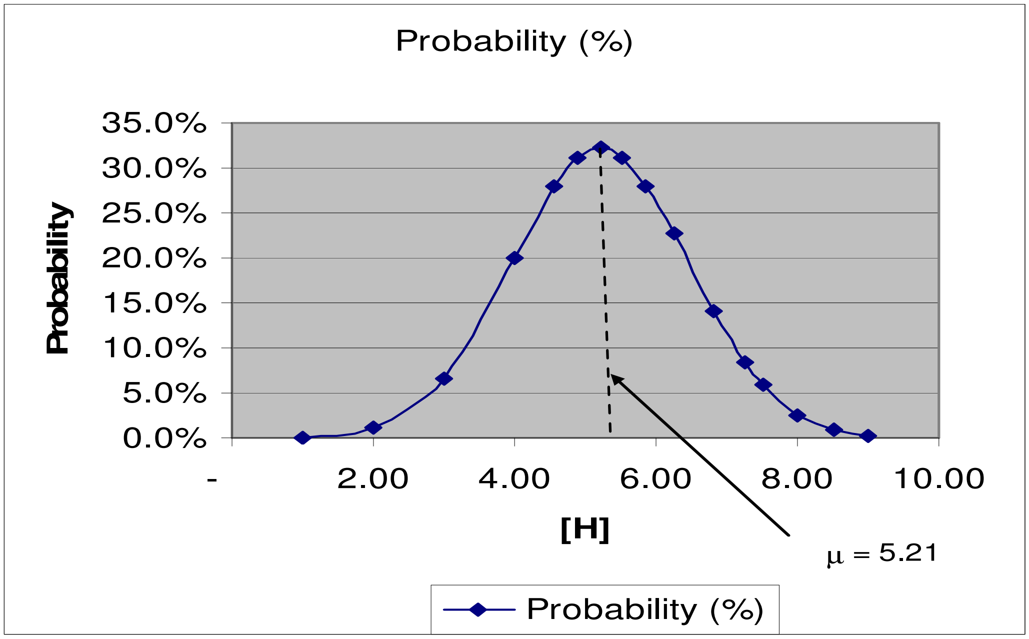

Fig 4.5: Probability Distribution of hydrogen in coal

3) Probability Inverse Value: - It is required to determine the *x*-value corresponding to a cumulative probability of 50%. This is normally achieved by finding the inverse function of the probability distribution function, i.e. $f^{-1}(x, \mu, \sigma)$, where $f(x, \mu, \sigma) = 1/\sqrt{(2\pi\sigma)}\exp\text{-}\{(x - x^m)^2/2\sigma^2$. However, by using MS-Excel GOALSEEK in conjunction with, Normal Probability Distr. = NORMDIST(x, μ, σ, cumulative) the process can be short-circuited. In this way, the average concentration of hydrogen in coal at a cumulative probability of 50% (NORMDIST(*x*, 5.21, 1.24, TRUE) = 50%) is found to be 5.21%. This is identical to the mean (μ) of the probability distribution and the chief reason for this is that P[f(*x*, μ, σ)] is a symmetrical distribution (Fig 4.5)

Therefore, the stochastic (average) concentration of hydrogen in coal is 5.21%

4.2.4.2 Constraints and Limitations

Constraints and Limitations can now be formulated or defined for the different production centres as follows (Key constraint equations and limits are **emboldened**):

A) Ammonia Production
Chemical Reaction: $N_2 + 3H_2 \leftrightarrow 2NH_3$

1) No 2 Ammonia (180 tons/day; 2.2 bar)

Overall Mass Balance: $\mathbf{A_2 + C_2 = R_2 + G_2 + (N2)}$
Nitrogen Balance: $0.75A_2 = 0.82(N2)$
Where N_2 mass fraction in Air = 75%
Where N_2 mass fraction in Ammonia = 82%
$\therefore$ $\mathbf{(N2) = 0.915A_2}$

Hydrogen Balance: $0.0521C_2 = (0.18)(N2)$
(*Stochastics 4.2.5.1*) Or $\mathbf{(N2) = 0.289C_2}$

Residual coal (R_2) $\mathbf{R_2 = 0.92C_2 + 0.05A_2}$
Gas Discharge (G_2) $\mathbf{G_2 = 0.08C_2 + 0.95A_2}$
} Approximations

Production Limitation: $\mathbf{(N2) \leq 180}$ **tons/day**

(N2) Ammonia Distribution: $\mathbf{(N2) = (N2)_S + (N2)_7 + (N2)_{ANS1}}$

2) No 4 Ammonia (1,000 tons/day; 6.0 bar)

Overall Mass Balance: $\mathbf{A_4 + C_4 = R_4 + G_4 + (N4)}$
Nitrogen Balance: $0.75A_4 = 0.82(N4)$
Where N_4 mass fraction in Air = 75%
Where N_4 mass fraction in Ammonia = 82%
$\therefore$ $\mathbf{(N4) = 0.915A_4}$

Hydrogen Balance: $0.0521C_4 = (0.18)(N4)$
(*Stochastics 4.2.4.1*) Or $\mathbf{(N4) = 0.289C_4}$

Residual coal (R_i) $\mathbf{R_4 = 0.92C_4 + 0.05A_4}$
Gas Discharge (G_i) $\mathbf{G_4 = 0.08C_4 + 0.95A_4}$
} Approximations

Production Limitation: $\mathbf{(N4) \leq 1{,}000}$ **tons/day**

No 4 Ammonia Distribution: $\mathbf{(N4) = (N4)_S + (N4)_9 + (N4)_{10} + (N4)_{11} + (N4)_{ANS2}}$

B) Nitric Acid Production
Chemical Reactions:

Oxidation: $5O_2 + 4NH_3 \leftrightarrow 4NO + 6H_2O$
Absorption: $2O_2 + 4NO \leftrightarrow 4NO_2$
Distillation: $4NO_2 + 4H_2O \leftrightarrow 4HNO_3 + 2H_2$

1) No 7 *POP* (55%) Nitric Acid (90 tons/day, 4.2 bar)

Overall Mass Balance: $\boldsymbol{(N2)_7 + A_7 + h_7 = T_7 + (HN)_7}$
Water Requirement: Water in final product – water produced in reaction
$h_7 = 0.45(HN)_7 - (6/4)[0.55(HN)_7/32](10)$
$= (0.45 - 0.258)(HN)_7 \Rightarrow$
$\boldsymbol{h_7 = 0.192(HN)_7}$
Tailgas: $\boldsymbol{T_7 = 0.79A_7}$
Molar equality: $NH_3/(HNO_3)$: $(N2)_7/10 = 0.55*((HN)_7/32) \Rightarrow$
$\boldsymbol{(N2)_7 = 0.172(HN)_7}$
Production Limitation: $\boldsymbol{(HN)_7 \leq 90}$ tons/day

2) No 9 *POP* (60%) Nitric Acid (275 tons/day, 8.7 bar)

Overall Mass Balance: $\boldsymbol{(N4)_9 + A_9 + h_9 = T_9 + (HN)_9}$
Water Requirement: Water in final product – water produced in reaction
$H_9 = 0.40(HN)_9 - (6/4)[0.6(HN)_9/32](10)$
$= (0.4 - 0.281)(HN)_9 \Rightarrow$
$\boldsymbol{h_9 = 0.119(HN)_9}$
Tailgas: $\boldsymbol{T_9 = 0.79A_9}$
Molar equality: $NH_3/(HNO_3)$: $(N4)_9/10 = 0.60*((HN)_9/32) \Rightarrow$
$\boldsymbol{(N4)_9 = 0.188(HN)_9}$
Production Limitation: $\boldsymbol{(HN)_9 \leq 275}$ tons/day

3) No 10 *POP* (60%) Nitric Acid (295 tons/day, 8.0 bar)

Overall Mass Balance: $\boldsymbol{(N4)_{10} + A_{10} + h_{10} = T_{10} + (HN)_{10}}$
Water Requirement: Water in final product – water produced in reaction
$h_{10} = 0.40(HN)_{10} - (6/4)[0.6(HN)_{10}/32](10)$
$= (0.4 - 0.281)(HN)_{10} \Rightarrow$
$\boldsymbol{h_{10} = 0.119(HN)_{10}}$
Tailgas: $\boldsymbol{T_{10} = 0.79A_{10}}$
Molar equality: $NH_3/(HNO_3)$: $(N4)_{10}/10 = 0.60*((HN)_{10}/32) \Rightarrow$
$\boldsymbol{(N4)_{10} = 0.188(HN)_{10}}$
Production Limitation: $\boldsymbol{(HN)_{10} \leq 295}$ **tons/day**

4) No 11 *DPOP* (60%) Nitric Acid (695 tons/day, 4.0 & 8.0 bar)

Overall Mass Balance: $\boldsymbol{(N4)_{11} + A_{11} + h_{11} = T_{11} + (HN)_{11}}$
Water Requirement: Water in final product – water produced in reaction
$h_{11} = 0.40(HN)_{11} - (6/4)[0.6(HN)_{11}/32](10)$
$= (0.4 - 0.281)(HN)_{11} \Rightarrow$
$\boldsymbol{h_{11} = 0.119(HN)_{11}}$
Tailgas: $\boldsymbol{T_{11} = 0.79A_{11}}$
Molar equality: $NH_3/(HNO_3)$: $(N4)_{11}/10 = 0.60^*((HN)_{11}/32) \Rightarrow$
$\boldsymbol{(N4)_{11} = 0.188(HN)_{11}}$
Production Limitation: $\boldsymbol{(HN)_{11} \leq 695}$ tons/day

5) Nitric Acid Distribution

55% Nitric Acid: $\boldsymbol{(HN)_7 = (HN)_{55}^S + (HN)_{ANS1}}$
60% Nitric Acid: $\boldsymbol{(HN)_9 + (HN)_{10} + (HN)_{11} = (HN)_{60}^S + (HN)_{ANS2}}$

C) 92% and 88% Ammonium Nitrate Solution (*ANS*) Production
Chemical Reaction: $NH_3 + HNO_3 \rightarrow NH_4NO_3$

1) No 1 *ANS*

Overall Mass Balance: $\boldsymbol{(HN)_{ANS1} + (N2)_{ANS1} = (ANS)_1 + (WV)_{ANS1}}$
Molar equality: $NH_3/(NH_4NO_3)$: $(N2)_{ANS1}/10 = 0.88^*((ANS)_1/42) \Rightarrow$
$\boldsymbol{(N2)_{ANS1} = 0.209(ANS)_1}$
Molar equality: $HNO_3/(NH_4NO_3)$: $0.55(HN)_{ANS1}/32 = 0.88^*((ANS)_1/42) \Rightarrow$
$\boldsymbol{(HN)_{ANS1} = 1.219(ANS)_1}$
Nitrogen Balance $0.55(7/32)(HN)_{ANS1} + (7/10)(N2)_{ANS1} =$
$0.88(14/42)(ANS)_1 \Rightarrow$
$0.12(HN)_{ANS1} + 0.7(N2)_{ANS1} = 0.293(ANS)_1$
$\boldsymbol{0.41(HN)_{ANS1} + 2.39(N2)_{ANS1} = (ANS)_1}$
Production Limitation: $\boldsymbol{(ANS)_1 \leq 350}$ tons/day

2) No 2 *ANS*

Overall Mass Balance: $\boldsymbol{(HN)_{ANS2} + (N4)_{ANS2} = (ANS)_2 + (WV)_{ANS2}}$
Molar equality: $NH_3/(NH_4NO_3)$: $(N4)_{ANS2}/10 = 0.92^*((ANS)_1/42) \Rightarrow$
$\boldsymbol{(N4)_{ANS2} = 0.219(ANS)_2}$
Molar equality: $HNO_3/(NH_4NO_3)$: $0.6(HN)_{ANS2}/32 = 0.92^*((ANS)_2/42) \Rightarrow$
$\boldsymbol{(HN)_{ANS2} = 1.168(ANS)_2}$
Nitrogen Balance $0.6(7/32)(HN)_{ANS2} + (7/10)(N2)_{ANS2} =$
$0.92(14/42)(ANS)_2 \Rightarrow$
$0.13(HN)_{ANS2} + 0.7(N2)_{ANS2} = 0.31(ANS)_2 \Rightarrow$
$\boldsymbol{0.427(HN)_{ANS2} + 2.28(N2)_{ANS2} = (ANS)_2}$
Production Limitation: $\boldsymbol{(ANS)_2 \leq 650}$ tons/day

3) 88% *ANS* Distribution

$$(ANS)_1 = (ANS)_S^{88} + (ANS)_{AN1} + (ANS)_{AN2} + (ANS)_{AN3}$$

4) 92% *ANS* Distribution

$$(ANS)_2 = (ANS)_{LAN} + (ANS)_{AN4} + (ANS)_S^{92}$$

D) Ammonium Nitrate (*AN*) Production

Evaporative Process: $NH_4NO_3.H_2O \rightarrow NH_4NO_3 + H_2O$

1) No 1 *AN*

Overall Mass Balance: $(ANS)_{AN1} = (AN)_{AN1} + (WV)_{AN1}$

Prill Tower Water Ejection: $(WV)_{AN1} = 0.12(ANS)_{AN1}$

Ammonium Nitrate Bal: $(AN)_{AN1} = 0.88(ANS)_{AN1}$

Production Limitation: $(AN)_{AN1} \leq 75$ tons/day

2) No 2 *AN*

Overall Mass Balance: $(ANS)_{AN2} = (AN)_{AN2} + (WV)_{AN2}$

Prill Tower Water Ejection: $(WV)_{AN2} = 0.12(ANS)_{AN2}$

Ammonium Nitrate Bal: $(AN)_{AN2} = 0.88(ANS)_{AN2}$

Production Limitation: $(AN)_{AN2} \leq 125$ tons/day

3) No 3 *AN*

Overall Mass Balance: $(ANS)_{AN3} = (AN)_{AN3} + (WV)_{AN3}$

Prill Tower Water Ejection: $(WV)_{AN3} = 0.12(ANS)_{AN3}$

Ammonium Nitrate Bal: $(AN)_{AN3} = 0.88(ANS)_{AN3}$

Production Limitation: $(AN)_{AN3} \leq 125$ tons/day

4) No 4 *AN*

Overall Mass Balance: $(ANS)_{AN4} = (AN)_{AN4} + (WV)_{AN4}$

Prill Tower Water Ejection: $(WV)_{AN3} = 0.08(ANS)_{AN3}$

Ammonium Nitrate Bal: $(AN)_{AN4} = 0.92(ANS)_{AN4}$

Production Limitation: $(AN)_{AN4} \leq 200$ tons/day

5) Ammonium Nitrate Distribution

$$(AN)_{AN1} + (AN)_{AN2} + (AN)_{AN3} + (AN)_{AN4} = (AN)_S$$

E) Limestone Ammonium Nitrate (*LAN*) Production

Physical Process: $NH_4NO_3.H_2O + (Ca/Mg)CO_3 \rightarrow LAN + H_2O$

Overall Mass Balance: $(ANS)_{LAN} + L = (LAN) + (WV)_{LAN}$

Ammonium Nitrate Bal: $0.92(ANS)_{LAN} = 0.975(LAN)$

Limestone Balance: $L = 0.025(LAN)$

Production Limitation: $(LAN) \leq 450$ tons/day

4.3. MSFMO Program

<u>Objective Functions</u>:

1) Maximise financial gross profit (*GP*) from the production and sales of Ammonia (NH_3), Nitric Acid (HNO_3), Ammonium Nitrate Solution (NH_4NO_3/H_2O), Ammonium Nitrate (NH_4NO_3) and Limestone Ammonium Nitrate (LAN):

$$\text{Max } [(GP)_{NH3}((N2)_s + (N4)_s) + (GP)^{55}{}_{HNO3}(\mathrm{HN})_S{}^{55} + (GP)^{60}{}_{HNO3}(\mathrm{HN})_S{}^{60} + (GP)_{ANS}(ANS)_S + (GP)_{AN}(AN)_S + P_{LAN}(LAN)_{PS}]$$

$$= \text{Max } [45(N2)_s + 75(N4)_s + 95(\mathrm{HN})_S{}^{55} + 125(\mathrm{HN})_S{}^{60} + 125(ANS)_S + 175(AN)_S + 95(LAN)_S]$$

2) Minimise the chief effluent flows in the production plants, notably tailgas from the Nitric Acid plants (NO/NO_2):

$$\text{Min } [(EEP)_7 + (EEP)_9 + (EEP)_{10} + (EEP)_{11}]$$

$$= \text{Min}[0.0746(HN)_7{}^2 - 11.16(HN)_7 + 461.39 + 0.013(HN)_9{}^2 - 7.130(HN)_9 + 1099.7 + 0.034(HN)_{10}{}^2 - 18.309(HN)_{10} + 2675.2 + 0.0064(HN)_{11}{}^2 - 7.765(HN)_{11} + 2416.6]$$

$$= \text{Min}[0.0746(HN)_7{}^2 - 11.16(HN)_7 + 461.39 + 0.013(HN)_9{}^2 - 7.130(HN)_9 + 1099.7 + 0.034(HN)_{10}{}^2 - 18.309(HN)_{10} + 2675.2 + 0.0064(HN)_{11}{}^2 - 7.765(HN)_{11} + 2416.6]$$

Subject to Common Constraints and Limitations (Table 4.7)::

T4.7 Constraints and Limitations

$A_2 + C_2 = R_2 + G_2 + (N2)$	$(N2) = 0.915A_2$
$(N2) = 0.289C_2$	$R_2 = 0.92C_2 + 0.05A_2$
$G_2 = 0.08C_2 + 0.95_2$	$(N2) = (N2)_S + (N2)_7 + (N2)_{ANS1}$
$A_4 + C_4 = R_4 + G_4 + (N4)$	$(N4) = 0.915A_4$
$(N4) = 0.289C_4$	$R_4 = 0.92C_4 + 0.05A_4$
$G_4 = 0.08C_4 + 0.95A_4$	$(N4) = (N4)_S + (N4)_9 + (N4)_{10} + (N4)_{11} + (N4)_{ANS2}$
$(N2)_7 + A_7 + h_7 = T_7 + (HN)_7$	$h_7 = 0.192(HN)_7$
$T_7 = 0.79A_7$	$(N2)_7 = 0.172(HN)_7$
$(N4)_9 + A_9 + h_9 = T_9 + (HN)_9$	$h_9 = 0.119(HN)_9$
$T_9 = 0.79A_9$	$(N4)_9 = 0.188(HN)_9$
$(N4)_{10} + A_{10} + h_{10} = T_{10} + (HN)_{10}$	$h_{10} = 0.119(HN)_{10}$
$T_{10} = 0.79A_{10}$	$(N4)_{10} = 0.188(HN)_{10}$
$(N4)_{11} + A_{11} + h_{11} = T_{11} + (HN)_{11}$	$h_{11} = 0.119(HN)_{11}$
$T_{11} = 0.79A_{11}$	$(N4)_{11} = 0.188(HN)_{11}$
$(HN)_7 = (HN)_{55}{}^S + (HN)_{ANS1}$	$(HN)_9 + (HN)_{10} + (HN)_{11} = (HN)_{60}{}^S + (HN)_{ANS2}$
$(HN)_{ANS1} + (N2)_{ANS1} = (ANS)_1 + (WV)_{ANS1}$	$(N2)_{ANS1} = 0.209(ANS)_1$
$(HN)_{ANS1} = 1.219(ANS)_1$	$(WV)_{ANS1} = 0.45(HN)_{ANS1} – 0.12(ANS)_1$
$0.41(HN)_{ANS1} + 2.39(N2)_{ANS1} = (ANS)_1$	$(HN)_{ANS2} + (N4)_{ANS2} = (ANS)_2 + (WV)_{ANS2}$
$(N4)_{ANS2} = 0.219(ANS)_2$	$(HN)_{ANS2} = 1.168(ANS)_2$
$(WV)_{ANS2} = 0.4(HN)_{ANS2} – 0.08(ANS)_2$	$0.427(HN)_{ANS2} + 2.28(N2)_{ANS2} = (ANS)_2$
$(ANS)_1 = (ANS)_S{}^{88} + (ANS)_{AN1} + (ANS)_{AN2} + (ANS)_{AN3}$	$(ANS)_2 = (ANS)_{LAN} + (ANS)_{AN4} + (ANS)_S{}^{92}$
$(ANS)_S = (ANS)_S{}^{88} + (ANS)_S{}^{92}$	$(ANS)_{AN1} = (AN)_{AN1} + (WV)_{AN1}$
$(WV)_{AN1} = 0.12(ANS)_{AN1}$	$(AN)_{AN1} = 0.88(ANS)_{AN1}$
$(ANS)_{AN2} = (AN)_{AN2} + (WV)_{AN2}$	$(WV)_{AN2} = 0.12(ANS)_{AN2}$
$(AN)_{AN2} = 0.88(ANS)_{AN2}$	$(ANS)_{AN3} = (AN)_{AN3} + (WV)_{AN3}$
$(WV)_{AN3} = 0.12(ANS)_{AN3}$	$(AN)_{AN3} = 0.88(ANS)_{AN3}$
$(ANS)_{AN4} = (AN)_{AN4} + (WV)_{AN4}$	$(WV)_{AN3} = 0.08(ANS)_{AN3}$
$(AN)_{AN4} = 0.92(ANS)_{AN4}$	$(AN)_{AN1} + (AN)_{AN2} + (AN)_{AN3} + (AN)_{AN4} = (AN)_S$
$(ANS)_{LAN} + L = (LAN) + (WV)_{LAN}$	$0.92(ANS)_{LAN} = 0.975(LAN)$
$L = 0.025(LAN)$	$(N2) \leq 180$
$(N4) \leq 1{,}000$	$(HN)_7 \leq 90$
$(HN)_9 \leq 275$	$(HN)_{10} \leq 295$
$(HN)_{11} \leq 695$	$(ANS)_1 \leq 350$
$(ANS)_2 \leq 650$	$(AN)_{AN1} \leq 75$
$(AN)_{AN2} \leq 125$	$(AN)_{AN3} \leq 125$
$(AN)_{AN4} \leq 200$	$(LAN) \leq 450$
$(N2) – (N2)_S \geq 0$	$(N4) – (N4)_S \geq 0$

4.3.1. MSFMO Model Solutions per Objective Function

T4.8 Optimum Solutions - Maximised Gross Profit and Minimised Effluent Discharge – Summary of Results

OBJECTIVE 1 - MAXIMISING GROSS PROFIT				OBJECTIVE 2 - MINIMISING EFFLUENT			
Decision Variable	Optimum Value	Decision Variable	Optimum Value	Decision Variable	Optimum Value	Decision Variable	Optimum Value
Optimum Gross Profit = R249,775				Optimum *EEP* = 438			
Corresponding *EEP* = 527				Corresponding Gross Profit = R233,971			
A_2	197	$(N2)_{ANS1}$	-	A_2	197	$(N2)_{ANS1}$	-
C_2	623	$(ANS)_1$	-	C_2	623	$(ANS)_1$	-
$(R)_2$	583	$(WV)_{ANS1}$	-	$(R)_2$	583	$(WV)_{ANS1}$	-
G_2	57	$(HN)_{ANS2}$	-	G_2	57	$(HN)_{ANS2}$	-0
$(N2)$	180	$(N4)_{ANS2}$	-	$(N2)$	180	$(N4)_{ANS2}$	0
A_4	886	$(ANS)_2$	-	A_4	886	$(ANS)_2$	-0
C_4	3,460	$(WV)_{ANS2}$	-	C_4	3,460	$(WV)_{ANS2}$	0
$(R)_4$	3,228	$(ANS)_{AN1}$	-	$(R)_4$	3,228	$(ANS)_{AN1}$	0
G_4	118	$(AN)_{AN1}$	-	G_4	118	$(AN)_{AN1}$	-0
$(N4)$	1,000	$(WV)_{AN1}$	-	$(N4)$	1,000	$(WV)_{AN1}$	-0
$(N2)_7$	16	$(ANS)_{AN2}$	-	$(N2)_7$	13	$(ANS)_{AN2}$	0
A_7	272	$(AN)_{AN2}$	-	A_7	226	$(AN)_{AN2}$	-
h_7	17	$(WV)_{AN2}$	-	h_7	14	$(WV)_{AN2}$	0
T_7	215	$(ANS)_{AN3}$	-	T_7	179	$(ANS)_{AN3}$	-0
$(HN)_7$	90	$(AN)_{AN3}$	-	$(HN)_7$	75	$(AN)_{AN3}$	-0
$(N4)_9$	52	$(WV)_{AN3}$	-	$(N4)_9$	52	$(WV)_{AN3}$	-0
A_9	908	$(ANS)_{AN4}$	-	A_9	905	$(ANS)_{AN4}$	0
h_9	33	$(AN)_{AN4}$	-	h_9	33	$(AN)_{AN4}$	0
T_9	717	$(WV)_{AN4}$	-	T_9	715	$(WV)_{AN4}$	0
$(HN)_9$	275	$(ANS)_{LAN}$	-	$(HN)_9$	274	$(ANS)_{LAN}$	-
$(N4)_{10}$	55	(LAN)	-	$(N4)_{10}$	51	(LAN)	-
A_{10}	974	L	-	A_{10}	889	L	-
h_{10}	35	$(WV)_{LAN}$	-	h_{10}	32	$(WV)_{LAN}$	-
T_{10}	769	$(N2)_S$	180	T_{10}	702	$(N2)_S$	180
$(HN)_{10}$	295	$(N4)_S$	1,000	$(HN)_{10}$	269	$(N4)_S$	1,000
$(N4)_{11}$	131	$(HN)_S^{55}$	90	$(N4)_{11}$	114	$(HN)_S^{55}$	75
A_{11}	2,294	$(HN)_S^{60}$	1,265	A_{11}	2,002	$(HN)_S^{60}$	1,150
h_{11}	83	$(ANS)_S^{92}$	-	h_{11}	72	$(ANS)_S^{92}$	0
T_{11}	1,812	$(ANS)_S^{88}$	-	T_{11}	1,582	$(ANS)_S^{88}$	0
$(HN)_{11}$	695	$(AN)_S$	-	$(HN)_{11}$	607	$(AN)_S$	-0
$(HN)_{ANS1}$	-			$(HN)_{ANS1}$	-		

4.3.2. Determination of Upper (U_k) and Lower Bounds (L_k)

According to the MSFMO procedure, once the optimum values of both the Objective Functions have been determined, the requirement is to determine the values of both the Objective Functions at the other function's decision variable set and label them U_k *(upper bound value = 'worst' value – In the case of a maximum objective, the 'worst' value equates to the lowest compared to all the other Objective Functions, whereas in the case of a minimum objective, the 'worst' value equates to the highest value compared to all the other objective functions*) and L_k (*lower bound value – vice versa of U_k*) per Objective Function accordingly. This is shown in Table 4.9:

T4.9 Upper (U_k) and Lower (L_k) Bound Optimum Values

Objective (*k*)	Nature	L_k ('Lower')	U_k ('Upper')
1	Max	233,971	249,775
2	Min	527	438

Once the upper and lower bound values have been determined, the requirement is to determine the Aspiration Level Functions (λ_k), which may then be optimised with the highest value one determining the final solution set.

4.3.3. Generation of Aspiration Level Functions (λ_k)

According to BIT et al (1993), the Aspiration Level Function per Objective Function (*k*) is defined as follows:

$\lambda_k = (U_k – Z_k)/(U_k – L_k)$

$\lambda_k = (U_k – Z_k)/(U_k – L_k)$

$\lambda_1 = \{234827 - [45_{NH3}(N2)_s + 75(N4)_s + 95(HN)_S^{55} + 125(HN)_S^{60} + 125(ANS)_S + 350(AN)_S + 200(LAN)_{PS}]\}/(234827 – 218788)$

$= \{234827 - [45_{NH3}(N2)_s + 75(N4)_s + 95(HN)_S^{55} + 125(HN)_S^{60} + 125(ANS)_S + 350(AN)_S + 200(LAN)_{PS}]\}/16039$

Therefore $\lambda_1 = 14.64 - 0.0028(N2)_s - 0.0047(N4)_s - 0.006(HN)_S^{55} - 0.0078(HN)_S^{60} – 0.0078(ANS)_S - 0.022(AN)_S - 0.012(LAN)_{PS}$

Similarly:

$\lambda_2 = \{526.47 - [0.0746(HN)_7^2 - 11.16(HN)_7 + 0.0064(HN)_9^2 - 7.765(HN)_9 + 0.034(HN)_{10}^2 - 18.309(HN)_{10} + 0.0064(HN)_{11}^2 - 7.765(HN)_{11} + 6652.7]/(526.47 - 436.85)$

$= \{526.47 - [0.0746(HN)_7^2 - 11.16(HN)_7 + 0.0064(HN)_9^2 - 7.765(HN)_9 + 0.034(HN)_{10}^2 - 18.309(HN)_{10} + 0.0064(HN)_{11}^2 - 7.765(HN)_{11} + 6652.7]/(89.62)$

$= \{5.87 - 0.00083(HN)_7^2 + 0.125(HN)_7 - 0.00007(HN)_9^2 + 0.0869(HN)_9 - 0.00038(HN)_{10}^2 + 0.204(HN)_{10} - 0.00007(HN)_{11}^2 + 0.0866(HN)_{11} - 74.232\}$

Therefore $\lambda_2 = -68.362 - 0.00083(HN)_7^2 + 0.125(HN)_7 - 0.00007(HN)_9^2 + 0.0866(HN)_9 + 0.00038(HN)_{10}^2 + 0.204(HN)_{10} - 0.00007(HN)_{11}^2 + 0.0866(HN)_{11}$

4.3.4. Maximisation of Aspiration Level Functions

According to BIT *et al* (1993), the procedure for maximising Aspiration Level Functions is identical to that for optimising the constituent objective functions. In other words:

a) Derive/define the objective functions, - λ_1 and λ_2
b) Define the constraints, which are given in Table 4.7
c) Specify the limits, which are also shown in Table 4.7
d) Populate the MS-Excel Solver program accordingly
e) Optimise the program – run Excel Solver
f) Display the results, which are summarised in Tables 4.10 and 4.11

T4.10 MSFMO Optimum Decision variables

Max (λ_1) = 14.64			
Max (λ_2) = 49.1			
Decision Variable	Optimum Value	Decision Variable	Optimum Value
Optimum Gross Profit = R248,379			
Corresponding *EEP* = 510			
A_2	197	$(N2)_{ANS1}$	-
C_2	623	$(ANS)_1$	-
$(R)_2$	583	$(WV)_{ANS1}$	-
G_2	57	$(HN)_{ANS2}$	-
$(N2)$	180	$(N4)_{ANS2}$	-
A_4	886	$(ANS)_2$	-
C_4	3,460	$(WV)_{ANS2}$	-
$(R)_4$	3,228	$(ANS)_{AN1}$	-
G_4	118	$(AN)_{AN1}$	-
$(N4)$	1,000	$(WV)_{AN1}$	-
$(N2)_7$	13	$(ANS)_{AN2}$	-
A_7	228	$(AN)_{AN2}$	-
h_7	14	$(WV)_{AN2}$	-
T_7	180	$(ANS)_{AN3}$	-
$(HN)_7$	75	$(AN)_{AN3}$	-
$(N4)_9$	52	$(WV)_{AN3}$	-
A_9	908	$(ANS)_{AN4}$	-
h_9	33	$(AN)_{AN4}$	-
T_9	717	$(WV)_{AN4}$	-
$(HN)_9$	275	$(ANS)_{LAN}$	-
$(N4)_{10}$	55	(LAN)	-
A_{10}	974	L	-
h_{10}	35	$(WV)_{LAN}$	-
T_{10}	769	$(N2)_S$	180
$(HN)_{10}$	295	$(N4)_S$	1,000
$(N4)_{11}$	131	$(HN)_S^{55}$	75
A_{11}	2,294	$(HN)_S^{60}$	1,265
h_{11}	83	$(ANS)_S^{92}$	-
T_{11}	1,812	$(ANS)_S^{88}$	-
$(HN)_{11}$	695	$(AN)_S$	-
$(HN)_{ANS1}$	-		

T4.11 Summary of MSFMO Optimum Results

Maximise Gross Profit and minimise *EEP*	
Maximum Objective Function: 1 - Total Gross Profit (Z_1) Minimum Objective Function: 2 - Total *EEP* (Z_2)	248,379 510
Max. Aspiration Level Function: 1 (λ_1) Max. Aspiration Level Function: 2 (λ_2)	14.64 49.1

4.3.5. Select the highest Aspiration Level Value

According to BIT *et al* (1993), the optimum solution for a multi-objective program is the solution set associated with the highest Aspiration Level Value and in this case, that is $\lambda_i = \lambda_2 = 49.1$.

4.3.6. Final MSFMO Optimum Solution

As can be seen from table 4.10, the Dual Objective Holistic (multi-sub-objective, stochastic, fuzzy, Minmax) optimum solution for the maximum gross production profit and minimum effluent discharge for an Ammonia and Nitrogen-derivatives (Nitric Acid, Ammonium Nitrate Solution, Ammonium Nitrate and Limestone Ammonium Nitrate) production facility is shown in Table 4.12:

T4.12 Optimised Production and Effluent Discharge

Objective Function (X_i)	**Category**	**Nature (Max/Min)**	**Result**
Z_1	Chemical Production – Gross Profit	Maximum	R248,379/day
Z_2	*EEP*	Minimum	510

The associated optimum solution set, x_i is shown in Table 4.7

4.3.6.1 Assessment of the Optimum Gross Profit of Production

According to the program solution, the optimum gross profit of production is R248, 379/day. This can be evaluated by comparing it with actual average values in Table 4.13

T4.13 Actual versus Optimum Production and Corresponding Gross Profit Figures

Product	Gross Profit (R/ton)	Actual Average Product Provision (t/day)	Actual Average Daily Gross Profit (R/day)	Optimum Product Provision (t/day)	Optimum Daily Gross Profit (R/day)
(N2)s	45	35	1,575	180	8,100
(N4)s	75	60	4,500	1000	75,000
$(HN)_S^{55}$	95	25	2,375	75	7,125
$(HN)_S^{60}$	125	45	5,625	1,265	158,125
(ANS)s	125	25	3,125		-
(AN)s	175	680	119,000		-
(LAN)	95	550	52,250		-
Total			188,450		248,350*

+ The difference between this calculated Gross Profit figure of R248,350 and the Optimised Gross Production figure of R248,379 is due to rounding errors.

It is interesting to note that under the Optimum Gross Profit scenario, neither Ammonium Nitrate nor Ammonium Nitrate Solution nor was Limestone Ammonium Nitrate sales realised, but that 60% Nitric Acid sales were extremely high. This would not be the case if an Optimum Demand study was done in parallel with this Optimum Supply analysis

4.3.6.2 Translation of the Optimum EEP Factor – Minimum Effluent

The *EEP* factor was defined in 4.2.3.2 as:

EEP (efficiency/effluent product) = R_e x [NOx];

Now the optimum EEP factor was determined to be 527 and this translates into a NOx concentration of 580 ppm as summarised in Table 4.14:

T4.14 *EEP*/NOx Conversion Table

Nitric Acid Plant	Optimum Production (t/day)	Corresponding Plant Efficiency
7	-	-
9	275	95.0%
10	295	87.5%
11	695	90.5%
Average Efficiency		90.8%
Optimum *EEP*		527
Corresponding NOx Effluent (ppm)		580

4.3.7. Discussion

The principal remarks pertaining to this holistic optimisation exercise relate to the comparison of these optimum results (580 ppm, R240, 837) against those of the actual production facility. The difficulty with this is that actual production gross profit and *NOx* effluent discharge figures are not available for confidentiality reasons, but a comparison of the nature of the actual plant data with the optimum solution set gives credence to the optimum objective values presented. For example the approximate NOx effluent discharge figures are shown in Table 4.15

T4.15 Actual NOx Discharge per *NA* Plant

NITRIC ACID PLANT	ACTUAL NOX DISCHARGE (PPM)
7	140
9	122
10	395
11	80
Total	737

The optimum effluent discharge figure was determined to be 580 ppm, which is 21% lower than the actual figure of 737 ppm.

Apart from the optimum objectives, a summary of all the optimum operating results is shown in Table 4.16

T4.16 Actual Plant Operational Status

Chemical Plant	Optimum Status	Typical Operational Status
No. 2 Ammonia	Live – 180 t/day	Live – 180 t/day
No. 4 Ammonia	Live – 1,000 t/day	Live – 1,000 t/day
Ammonia Sales	35 t/day	60 t/day
No. 7 *NA*	Offline	Live 90 t/day
No. 9 *NA*	Live – 275 t/day	Live – 275 t/day
No. 10 *NA*	Live – 295 t/day	Live – 295 t/day
No. 11 *NA*	Live – 695 t/day	Live – 720 t/day
55% Nitric Acid Sales	25 t/day	25 t/day
60% Nitric Acid Sales	1,265 t/day	50 t/day
No. 1 *ANS*	Offline	Live – 350 t/day
No. 2 *ANS*	Live – 84 t/day	Live – 650 t/day
No. 1 *AN*	Live – 31 t/day	Live – 75 t/day
No. 2 *AN*	Offline	Live – 125 t/day
No. 3 *AN*	Offline	Live – 240 t/day
No. 4 *AN*	Offline	Live – 240 t/day
LAN	Offline	Live - 550 t/day

Another interesting point is that the optimisation procedure has determined an operational status of the production plants that is not totally consistent with actual practise at the time, which is not surprising for the following reasons:

a) The production and sales facilities had never before been subjected to an Optimisation exercise.
b) There are frequently many varied factors which influence production and sales that were not or could not be taken into account in such an Optimisation exercise, e.g. labour unrest, availability of raw materials, business priorities, state of the market, political situation etc. It is

entirely possible to conduct such a comprehensive Optimisation exercise but that would fall way beyond the scope of this exercise.

It is also interesting to note that for the Maximum Gross Profit of Production and the Minimum Effluent scenarios as well as the final Minmax optimisation scenario that the sale of 60% Nitric Acid was repeatedly maximised (~ 1,265 t/day) to the exclusion of the downstream production and sale of other Nitrogen-derivatives like Ammonium Nitrate and Limestone Ammonium Nitrate. This quantity of Nitric Acid sold could have been limited to a much lower figure (e.g. 60 tons/day), which would have definitely incurred the production and sales of the downstream nitrogen-derivatives but that would have defeated the purpose of this Optimisation exercise. This difficulty could be overcome by either decreasing the gross profit margin of Nitric Acid or by increasing the gross profit margins of the other downstream products or, lastly, by extending the Optimisation exercise to include a complementary holistic analysis of the local Explosives and Fertiliser markets.

4.3.8. MSFMO – Software Simulation

It was decided to develop a personal computer software program to effectively simulate and demonstrate the Holistic Optimisation of the Ammonia and Nitrogen-derivatives production facility. The software program was developed using Delphi 6.0 Professional. The reason for this is that Delphi is an excellent software development tool because it is object-oriented, powerful and flexible and logically straightforward and easy to use. The Delphi program code is available in Appendix A. The program follows the basic MSFMO development methodology and is shown below:

<u>Program Structure</u>

1) Introduction – Brief summary of MSFMO and its application
2) Flowchart – Fairly detailed flow diagram of the interrelated ammonia and nitrogen-derivative production facility.
3) Objectives: -
   a) Maximise Gross Production Profit
   b) Minimise total Effluent Discharge rate
4) MSFMO Program: -
   a) Decision Variables
   b) Objective Functions
   c) Constraints and Limitations
   d) Maximum Gross Profit Solution
   e) Minimum Effluent Solution
   f) Aspiration Level Functions
   g) Maximise Aspiration Levels
5) MSFMO Solution
6) Conclusion

<u>Software Installation</u>

The Delphi runtime program, ***MSFMO.exe***, together with a few associated MS-Excel files, Gross Profit.xls, MaxGP.xls, MinEff.xls, Decision Variables.xls, AspVariables.xls, Optimum Decision Variables.xls and U & L Values.xls has been provided on the attached 1.4 MB disk

The Delphi program, ***MSFMO.exe***, is typically installed on a *Windows* desktop as a Delphi *7* icon (it does not matter where this is installed) whereas all the MS-Excel files <u>must</u> be copied into the primary *Windows*, '*Documents and Settings*' folder.

Double-Click the Delphi 7 icon to start the program.

5. CONCLUSIONS AND RECOMMENDATION

5.1 Conclusions

There were two principal aims of this research:

a) The derivation of a Dual Objective Holistic (multi-sub-objective stochastic fuzzy Minmax) optimisation methodology that can be applied to most operational processes for the purpose of obtaining the most advantageous solutions

b) The successful application of this methodology into a complex, interrelated chemical production environment with multiple objectives, i.e. ammonia and nitrogen-derivatives (NH_3, HNO_3, NH_4NO_3) production

The derivation of a Dual Objective Holistic optimisation methodology was achieved in that the procedure was successfully derived and then, as discussed further below, successfully applied to a complex operational facility (ammonia and nitrogen-derivative production). Success with regard to both objectives could be measured in terms of the ease of use and accuracy of implementation as well as the realism of the results obtained (i.e. maximum production profit and minimum effluent discharge), both of which, as seen below, were very good.

The derivation procedure involved the extraction and subsequent integration of the 'Best' and appropriate component processes from separate and distinctive class (stochastic fuzzy multi-objective etc.) optimisation methodologies. The 'Best' component processes were regarded as those that were the most integrable, robust and reliable. This was not a particularly difficult procedure as most selected component processes were already integrable. The resulting Dual Objective Holistic optimisation methodology is a step-wise, easily implementable procedure.

Further, the application of the methodology to an Ammonia and Nitrogen-Derivatives Production facility consisting of an interrelated number of chemical plants (Nitric Acid, Ammonium Nitrate Solution, Ammonium Nitrate and Limestone Ammonium Nitrate) was successfully achieved. The main optimised results were as follows:

a) Maximum Daily Gross Profit of production = R240,837/day

b) NOx Tailgas effluent discharge = 527 ppm

These figures are not easily comparable with actual production statistics because of confidentiality but there is definitely an improvement in NOx discharge of which the total is often in excess of 1,200 ppm under normal plant operating conditions.

The following conclusions can be drawn from the work:
:

- The derivation of a Multi-sub-objective Stochastic Fuzzy Minmax optimisation methodology has been successfully accomplished.

- The creation of an *EEP* (Effluent/Efficiency Product) factor that enables the successful minimisation of a chemical plant's effluent discharge rate whilst simultaneously maintaining reasonable plant efficiency. An *EEP* versus production curve typically has a concave shape on all four Nitric Acid plants, which ideally lends itself to quadratic function emulation and consequent effluent minimisation procedures, whereas a typical effluent-only curve would not have such features.

- Minmax Capability enables one to successfully adapt a multiple objective minima or maxima procedural technique to a combinational maxima and minima scenario.

- A powerful Delphi program to simulate and demonstrate the Dual Objective Holistic optimisation of an Ammonia and Nitrogen-derivatives (i.e. HNO_3, NH_4NO_3 and Limestone Ammonium Nitrate) production facility has been developed.

- It was demonstrated that MS-Excel Solver is not only able to perform standard, fairly complex optimisation routines, but also to perform a complex combinational minimum/maximum optimisation scenario. Although MS-Excel Solver was originally designed to optimise linear programs, a complex polynomial objective function, e.g. the EEP_i function, was successfully optimised.

- Due to the complexity of the Multi-sub-objective Stochastic Fuzzy Minmax Optimisation program for Ammonia and Nitrogen-derivatives production and the nature of the MS-Excel Solver solution routine, it was vital that the mathematical modeling of the entire operation must be absolutely correct. The effect of any mistakes or errors in the program was greatly magnified in the final result. A procedure was developed whereby any changes to the program had to be integrated on a piecemeal basis otherwise the cause of any errors could not be determined.

In conclusion, the hypothesis:

'It should be possible to derive and apply a Dual Objective Holistic optimisation methodology in a complex, inter-related chemical production environment that involves conditions of multiple objectivity, uncertainty (fuzzy), probability (stochastics) and Minmax (simultaneous maxima and minima)', .

was successfully proven in that the methodology was successfully derived and then successfully applied to an interrelated ammonia and downstream nitrogen-derivatives production facility.

5.2 Recommendation

It is interesting to note that under the Optimum Gross Profit scenario, neither Ammonium Nitrate nor Ammonium Nitrate Solution nor was Limestone Ammonium Nitrate sales realised, but that 60% Nitric Acid sales were extremely high. This would not be the case if an Optimum Demand study was done in parallel with this Optimum Supply analysis

It would be extremely interesting and beneficial to extend the scope of this Dual Objective Holistic optimisation exercise to include a combinational Dual Objective Holistic (Multi-sub-objective Stochastic Fuzzy Minmax) Optimisation analysis of the Explosives and Fertiliser markets that this Ammonia and Nitrogen-derivatives Production facility supplied in the 1980's. If this were possible, a comprehensive business case (Profitability, ROI etc.) could be prepared.

This last route would be far preferable because, in this way, a realistic and comprehensive *business* analysis of a similar Explosives and Fertiliser enterprise could have been achieved. Such an exercise is outside the scope of this project but should be done to determine the viability of the business model.

5.3 Contributions to Science

An Dual Objective Holistic (Multi-sub-objective Stochastic Fuzzy Minmax - MSFM) Optimisation initiative, either the methodology derivation or the application itself, was not found after a comprehensive survey of the available literature in a number of related and associated areas.

The optimisation projects, uncovered in the literature survey, tended to be limited to Solo or Dual (combinatorial) optimisation initiatives, such as:

a) (Single Objective) Fuzzy Optimisation
b) Multiple Objective Fuzzy Optimisation
c) Stochastic Optimisation
d) Multiple Objective Stochastic Optimisation
e) Stochastic Fuzzy Optimisation
f) Multi-sub-objective Stochastic Fuzzy Optimisation
g) Minmax Fuzzy Optimisation

(*Note: Optimisation methodologies must either be single or multiple objective initiatives. If nothing is stated in this regard, then single objective is implie*d.)
However, the concept, derivation and application of truly Dual Objective Holistic (Multi-sub-objective Stochastic Fuzzy Minmax) Optimisation was never discovered.

Clearly therefore, an Dual Objective Holistic (MSFM) optimisation technique had never been applied to a chemical production operation before. In fact, little evidence could be found of even any partially holistic initiative in the chemical engineering industry and, therefore, this research would constitute one of the first attempts in this regard.

As part of the derivation and application of Dual Objective Holistic Multi-sub-objective Stochastic Fuzzy Minmax Optimisation in the chemical industry, this research initiative also necessitated the derivation of a proper, workable component 'Minmax' optimisation technique. In this regard, the approaches discovered during the literature survey were, generally, far too theoretical and simply not practical. Based on certain similarities with the Multi-sub-objective Optimisation technique, it was decided to derive a Minmax optimisation technique, using the former as a development template. The application results obtained indicated a successful derivation, and a significant contribution to the optimisation of any chemical production process or plant

6. SYMBOLS AND ABBREVIATIONS

The symbols and abbreviations used in this report are defined in Table 7.1

Table 7.1 Symbols and Abbreviations

Decision Variable	**Description**
Overall Definitions	
h	Total input distilled water for all process requirements
C	Total coal input for NH_3 Plants
A	Total input air for NH_3 Plants
R	Total coal residue and gas discharge from NH_3 Plants
Ammonia (NH_3) Production and Sales	
P_{NH3}	Selling Price per ton of NH_3
No 2 Ammonia Production Plant	
C_2	Input Coal for No 2 NH_3
$N2$	Total NH_3 produced from No. 2 NH_3 Plant
$(N2)_s$	Total NH_3 external sales from No 2 NH_3
A_2	Supply of air to No 2 NH_3
R_2	Coal residue from No 2 NH_3
G_2	CO/CO_2 discharge from No 2 NH_3
No 4 Ammonia Production Plant	
C_4	Input Coal for No 4 NH_3
$N4$	Total NH_3 produced from No. 4 NH_3 Plant
$(N4)_s$	Total NH_3 external sales from No 4 NH_3
A_4	Supply of air to No 4 NH_3
R_4	Coal residue from No 4 NH_3
G_4	CO/CO_2 discharge from No 4 NH_3
Nitric Acid Production and Sales	
P^{55}_{HNO3}	Selling price per ton 55% HNO_3
P^{60}_{HNO3}	Selling price per ton 60% HNO_3
$(HN)_S^{60}$	Sales of 55% HNO_3 from 7 *NA*
$(HN)_S^{55}$	Sales of 60% HNO_3 from 9, 10 & 11 *NA*
No 7 Nitric Acid Production Plant	
h_1	Distilled water for No 7 Nitric Acid Plant (7 *NA*)
$(N2)_7$	NH_3 produced from No 2 NH_3 going to No 7 *NA*
$(HN)_7$	Total 55% HNO_3 produced on No 7 *NA*
T_7	NO/NO_2 Tailgas discharge from No 7 *NA*

No 9 Nitric Acid Production Plant	
h_2	Distilled water for No 9 *NA*
$(N4)_9$	NH_3 produced from No 4 NH_3 going to No 9 *NA*
$(HN)_9$	Total 60% HNO_3 produced on No 9 *NA*
T_9	*NO/NO₂* Tailgas discharge from No 9 *NA*
No 10 Nitric Acid Production Plant	
h_3	Distilled water for No 10 *NA*
$(N4)_{10}$	NH_3 produced from No 4 NH_3 going to No 10 *NA*
$(HN)_{10}$	Total 60% HNO_3 produced on No 10 *NA*
T_{10}	NO/NO_2 Tailgas discharge from No 10 *NA*
No 11 Nitric Acid Production Plant	
h_4	Distilled water for No 11 *NA*
$(N4)_{11}$	NH_3 produced from No 4 NH_3 going to No 11 *NA*
$(HN)_{11}$	Total 60% HNO_3 produced on No 11 *NA*
T_{11}	NO/NO_2 Tailgas discharge from No 11 *NA*
Ammonium Nitrate Solution (ANS) Production and Sales	
$(ANS)_S$	Total external *ANS* sales
P_{ANS}	Selling price of *ANS* per ton
No 1 ANS Production Plant	
$(N2)_{ANS1}$	NH_3 produced from No 2 NH_3 going to No 1 *ANS*
$(HN)_{ANS1}$	55% HNO_3 produced from No 7 *NA* going to No. 1 *ANS*
$(ANS)_1$	ANS produced on No 1 *ANS*
No 2 ANS Production Plant	
$(N4)_{ANS2}$	NH_3 produced from No 4 NH_3 to No 2 *ANS*
$(HN)_{ANS2}$	60% HNO_3 produced from 9, 10 & 11 *NA* going to No 2 *ANS*
$(ANS)_2$	ANS produced on No 2 *ANS*
Ammonium Nitrate (AN) Production and Sales	
$(AN)_S$	Total external sales of ammonium nitrate
P_{AN}	Selling price of *AN* per ton
No I Ammonium Nitrate (AN) Production	
$(ANS)_{AN1}$	ANS transferred to No 1 *AN*
$(AN)_{AN1}$	AN produced on No. 1 *AN*
$(WV)_{AN1}$	Water Vapour released from No 1 *AN*
No 2 Ammonium Nitrate (AN) Production	
$(ANS)_{AN2}$	ANS transferred to No 2 *AN*
$(AN)_{AN2}$	AN produced on No. 2 *AN*
$(WV)_{AN2}$	Water Vapour released from No 2 *AN*
No 3 Ammonium Nitrate (AN) Production	

$(ANS)_{AN3}$	ANS transferred to No 3 *AN*
$(AN)_{AN3}$	AN produced on No. 3 *AN*
$(WV)_{AN3}$	Water Vapour released from No 3 *AN*
No 4 Ammonium Nitrate (AN) Production	
$(ANS)_{AN4}$	ANS transferred to No 4 *AN*
$(AN)_{AN4}$	AN produced on No. 4 *AN*
$(WV)_{AN4}$	Water Vapour released from No 4 *AN*
Limestone Ammonium Nitrate (LAN) Production and Sales	
P_{LAN}	Selling price of *LAN* per ton
$(ANS)_{LAN}$	ANS transferred to *LAN*
$(LAN)_{S}$	*LAN* produced and sold on *LAN*
$(WV)_{LAN}$	Water Vapour released from *LAN*
(L)	Limestone required for the production of *LAN*

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APPENDIX A: MSFMO SOFTWARE – DELPHI CODE

```
unit MSFMO;

interface

uses
  Windows, Messages, SysUtils, Variants, Classes, Graphics, Controls, Forms,
  Dialogs, Menus, StdCtrls, ExtCtrls;

type
  TOpeningScreen = class(TForm)
    MainMenu: TMainMenu;
    Flowchart1: TMenuItem;
    Objectives1: TMenuItem;
    Introduction1: TMenuItem;
    DecisionVariables1: TMenuItem;
    ObjFunctions1: TMenuItem;
    Constraints1: TMenuItem;
    Label1: TLabel;
    Label2: TLabel;
    Panel3: TPanel;
    Panel9: TPanel;
    ObjectiveFunctions1: TMenuItem;
    Constraints2: TMenuItem;
    MaximiseGrossProfit1: TMenuItem;
    MinimiseEffluent1: TMenuItem;
    AspirationLevelFunctions1: TMenuItem;
    OptimumAspirationLevel1: TMenuItem;
    Exit: TButton;
    Label3: TLabel;
    Label4: TLabel;
    Label5: TLabel;
    Label6: TLabel;
    Label7: TLabel;
    Label8: TLabel;
    GrossProductionProfit1: TMenuItem;
    Effluent1: TMenuItem;
    DecisionVariables2: TMenuItem;
    procedure Introduction1Click(Sender: TObject);
    procedure Flowchart1Click(Sender: TObject);
    procedure ObjectiveFunctions1Click(Sender: TObject);
    procedure ProfitClick(Sender: TObject);
    procedure GrossProductionProfit1Click(Sender: TObject);
    procedure Effluent1Click(Sender: TObject);
    procedure ExitClick(Sender: TObject);
    procedure MaximiseGrossProfit1Click(Sender: TObject);
    procedure MinimiseEffluent1Click(Sender: TObject);
    procedure Constraints2Click(Sender: TObject);
```

```
    procedure DecisionVariables2Click(Sender: TObject);
    procedure AspirationLevelFunctions1Click(Sender: TObject);
    procedure OptimumAspirationLevel1Click(Sender: TObject);
    procedure ObjFunctions1Click(Sender: TObject);
    procedure Constraints1Click(Sender: TObject);
  private
    { Private declarations }
  public
    { Public declarations }
  end;

var
  OpeningScreen: TOpeningScreen;

implementation

uses IntroductionF, FlowChartP, O_FunctionsF, ProfitF, PEffluentF, MaxGPF,
  MinEffF, Limits, VariablesF, ASPFunF, OptimiseASPF, MSFMOfs, ConclusionF;

{$R *.dfm}

procedure TOpeningScreen.Introduction1Click(Sender: TObject);
begin
  IntroductionForm.Visible:= True;
end;


procedure TOpeningScreen.Flowchart1Click(Sender: TObject);
begin
  FlowChart.Visible:= True;
end;


procedure TOpeningScreen.ObjectiveFunctions1Click(Sender: TObject);
begin
  O_Functions.Visible:= True;
end;

procedure TOpeningScreen.ProfitClick(Sender: TObject);
begin
  IntroductionForm.Visible:= True;
end;


procedure TOpeningScreen.GrossProductionProfit1Click(Sender: TObject);
begin
  GProfit.Visible:= True;
end;

procedure TOpeningScreen.Effluent1Click(Sender: TObject);
```

```
begin
  PEffluent.Visible:= True;
end;

procedure TOpeningScreen.ExitClick(Sender: TObject);
begin
  OpeningScreen.Close;
end;


procedure TOpeningScreen.MaximiseGrossProfit1Click(Sender: TObject);
begin
  MaxGP.Visible:= True;
end;

procedure TOpeningScreen.MinimiseEffluent1Click(Sender: TObject);
begin
  MinEffluent.Visible:= True;
end;

procedure TOpeningScreen.Constraints2Click(Sender: TObject);
begin
  Limitations.Visible:= True;
end;

procedure TOpeningScreen.DecisionVariables2Click(Sender: TObject);
begin
  DVariables.Visible:= True;
end;

procedure TOpeningScreen.AspirationLevelFunctions1Click(Sender: TObject);
begin
  ASP_Functions.Visible:= True;
end;

procedure TOpeningScreen.OptimumAspirationLevel1Click(Sender: TObject);
begin
  Optimise_ASP.Visible:= True;
end;

procedure TOpeningScreen.ObjFunctions1Click(Sender: TObject);
begin
  MSFMO_Final_Solution.Visible:= True;
end;

procedure TOpeningScreen.Constraints1Click(Sender: TObject);
begin
  Conclusion.Visible:= True;
end;
```

```
end.

unit IntroductionF;

interface

uses
  Windows, Messages, SysUtils, Variants, Classes, Graphics, Controls, Forms,
  Dialogs, StdCtrls;

type
  TIntroductionForm = class(TForm)
    Exit: TButton;
    Memo1: TMemo;
    Label1: TLabel;
    procedure ExitClick(Sender: TObject);
  private
    { Private declarations }
  public
    { Public declarations }
  end;

var
  IntroductionForm: TIntroductionForm;

implementation

{$R *.dfm}

procedure TIntroductionForm.ExitClick(Sender: TObject);
begin
  IntroductionForm.Visible:= False;
end;

end.

unit FlowChartP;

interface

uses
  Windows, Messages, SysUtils, Variants, Classes, Graphics, Controls, Forms,
  Dialogs, StdCtrls, ExtCtrls, Menus;

type
  TFlowChart = class(TForm)
    Panel1: TPanel;
    Panel2: TPanel;
    Panel3: TPanel;
    Panel4: TPanel;
```

```
Panel5: TPanel;
Panel6: TPanel;
Panel7: TPanel;
Panel8: TPanel;
Edit1: TEdit;
Panel9: TPanel;
Panel10: TPanel;
Panel11: TPanel;
Edit2: TEdit;
Panel12: TPanel;
Panel13: TPanel;
Panel14: TPanel;
Label1: TLabel;
Panel15: TPanel;
Panel16: TPanel;
Edit3: TEdit;
Panel17: TPanel;
Panel18: TPanel;
Panel19: TPanel;
Panel20: TPanel;
Edit4: TEdit;
Panel21: TPanel;
Panel22: TPanel;
Panel23: TPanel;
Panel24: TPanel;
Panel25: TPanel;
Panel26: TPanel;
Panel28: TPanel;
Edit5: TEdit;
Panel29: TPanel;
Edit6: TEdit;
Panel30: TPanel;
Exit: TButton;
Edit7: TEdit;
Panel31: TPanel;
Panel32: TPanel;
Panel33: TPanel;
Panel34: TPanel;
Edit8: TEdit;
Panel35: TPanel;
Panel36: TPanel;
Panel37: TPanel;
Panel38: TPanel;
Panel39: TPanel;
Edit9: TEdit;
Panel40: TPanel;
Panel41: TPanel;
Panel42: TPanel;
Edit10: TEdit;
Panel43: TPanel;
```

```
Panel44: TPanel;
Panel45: TPanel;
Panel46: TPanel;
Panel47: TPanel;
Panel49: TPanel;
Edit11: TEdit;
Panel50: TPanel;
Edit12: TEdit;
Panel51: TPanel;
Panel52: TPanel;
Edit13: TEdit;
Panel54: TPanel;
Panel48: TPanel;
Panel53: TPanel;
Edit14: TEdit;
Panel55: TPanel;
Edit15: TEdit;
Panel56: TPanel;
Edit16: TEdit;
Panel57: TPanel;
Panel58: TPanel;
Panel59: TPanel;
Panel60: TPanel;
Edit17: TEdit;
Panel61: TPanel;
Edit18: TEdit;
Panel62: TPanel;
Panel63: TPanel;
Panel64: TPanel;
Panel65: TPanel;
Edit19: TEdit;
Panel66: TPanel;
Panel67: TPanel;
Panel68: TPanel;
Panel69: TPanel;
Panel70: TPanel;
Panel71: TPanel;
Edit20: TEdit;
Panel72: TPanel;
Edit21: TEdit;
Panel73: TPanel;
Panel74: TPanel;
Panel75: TPanel;
Panel76: TPanel;
Panel77: TPanel;
Panel78: TPanel;
Panel79: TPanel;
Panel80: TPanel;
Panel81: TPanel;
Panel82: TPanel;
```

```
Panel83: TPanel;
Edit22: TEdit;
Edit23: TEdit;
Edit24: TEdit;
Panel84: TPanel;
Edit25: TEdit;
Panel85: TPanel;
Panel86: TPanel;
Edit26: TEdit;
Panel87: TPanel;
Panel88: TPanel;
Panel89: TPanel;
Panel90: TPanel;
Panel91: TPanel;
Panel92: TPanel;
Edit27: TEdit;
Edit28: TEdit;
Edit29: TEdit;
Panel93: TPanel;
Edit30: TEdit;
Panel94: TPanel;
Panel95: TPanel;
Panel96: TPanel;
Panel97: TPanel;
Panel98: TPanel;
Panel99: TPanel;
Panel100: TPanel;
Edit31: TEdit;
Panel101: TPanel;
Panel102: TPanel;
Edit32: TEdit;
Edit33: TEdit;
Panel103: TPanel;
Panel104: TPanel;
Panel105: TPanel;
Panel106: TPanel;
Edit34: TEdit;
Panel107: TPanel;
Edit35: TEdit;
Panel109: TPanel;
Panel110: TPanel;
Panel111: TPanel;
Panel112: TPanel;
Panel113: TPanel;
Panel114: TPanel;
Edit36: TEdit;
Panel115: TPanel;
Edit37: TEdit;
Panel116: TPanel;
Panel117: TPanel;
```

```
    Panel108: TPanel;
    Edit38: TEdit;
    Panel118: TPanel;
    Panel119: TPanel;
    Edit39: TEdit;
    Panel120: TPanel;
    Panel121: TPanel;
    Edit40: TEdit;
    Panel124: TPanel;
    Panel122: TPanel;
    Edit41: TEdit;
    Panel123: TPanel;
    Panel125: TPanel;
    Panel126: TPanel;
    Edit42: TEdit;
    Panel127: TPanel;
    Panel128: TPanel;
    MainMenu1: TMainMenu;
    procedure ExitClick(Sender: TObject);
    procedure FormCreate(Sender: TObject);
  private
    { Private declarations }
  public
    { Public declarations }
  end;

var
  FlowChart: TFlowChart;

implementation

{$R *.dfm}

procedure TFlowChart.ExitClick(Sender: TObject);
begin
  FlowChart.Visible:= False;
end;

procedure TFlowChart.FormCreate(Sender: TObject);
begin
  Edit1.Text:= 'C2';
  Edit2.Text:= 'A2';
  Edit3.Text:= 'A4';
  Edit4.Text:= 'C4';
  Edit5.Text:= 'A7';
  Edit6.Text:= '(N2)7';
  Edit7.Text:= '(HN)7';
  Edit8.Text:= '(N2)ANS1';
  Edit9.Text:= '(ANS)AN1';
  Edit10.Text:= '(WV)AN1';
```

```
  Edit11.Text:= '(N4)9';
  Edit12.Text:= '(N4)10';
  Edit13.Text:= '(N4)11';
  Edit14.Text:= 'A9';
  Edit15.Text:= 'A10';
  Edit16.Text:= 'A11';
  Edit17.Text:= 'h7';
  Edit18.Text:= 'h9';
  Edit19.Text:= 'h10';
  Edit20.Text:= 'h11';
  Edit21.Text:= '(NOx)9';
  Edit22.Text:= '(HN)9';
  Edit23.Text:= '(HN)10';
  Edit24.Text:= '(HN)11';
  Edit25.Text:= '60(HN)S';
  Edit26.Text:= '(HN)ANS2';
  Edit27.Text:= '(ANS2)AN2';
  Edit28.Text:= '(ANS2)AN3';
  Edit29.Text:= '(ANS2)AN4';
  Edit30.Text:= '(AN2)';
  Edit31.Text:= 'AN1';
  Edit32.Text:= 'AN3';
  Edit33.Text:= 'AN4';
  Edit34.Text:= '(ANS2)LAN';
  Edit35.Text:= 'LAN';
  Edit36.Text:= '(WV)LAN';
  Edit37.Text:= '(WV)AN4';
  Edit38.Text:= '(WV)AN2';
  Edit39.Text:= '(WV)AN3';
  Edit40.Text:= '(NOx)10';
  Edit41.Text:= '(NOx)7';
  Edit42.Text:= '(NOx)11';
end;

end.

unit O_FunctionsF;

interface

uses
  Windows, Messages, SysUtils, Variants, Classes, Graphics, Controls, Forms,
  Dialogs, StdCtrls;

type
  TO_Functions = class(TForm)
    Label1: TLabel;
    Label2: TLabel;
    Label3: TLabel;
    Label4: TLabel;
```

```
    Edit1: TEdit;
    Edit2: TEdit;
    Exit: TButton;
    procedure FormCreate(Sender: TObject);
    procedure ExitClick(Sender: TObject);
  private
    { Private declarations }
  public
    { Public declarations }
  end;

var
  O_Functions: TO_Functions;

implementation

{$R *.dfm}

procedure TO_Functions.FormCreate(Sender: TObject);
begin
  Edit1.Text:= 'Max[45(N2) + (N2)S + 75(N4)S + 95(HN)55S + 125(HN)60S +
350(AN)S + 200(LAN)S';
  Edit2.Text:= 'Min[0.0746(HN7)(HN7) - 11.16(HN7) + 0.013(HN9)(HN9) -
7.13(HN9) + 0.034(HN10)(HN10) - 18.309(HN10) + 0.0064HN11)(HN11) -
7.785(HN11) + 6652.89';
end;

procedure TO_Functions.ExitClick(Sender: TObject);
begin
  O_Functions.Visible:= False;
end;

end.

unit ProfitF;

interface

uses
  Windows, Messages, SysUtils, Variants, Classes, Graphics, Controls, Forms,
  Dialogs, Grids, DBGrids, DB, ADODB, StdCtrls;

type
  TGProfit = class(TForm)
    ADODataSet1: TADODataSet;
    DataSource1: TDataSource;
    DBGrid1: TDBGrid;
    Label1: TLabel;
    Label2: TLabel;
    Exit: TButton;
```

```
    Obj_Fn: TButton;
    Edit1: TEdit;
    procedure ExitClick(Sender: TObject);
    procedure Obj_FnClick(Sender: TObject);
    procedure FormCreate(Sender: TObject);
  private
    { Private declarations }
  public
    { Public declarations }
  end;

var
  GProfit: TGProfit;

implementation

{$R *.dfm}

procedure TGProfit.ExitClick(Sender: TObject);
begin
  GProfit.Visible:= False;
end;

procedure TGProfit.Obj_FnClick(Sender: TObject);
begin
  Edit1.Text:= 'Max[45(N2) + (N2)S + 75(N4)S + 95(HN)55S + 125(HN)60S +
350(AN)S + 200(LAN)S';
end;

procedure TGProfit.FormCreate(Sender: TObject);
begin
  Edit1.Text:= '';
end;

end.

unit PEffluentF;

interface

uses
  Windows, Messages, SysUtils, Variants, Classes, Graphics, Controls, Forms,
  Dialogs, StdCtrls;

type
  TPEffluent = class(TForm)
    Memo1: TMemo;
    Label1: TLabel;
    Label2: TLabel;
    Memo2: TMemo;
```

```
    Exit: TButton;
    EEP: TButton;
    procedure ExitClick(Sender: TObject);
    procedure EEPClick(Sender: TObject);
  private
    { Private declarations }
  public
    { Public declarations }
  end;

var
  PEffluent: TPEffluent;

implementation

uses EEP_F;

{$R *.dfm}

procedure TPEffluent.ExitClick(Sender: TObject);
begin
  PEffluent.Visible:= False;
end;

procedure TPEffluent.EEPClick(Sender: TObject);
begin
  EffEffProd.Visible:= True;
end;

end.

unit MaxGPF;

interface

uses
  Windows, Messages, SysUtils, Variants, Classes, Graphics, Controls, Forms,
  Dialogs, StdCtrls, DB, ADODB, Grids, DBGrids;

type
  TMaxGP = class(TForm)
    Exit: TButton;
    DataSource1: TDataSource;
    DBGrid1: TDBGrid;
    ADODataSet1: TADODataSet;
    Label1: TLabel;
    Label2: TLabel;
    Label3: TLabel;
    Edit1: TEdit;
    Edit2: TEdit;
```

```
    procedure ExitClick(Sender: TObject);
    procedure FormCreate(Sender: TObject);
  private
    { Private declarations }
  public
    { Public declarations }
  end;

var
  MaxGP: TMaxGP;

implementation

{$R *.dfm}

procedure TMaxGP.ExitClick(Sender: TObject);
begin
  MaxGP.Visible:= False;
end;

procedure TMaxGP.FormCreate(Sender: TObject);
begin
  Edit1.Text:= 'R240,837';
  Edit2.Text:= '527 t/day';
end;

end.

unit MinEffF;

interface

uses
  Windows, Messages, SysUtils, Variants, Classes, Graphics, Controls, Forms,
  Dialogs, Grids, DBGrids, DB, ADODB, StdCtrls;

type
  TMinEffluent = class(TForm)
    DataSource1: TDataSource;
    ADODataSet1: TADODataSet;
    DBGrid1: TDBGrid;
    Label1: TLabel;
    Exit: TButton;
    Edit1: TEdit;
    Edit2: TEdit;
    Label2: TLabel;
    Label3: TLabel;
    procedure ExitClick(Sender: TObject);
    procedure FormCreate(Sender: TObject);
  private
```

```
    { Private declarations }
  public
    { Public declarations }
  end;

var
  MinEffluent: TMinEffluent;

implementation

{$R *.dfm}

procedure TMinEffluent.ExitClick(Sender: TObject);
begin
  MinEffluent.Visible:= False;
end;

procedure TMinEffluent.FormCreate(Sender: TObject);
begin
  Edit1.Text:= '477 t/day';
  Edit2.Text:= 'R235,129';
end;

end.

unit Limits;

interface

uses
  Windows, Messages, SysUtils, Variants, Classes, Graphics, Controls, Forms,
  Dialogs, StdCtrls;

type
  TLimitations = class(TForm)
    Exit: TButton;
    Memo1: TMemo;
    Label1: TLabel;
    procedure ExitClick(Sender: TObject);
  private
    { Private declarations }
  public
    { Public declarations }
  end;

var
  Limitations: TLimitations;

implementation
```

```
{$R *.dfm}

procedure TLimitations.ExitClick(Sender: TObject);
begin
  Limitations.Visible:= False;
end;

end.

unit VariablesF;

interface

uses
  Windows, Messages, SysUtils, Variants, Classes, Graphics, Controls, Forms,
  Dialogs, StdCtrls, Grids, DBGrids, DB, ADODB;

type
  TDVariables = class(TForm)
    Exit: TButton;
    ADODataSet1: TADODataSet;
    DataSource1: TDataSource;
    DBGrid1: TDBGrid;
    procedure ExitClick(Sender: TObject);
  private
    { Private declarations }
  public
    { Public declarations }
  end;

var
  DVariables: TDVariables;

implementation

{$R *.dfm}

procedure TDVariables.ExitClick(Sender: TObject);
begin
  DVariables.Visible:= False;
end;

end.

unit ASPFunF;

interface

uses
  Windows, Messages, SysUtils, Variants, Classes, Graphics, Controls, Forms,
```

```
  Dialogs, StdCtrls, Grids, DBGrids, DB, ADODB;

type
  TASP_Functions = class(TForm)
    Exit: TButton;
    Memo1: TMemo;
    Label1: TLabel;
    Label2: TLabel;
    Memo2: TMemo;
    DataSource1: TDataSource;
    ADODataSet1: TADODataSet;
    Memo3: TMemo;
    DBGrid1: TDBGrid;
    Label3: TLabel;
    ShowASP: TButton;
    procedure ExitClick(Sender: TObject);
    procedure FormCreate(Sender: TObject);
    procedure ShowASPClick(Sender: TObject);
  private
    { Private declarations }
  public
    { Public declarations }
  end;

var
  ASP_Functions: TASP_Functions;

implementation

{$R *.dfm}

procedure TASP_Functions.ExitClick(Sender: TObject);
begin
  ASP_Functions.Visible:= False;
end;

procedure TASP_Functions.FormCreate(Sender: TObject);
begin
  Memo3.Text:= 'The Aspiration Level Functions per Objective Function are defined
as follows: Asp(k) = (Uk - Zk)/(Uk - Lk)';
  Memo1.Text:= 'Asp(1) = [427 - (0.0064(HN)11(0.0064(HN)11) - 7.7654(HN)11 +
2416.5) + (0.034(HN)10(0.034(HN)10 - 18.309(HN)10 +2675.2) +
(0.013(HN)9(0.013(HN)9 -7.1301(HN)9 + 1099.7) + (0.0746(HN)7(0.0746(HN)7) -
11.167(HN)7 + 461.39]/(427 - 527)]';
  Memo2.Text:= 'Asp(2) = [-4.28 + (0.000064(HN)11(0.000064(HN)11) -
0.078(HN)11 + 24.26) - (0.00034(HN)10(0.00034(HN)10) - 0.184(HN)10 + 26.85) -
(0.00013(HN)9(0.00013(HN)9 - 0.0716(HN)9 + 11.04) -
(0.00075(HN)7(0.00075(HN)7) -0.112(HN)7 + 4.632)]';
  Memo1.Visible:= False;
  Memo2.Visible:= False;
```

```
  Label1.Visible:= False;
  Label2.Visible:= False;
end;

procedure TASP_Functions.ShowASPClick(Sender: TObject);
begin
  Label1.Visible:= True;
  Memo1.Visible:= True;
  Label2.Visible:= True;
  Memo2.Visible:= True;
end;

end.

unit OpAspirationF;

interface

uses
  Windows, Messages, SysUtils, Variants, Classes, Graphics, Controls, Forms,
  Dialogs, StdCtrls, DB, ADODB, Grids, DBGrids;

type
  TOpAspiration = class(TForm)
    Exit: TButton;
    Memo1: TMemo;
    Label1: TLabel;
    Edit1: TEdit;
    Label2: TLabel;
    Memo2: TMemo;
    Label3: TLabel;
    Label4: TLabel;
    DataSource1: TDataSource;
    ADODataSet1: TADODataSet;
    DBGrid1: TDBGrid;
    procedure ExitClick(Sender: TObject);
    procedure FormCreate(Sender: TObject);
  private
    { Private declarations }
  public
    { Public declarations }
  end;

var
  OpAspiration: TOpAspiration;

implementation

{$R *.dfm}
```

```
procedure TOpAspiration.ExitClick(Sender: TObject);
begin
  OpAspiration.Visible:= False;
end;

procedure TOpAspiration.FormCreate(Sender: TObject);
begin
  Edit1.Text:= '112.5';
end;

end.

unit MSFMOfs;

interface

uses
  Windows, Messages, SysUtils, Variants, Classes, Graphics, Controls, Forms,
  Dialogs, StdCtrls, Grids, DBGrids, DB, ADODB;

type
  TMSFMO_Final_Solution = class(TForm)
    Exit: TButton;
    DataSource1: TDataSource;
    ADODataSet1: TADODataSet;
    Label1: TLabel;
    Edit1: TEdit;
    Edit2: TEdit;
    Label2: TLabel;
    Label3: TLabel;
    Label5: TLabel;
    DBGrid1: TDBGrid;
    procedure ExitClick(Sender: TObject);
    procedure FormCreate(Sender: TObject);
  private
    { Private declarations }
  public
    { Public declarations }
  end;

var
  MSFMO_Final_Solution: TMSFMO_Final_Solution;

implementation

{$R *.dfm}

procedure TMSFMO_Final_Solution.ExitClick(Sender: TObject);
begin
  MSFMO_Final_Solution.Visible:= False;
```

```
end;

procedure TMSFMO_Final_Solution.FormCreate(Sender: TObject);
begin
  Edit1.Text:= 'R 240,837';
  Edit2.Text:= '527 ppm';
end;

end.

unit ConclusionF;

interface

uses
  Windows, Messages, SysUtils, Variants, Classes, Graphics, Controls, Forms,
  Dialogs, StdCtrls;

type
  TConclusion = class(TForm)
    Memo1: TMemo;
    Exit: TButton;
    Label1: TLabel;
    procedure ExitClick(Sender: TObject);
  private
    { Private declarations }
  public
    { Public declarations }
  end;

var
  Conclusion: TConclusion;

implementation

{$R *.dfm}

procedure TConclusion.ExitClick(Sender: TObject);
begin
  Conclusion.Visible:= False;
end;

end.
```