DEVELOPING AN INTEGRATED DECISION SUPPORT SYSTEM FOR AN OIL REFINERY

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ABSTRACT

This thesis considers the problem of residue upgrading operations in an oil refinery. Visbreaking is a residue-upgrading process that improves profitability of a refinery. The economics of converting the heavy residue into the lighter and more valuable streams, coupled with the installation of a modern visbreaker unit at the Engen Refinery in Durban, provides sufficient motives to develop a mathematical model to simulate the unit's capability and estimate the economics of the visbreaking process and fuel oil operations. Furthermore, the proposed model should provide a crude-dependent visbreaking yield that can be used in the refinery's global linear programme (LP), employed to evaluate and select the crude and to optimise refinery's operations.

Traditionally, kinetically based models have been used to simulate and study the refining reaction processes. In this case, due to the complexity of the process and some unknown reactions, the performances of existing visbreaking simulators are not fully satisfactory. Consequently, a neural network model of the visbreaking process and fuel oil blending operation is developed.

The proposed model is called the adaptive visbreaker paradigm, since it is formed using neuroengineering, a technique that fabricates empirically-based neural network models. The network operates in supervised mode to predict the visbreaking yields and the residue quality.

It was observed that due to the fluctuation in the quality of feedstock, and plant operating conditions, the prediction accuracy of the model needs to be improved. To improve the system's predictability, a network reciprocation procedure has been devised. Network reciprocation is a mechanism that controls and selects the input data used in the training of a neural network system. Implementation of the proposed procedure results in a considerable improvement in the performance of the network.

To facilitate the interaction between the simulation and optimisation routines, an integrated system to incorporate the fuel oil blending with the neurally-based module is constructed. Under an integrated system, the economics of altering the models' decision variables can be monitored.

To account for the visbreakability of the various petroleum crudes, the yield predicted by the adaptive visbreaker paradigm should enter into the visbreaker's sub-model of the global refinery LP. To achieve this, a mechanism to calculate and update the visbreaking yields of various crude oils is also developed.

The computational results produced by the adaptive visbreaker paradigm prove that the economics of the visbreaking process is a multi-dimensional variable, greatly influenced by the feed quality and the unit's operating condition. The results presented show the feasibility of applying the proposed model to predict the cracking reaction yields. Furthermore, the model allows a dynamic monitoring of the residue properties as applicable to fuel oil blending optimisation.

In summary, the combination of the proposed models forms an integrated decision support system suitable for studying the visbreaking and associated operations, and to provide a visbreaking yield pattern that can be incorporated into the global refinery LP model. Using an integrated decision support system, refinery planners are able to see through the complex interactions between business and the manufacturing process by performing predictive studies using these models.

PREFACE

The research work presented in this thesis was carried out in the Department of Mathematics and Applied Mathematics, University of Natal, Pietermaritzburg, from 1994 to 1998, under supervision of Professor John Hearne.

These studies represent original work by the author and have not otherwise been submitted in any form for any degree or diploma to any University. Where use has been made of the work of others it is duly acknowledged in the text.

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CHAPTER 1

INTRODUCTION

This chapter provides some information on the background to the world-wide problem of refining heavy petroleum crude and the incentives behind the residue upgrading process. Visbreaking is a refinery process unit that allows refiners to upgrade the crude's residue. It briefly discusses different visbreaking models and the motives for the introduction of a new modelling concept that simulates the visbreaking process and provides the necessary yield data required by the refinery linear programme. The refinery linear programme is a mathematical representation of a refinery that is used in crude selection and plant-wide optimisation of a refinery. In this respect, an introduction into refinery planning system and the application of the refinery linear programme as a managerial decision support is also presented.

1.1 Background

Petroleum crude – Overview & Economics

Crude oils are complex mixtures of different species of chemical compounds. In addition to the hydrocarbons, a number of elements appear in crude oil. From the refiners point of view, some of these elements (such as sulphur, sodium, vanadium...) are undesirable and must be removed from the petroleum products. There has been an understandable tendency among refiners to select from the crude's available those with the lower amounts of these undesirable materials. As a result, the world reserves of more desirable crude's decline while the reserves of less desirable and inevitably more viscous crudes grow (Hermes, 1998).

For a better understanding of crude processing and typical refinery products yield, a simplified schematic of crude processing is shown below:

Decision Making Levels

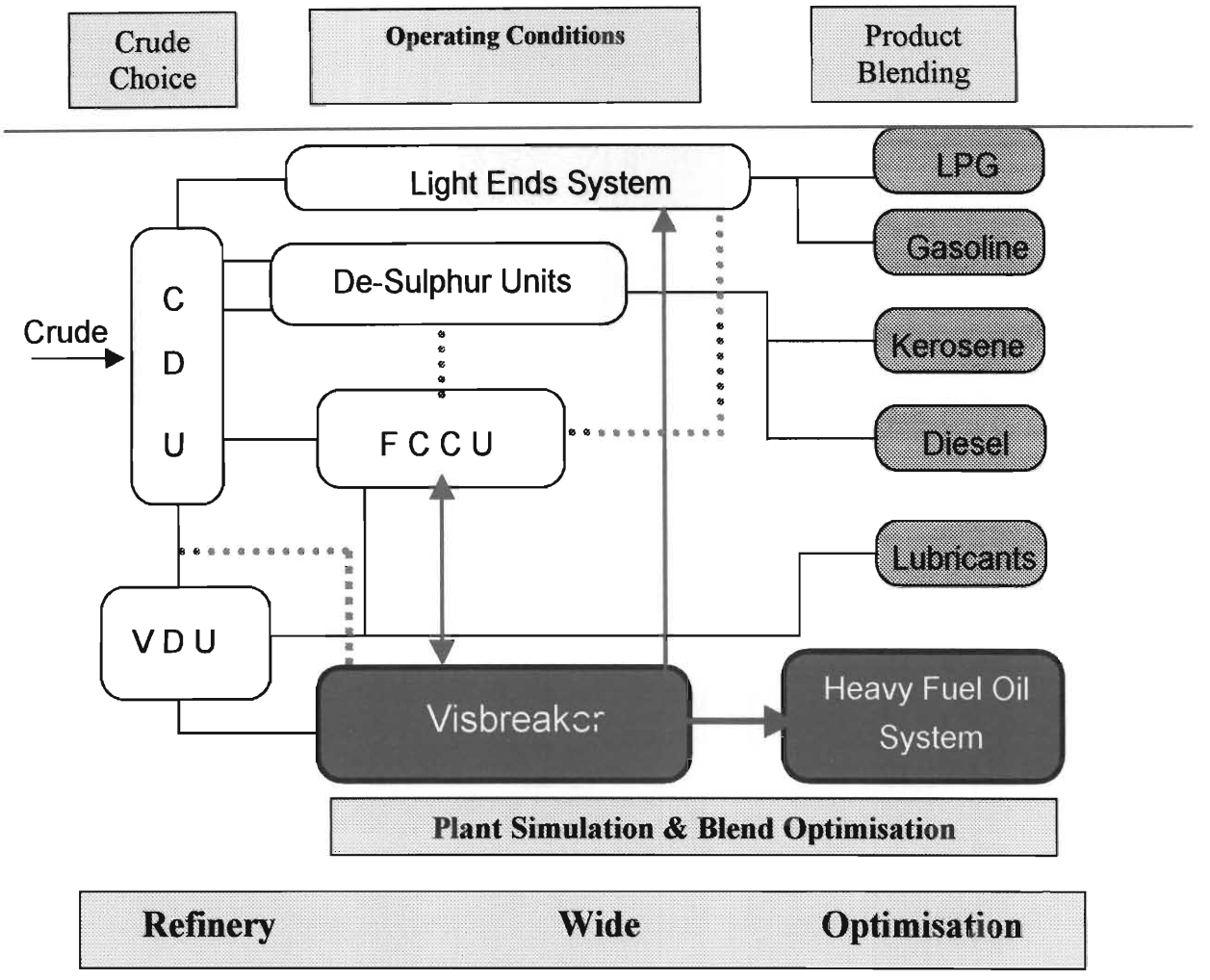


Figure 1-1 A simplified schematic of a petroleum refinery

CDU = Crude Distillation Unit

VDU = Vacuum Distillation Unit

Light Ends System = Combination of several plants to process the light hydrocarbons

De-Sulphur Units = Sulphur Removing Process Units.

FCCU = Fluid Catalytic Cracker Unit

Visbreaker = Residue Upgrading Unit.

LPG = Liquid Petroleum Gas.

Fuel Oil System = Heavy Fuel Oil Blending (fuel oil blending pool) and Optimisation systems.

For the sake of clarity, the complete picture of the crude refining plants and processes is not shown.

An internationally accepted yardstick to measure the specific gravity of the crude is the API degrees, adopted by American Petroleum Institute. This is based on the following equation:

$$API = \frac{141.5}{SPG} - 131.4 \qquad (1.1)$$

where the **SPG**. is the specific gravity of crude oil; a ratio of the density of the materials at 60° Fahrenheit (15.5C) to the density of water at that same temperature that is; the lower the API gravity, the more viscous or heavier the crude oil.

On average, crude oils available to the refiners are becoming heavier and therefore more difficult to convert to the light products, such as gasoline, kerosene, or diesel fuel (Tamburrano, 1994). This is shown in the Figure 1-2, where the trend of the crude's API during the years' 1975-1990 is depicted.

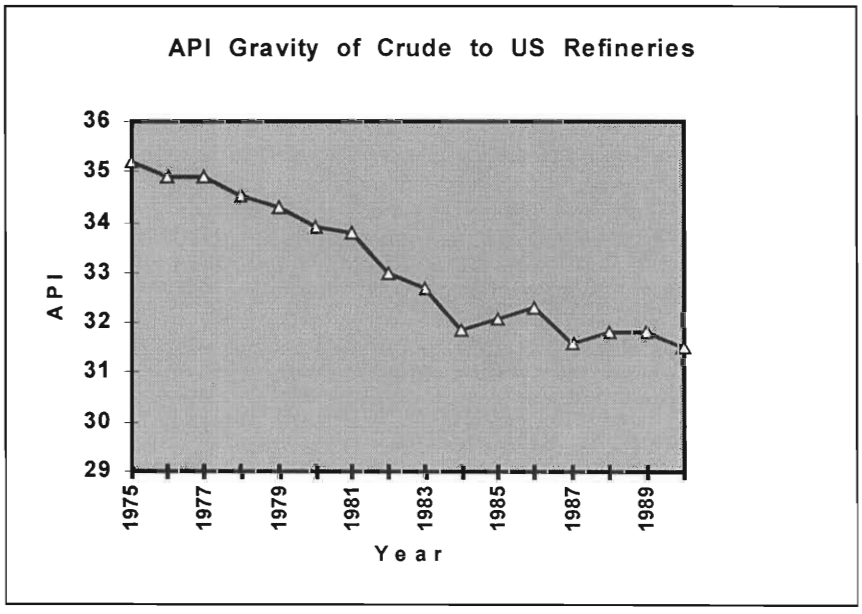


Figure 1-2 API gravity of the crude. Source : Oil and Gas Journal September 9, 1991

In the past, demand for highly refined products such as transportation fuels has largely been satisfied by processing relatively high quality, high API crudes. This is no longer the case as the quality of crude oils processed around the world is worsening (Tebbal *et al*, 1997).

There has been a decline in the world reserves of the high quality crudes. There is also a decreasing demand for heavy fuel oil and an increasing demand for gasoline and distillates (also called white oil). This has resulted in a renewed interest in converting the residual portion of the crude barrel. Consequently, the change in the product slate has created a world-wide product imbalance. This is shown in the Figure 1-3.

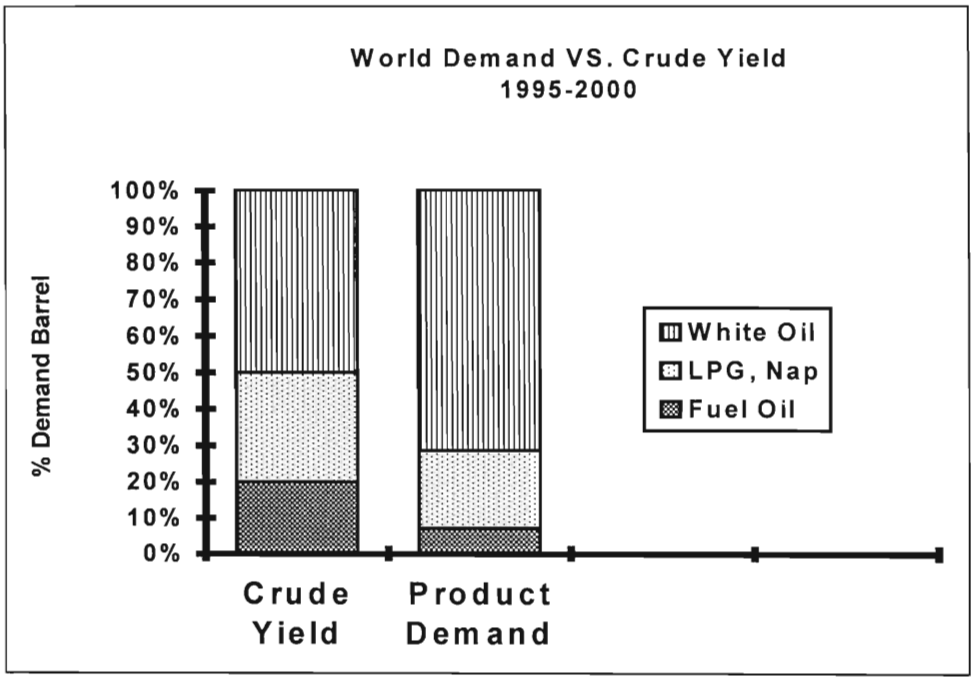


Figure 1-3 Product Demand VS. Crude Yield. Source: Bonner & Moore NPRA March 1995. AM-95-06 (presented by G. Guariguata)

Anticipated changes in crude quality and the product slate are expected to result in:

- Wider price differential between heavy and light crudes.
- Wider price differential between the white oils and heavy fuel oils.

To illustrate the impact of a change in crude quality, Table 1-1 compares the residue yields from two Arabian based crudes. Arab light crude contains roughly 45 volume percent of residue (crude bottom).

Progressing to the Arab heavy crude increases the amount of the crude residue by approximately 30 volume percent. In addition, the amount of undesirable contaminants present in the residue also increases dramatically as the crude becomes heavier (Hennico *et al*, 1994). Obviously, refining a crude with such characteristics is a cumbersome task.

Additionally, due to the higher contaminates (or undesirable materials) of the heavy crude, the refining cost of a heavy crude is higher than that of a light crude.

The expected product spectrum and the selling price of various petroleum products are compared in Table 1-1. The residue upgrading incentive is based on the given price and the volume of major products obtained from processing of Arab Light and Heavy crudes. It is shown that the upgrading incentive of Arab Heavy is greater than that of Arab Light.

Table 1-1 Estimation of residue-upgrading incentive

Source: Hydrocarbon Technologies Inc. (HTI) Quarterly: Spring 1995 (Presented by E. Houde *et al*, 1995)

Crude Type	Arab Light	Arab Heavy
Crude API °	33.8	27.9
Crude Residue (bottom) %	45	54
Vacuum residue Volume %	15	28
Average Crude Price $/bbl spot Europe 1994	14.18	12.25
Average Gasoline Price $/bbl spot Europe 1994	19.28	19.28
Average Jet fuel Price $/bbl spot Europe 1994	22.22	22.22
Average Diesel fuel Price $/bbl spot Europe 1994	20.75	20.75
Average Fuel Oil Price $/bbl spot Europe 1994	9.70	9.70
Expected Fuel Oil Yield Volume % (No-Visbreaker)	20.8	28.3
Expected Fuel Oil Yield Volume % (With-Visbreaker)	16	21
Estimated Upgrading Incentive $ per barrel of crude	0.55	0.82

Clearly, it can be seen that the economics of petroleum refining are based on ratio, or degree, of converting the heavy crude's residue to white oil (gasoline, jet, diesel fuel). This is because of the higher marginal value of white oil versus the petroleum crude as shown in the Table 1-2 below:

Table 1-2 Crude and Product Pricing Profile

The price of petroleum crude is shown as P. The marginal values are the average pricing obtained from various petroleum trading bulletins during 1996-1997.

White oil: Products such as Gasoline -Jet-Diesel	High-selling price $/bbl	P+9
	Low selling price $/bbl	P+2
Crude petroleum	Benchmark price $/bbl	P
Black oil: Asphalt – Heavy Fuel Oils	High selling price $/bbl	P–1
	Low selling price $/bbl	P–11

It should be noted that the crude price itself is steadily increasing. Burk (1995) has estimated that the median price of crude petroleum (in 1994 dollars) for the years 2000 to 2004 is about 20 to 24 Dollar per barrel respectively.

In summary, residue upgrading increases the white oil production, that in turn results in an increase in the income of the refinery. This is demonstrated in the Figure 1-4 below:

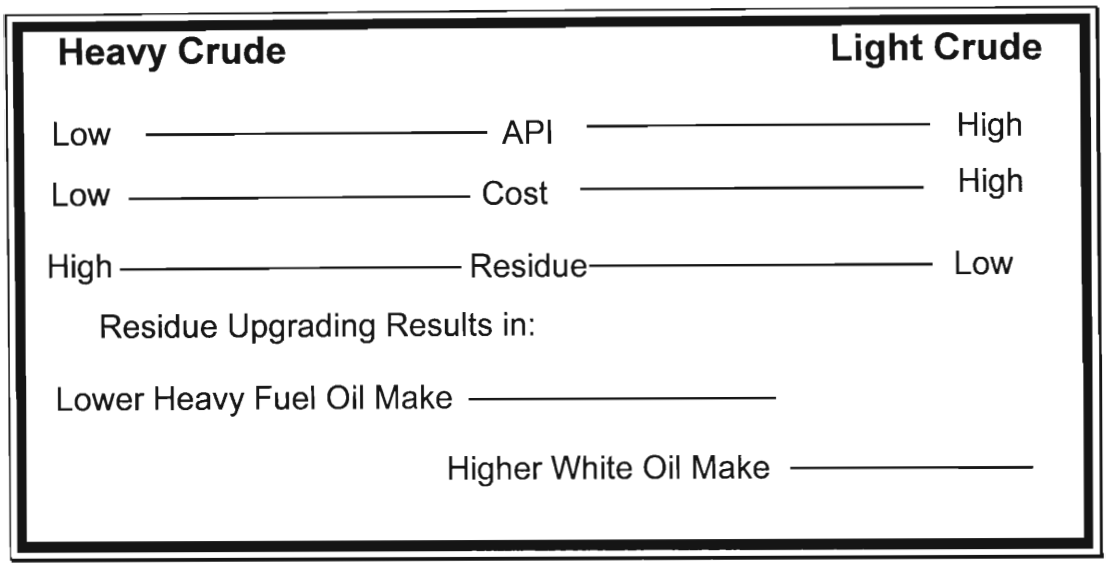


Figure 1-4 Schematic of the Residue Upgrading Incentive

Some words must be also said about the application of the residue upgrading units (such as the visbreaking process) in South Africa. The South African petroleum refineries produce the bulk of the fuel needed by the country. The total crude usage of some 400,000 barrels per day must be imported. The application of the residue conversion units, such as visbreaking, enables a refiner to purchase heavier and cheaper crude thus saving much needed hard currency for social upliftment projects.

Visbreaking Models – An overview

From the above discussion, we conclude that the key to economical refining is in maximising the white oil to black oil ratio. To achieve this, many refineries have embarked on various residue conversion schemes (Dawson, 1995). There are many ways to convert the crude's heavy residue into the light products, among them visbreaking; a non-catalytic thermal process widely used by petroleum refiners (Hofmann, 1984). According to a survey by Bonnifay (1992), about 22 percent of the world's residue upgrading units in use are visbreakers.

Kinetic models have traditionally been used to simulate and study the chemical reactions in the petroleum and petrochemical industry. In recent years, few visbreaking simulation models have been developed. These models are generally based on the empirical relationships derived from kinetic equations of the thermal decomposition of the hydrocarbons. Among the most well known visbreaker simulation models are Vistop™ and Vispo™; discussed below.

Vistop, a kinetic visbreaker simulator from KBC Process Technology Ltd, is designed to monitor and optimise the furnace, transfer line, main fractionator and the fuel oil blending facilities of visbreaking units. According to KBC Technology, either coil or soaker units may be simulated and Vistop is capable of predicting the visbreaker residue conversion based on the feedstocks quality.

Vispo simulator, from KTI-Spa Inc, is a computer program that simulates the thermal process in a visbreaking furnace and joint soaking unit. According to Bussani *et al* (1995), based on the coil and soaking unit geometry, feed characterisation and operating conditions, the program can estimate the visbreaking yields and some properties of the visbreaking effluents.

The kinetic models of the visbreaker have not been widely used by the petroleum industry. This is due to the complexity of the modern visbreaking process, where the relationships between the various process parameters are often unknown or unattainable. It should be noted that, in the absence of a catalyst, the visbreaking process of the heavy residues cannot be efficiently controlled. In other words, the nature and composition of the free radicals (Atkins, 1994) formed during the thermal decomposition of the heavy hydrocarbons are often unknown and difficult to estimate.

Another problem associated with these models is their high dependency on the layout of the visbreaking equipment. Thus, they are not easily adaptable to a new environment.

The estimation of visbreaking yields is often a difficult task because the product is a mixture that cannot be completely analysed, and because the viscosity of the residue cannot be accurately predicted (Orbey, *et al*, 1993). Laboratory-based yields (pilot plant) are in many instances worthless because commercial conditions cannot be adequately simulated by the laboratory procedures.

The overall reaction of visbreaking involves the decomposition of heavy oil into gas, light naphtha, distillates, and heavy condensation products. Because of the process's complexity as well as some unknown and uncontrollable reactions, the conventional models based on the theory of thermo-kinetics have not been truly satisfactory. Furthermore, these models do not generally account for the quality of the fuel oil nor the economics associated with the visbreaking process and fuel oil blending.

As a result, the predicting quality and applicability of the existing visbreaking simulation model(s) is often poor and does not resemble the real world of the visbreaking process and fuel oil blending operation. Additionally, these models have traditionally been expensive to purchase and maintain.

Refinery Linear Programming Model - An overview

Industrial operations of any complexity require some degrees of planning. This involves anticipating future problems and situations and deciding in advance what steps need to be taken to deal with them.

In the petroleum refining industry the analysis of the economic aspects of a chemical process provides an essential basis for process and plant decisions to determine what, in any particular situation is the best thing to do. In this respect, planning is broadly concerned with identifying courses of action and selecting the best suited to the particular circumstances. In an economic context this means finding the particular plan which is likely to be the most profitable (or the least costly). The search for a "best" or "right" economic plan is referred to as a procedure of optimisation.

For a plant or process the range of possible alternative plans and the scope for optimisation depends on what flexibility exists in the way it can be run. There may be flexibility in operating conditions, in feedstocks that can be used and in relative amounts of different products that can be made. It should be noted that each refinery has its own unique processing schemes, which are determined by the equipment available, operating costs, and product demand. The optimum flow pattern for any refinery is dictated by economic considerations and no two refineries are identical in their operations.

It is against this background that mathematical techniques such as the Linear Programming (LP) can be particularly helpful in planning and scheduling applications. Linear programming (and associated techniques) enables a wide variety of planning data to be properly evaluated. It enables the "best" economic plan to be selected with confidence and provides valuable insight into alternative plans and involved interactions, which occur in complex planning situations.

In many ways the refining industry was the investor and leader in the early development of linear programming in the industrial sector (Coxhead, 1992). Almost every refinery in the world is using the linear programming technique to optimise its operation. This so called Refinery LP or Global Refinery LP (GLP) usually consist of several sub-models, each representing a refinery process unit or the product blending operation. The objective function is to maximise profit (or minimise cost) of the refining operation by selecting the optimum quantity of the petroleum crude, or mix of crude's, to satisfy a product slate. Additionally, the Refinery LP is capable of blending these products according to the specification stipulated by the refiner. The global LP is a mathematical representation of the refinery. However, extensive knowledge of process modelling, process chemistry, yield accounting, computer science, refinery economics and finance is often needed to understand and address the various planning issues arising in the petroleum industry. Detailed discussion of this very important planning tool is presented in Appendix -4 of this thesis.

1.2 Problem Statement

As stated earlier, petroleum crude is the primary feedstock of the refinery. As the petroleum crude available to the refining industry becomes expensive and heavier, the more refiners will apply residue upgrading such as the visbreaking process to convert heavy materials to more economically desirable products. The refinery profitability is therefore highly sensitive to the optimality of the visbreaking and fuel oil blending operation.

In addition to reducing the viscosity of the heavy residue, the modern visbreaker units provide feed to the Catalytic Cracker unit, where the refinery's most valuable products (gasoline and diesel stocks) are produced. In this respect, the interaction between the visbreaker, catalytic cracker, and the heavy fuel oil system plays a great role in the refinery's profitability.

These interactions are mathematically modelled into the Global Refinery LP. The yield and quality pattern of different crude dependent feedstocks and other non-linear relationships, however, cannot be accurately modelled. The main reasons for this deficiency are listed below:

- The Global Refinery LP is concerned with the global optimisation of a refinery and thus can not satisfactorily be used to simulate the operation of a specific unit, or for product blending, where the relationships are often non-linear (Patterson, 1971).

- In primary upgrading of heavy oils (residue) to distillates (gas oils), highly condensed aromatic rings are involved in a complex chemistry that is not well understood (Rahimi & Dettman, 1997).

- More than 200 visbreaking units are now in operation. In spite of the large number of publications on this process, many questions are still unanswered. The role of asphaltenes in the thermal transformation of oil residues, the interdependencies between the asphaltenes content, stability, viscosity and other properties of feedstocks, and their effects on the products of visbreaking are not clear (Brauch *et al*, 1996).

The cost of purchasing petroleum crude is the highest single cost to a refiner. In order to economically evaluate the crude and other refinery feedstocks, it is necessary to account for the visbreaking yields and properties. In this respect, mathematical models can be used to evaluate various refinery feedstocks, and to quantify the economics of refinery operations. In scientific terms " model" is used to describe a contrived representation of real processes or phenomena (Rice *et al*, 1995). Models are used both to quantify our knowledge of reality and to make inferences about that reality (Malik, 1991). Reaction simulation models are often used to predict the yields of refinery process units. In practice many assumptions about the reaction course are normally made. In some cases a "black-box" model is used with parameters gained from experimental runs. These models are essentially based on detailed reaction

engineering principles and thus are widely different from planning models which are used in optimisation and process economics (Friedman, 1995). The results produced from running this type of reaction simulation model can, however, be used as the starting point in the refinery global LP model.

The search for the kinetically based visbreaker simulation model indicated that the performances of the commercial visbreaker reaction simulation models are not fully satisfactory; thus these models are not widely used by petroleum refiners.

In view of the above, our aim to simulate the visbreaking process, optimise the fuel oil blending operation, and to equip the refinery LP with the crude's visbreakability relationships. It is, therefore, necessary to develop an alternative mathematical model that can predict the visbreaking yields and properties. The output of this model is used to update the visbreaking yield of the global refinery LP model. The integrated system is used to economically evaluate the various refinery feedstocks.

1.3 Motivation of the research and objective of the thesis

The work presented here is part of an ongoing research effort, to understand the visbreaking operations and its effect on the refinery's economics, and to improve the accuracy of the refinery LP model that is used in refinery-wide optimisation. To achieve this objective, it is necessary to develop computational methods to model the visbreakability of different crude oils and other refinery streams used as the visbreaker's feedstocks. It is also necessary to represent the fuel oil blending system and it's influences on the visbreaking operations.

In recent years, through the business transformation process, the refining industry has evolved into a commercial entity, where profit improvement and survivability are the major issues facing refinery management (Brice, 1996). As a result, optimisation of the decision making process requires constant evaluation of available resources. Against this background, it might be said that the cornerstone of a modern refinery is a sophisticated planning system (Tobin, 1997). Accordingly, the perspective that orients this work comes from a need to develop some decision-making tool(s) for a multi-disciplinary problem, at an oil refinery. Given that motivation, the emphasis is however, on the practicality of the concept and decision analysis.

Many practical applications require a multitude of mathematical models interacting not only with each other but also with a database, with a user interface, and with models from other modelling traditions. In this respect, the basic idea is to produce an integrated decision support system comprising an artificial neural network model of a visbreaker process unit, a fuel oil blending optimisation, and the global refinery LP model.

Decision support systems (DSS) are computer programs designed to improve the process and outcome of industrial or business decision making. DSS incorporate both data and models (Saaty, 1994). They are designed to assist

managers in their decision process (Goodwin *et al*, 1997). Using an integrated decision support system, refinery planners are able to see through the complex interactions between business and the manufacturing process by performing predictive studies using these models.

The simulation model developed for this study will be called the "Adaptive Visbreaker Paradigm" (AVP) that is based on the mechanism of neuroengineering. Broadly speaking, neuroengineering is a term applied to any empirically-based neural network model (Holt, 1994). In this thesis we classify and use neuroengineering as the technique employed in building an empirical Artificial Neural Network System (ANNs) that can predict the yields of a petroleum process unit. Neural network technology mimics the brain's own problem solving process. Just as humans apply knowledge gained from past experience to new problems or situations, a neural network takes previously-solved examples to build a system of "neurons" that makes new decisions, classifications, and forecasts (Hertz *et al*, 1991). The reason for much excitement about neural networks is their ability to generalise to new situations. After being trained on a number of plant and laboratory examples, they can often induce a complete relationship that interpolates and extrapolates from the input examples in a sensible way. Consequently, neural networks are widely used in a variety of business applications (Sharda, 1994).

In recent years, artificial neural network systems have successfully been used for many chemical processing applications. Among the earlier works, a paper by Reinschmidt, (1990) titled "Neural Networks for Process Forecasting" is of particular interest. Baratti *et al.*(1995) have successfully designed a neural network system to control the butane splitter column at the SARAS refinery in Italy. Ramasamy from the University of Louisville, and Paxton from Exxon Chemicals (1995) have produced a non-linear "phenomenological model" that is capable of explaining the underlying physics of the process identification problem. Brambilla *et al.* (1996) had limited success in using artificial neural networks to estimate product quality. Another interesting piece of work in the field of refinery process control is by Jyh-Ming Horng *et al* (1995) from

National Tsing Hua University in Taiwan. Here the researchers have used neural network systems to determine the operating conditions of a crude distillation tower.

However, so far, not many integrated simulation-optimisation models of the petroleum refinery processes have been reported. This is partly due to the fact that in the refining industry, the artificial neural network is a new and unproved tool. Moreover, developing a neural network system requires access to extensive plant and laboratory data, often difficult to acquire.

This thesis comprises a host of related, but somewhat separate problems. For example, the visbreaking operation concerns the optimal production of light hydrocarbons, while the fuel oil blending operation is essentially an optimisation problem concerned with the allocation of refinery streams to produce a blend. Since the overall objective is to improve the accuracy of the refinery LP model, it is imperative to frequently update and revise its visbreaking yields, and these can be derived from the proposed adaptive visbreaker paradigm.

In essence, the visbreaker paradigm is a neural network model of a visbreaker unit, combined with the fuel oil blending operations. The objective of AVP is to predict the visbreaking yield and quality, and to optimise the fuel oil blending pool on an ongoing basis. This type of model delivers it's best results when it has access to a large population of raw data. This is not a problem, as the refinery's operation is a continuous process. The foundation of the Visbreaker Adaptive Paradigm is based on the operation of the visbreaker unit at the Engen Refinery in Durban. However, it is possible to re-train the neural network paradigm and to learn other visbreaking process data in other working environments. In other words, the application of the proposed neuroengineering technique is not limited to the visbreaking operation nor to the existing Engen refinery configuration. In essence, the underlying structure of the proposed model provides sufficient flexibility for further refinement or usage at other

locations. Similarly, the combination of the various mathematical models developed for this study can be modified to suit other petroleum refineries.

This motivation leads us to define the project's objective as follows:

The primary objective of this project is to develop an integrated decision support system that can be used to study the economics of the visbreaking process and fuel oil blending operation. The system should be capable of improving the accuracy of the refinery LP model that is used in the global optimisation of the refinery.

The project consists of the following steps:

- To construct a mathematical model that can be used to simulate the visbreaking process and to generate product yields, using a neuroengineering technique.

- To develop a fuel oil blending optimisation model, since the visbreaking operation is closely related to that of fuel oil blending.

- The integration of simulation optimisation models to study the economics of the visbreaking operations.

- To test the interaction with the global refinery LP model by using the data generated by the above mentioned integrated system and to develop a mechanism to account for the visbreakability of various crude petroleum.

CHAPTER 2

DESCRIPTION & DEFINITION

This chapter is organised into the following sections:

Product blending: Product blending is one of the most important steps in the transformation of crude petroleum into finished petroleum products. However, for better understanding, the technical terms used in product blending should be reviewed. This is presented in Appendix 1.

The fundamentals of product blending are discussed under the headings of section 2.1.

Section 2.2: presents an overview of the visbreaking process and the fuel oil blending operation. Further information on residue decomposition theory is presented in Appendix-2.

For a better understanding of the visbreaking process and fuel oil blending, this section begins by defining the general terms applied to the visbreaking operations as outlined below:

Aromatic Hydrocarbons: Hydrocarbons derived from or characterised by the presence of the benzene ring. Many of this large class of cyclic and polycyclic organic compound are odorous.

Asphalt – also know as bitumen, pitch

Asphaltenes – Asphaltic – Asphaltene: Are the coal-like materials which occur in the residues obtained from refining petroleum crude oil. The asphaltenes are rich in the undesirable elements (e.g. sulphur, nitrogen...) that occur in fuel oil. It is generally believed that the visbreaking yield reduces with an increase in the asphaltenes content of the feedstocks.

ASTM: The acronym of The American Society for Testing Materials. The test procedures and specifications developed by ASTM for petroleum products are used world-wide.

Atmospheric Residue (AR): A stream drawn from the bottom of the crude distillation tower. It is also referred to as the crude tower bottom or long residue. This product can be routed to vacuum distillation or alternatively, the visbreaker unit.

Barrel: For statistical purposes, the petroleum industry uses a barrel (bbl) containing 42 US standard gallons as volumetric unit of measure for crude oil and petroleum products. The barrel is equivalent to 0.159 cubic meters.

Blending Stock(s): Materials suitable for blending into a refinery product.

Bottoms (Visbreaker Bottoms, Residue or Heavy Residue, Visbreakate, Heavy Residual Oil, Heavy Oils): In distilling operations, that portion of charge remaining in the still or flask at the end of the run. Also known as residue, residuum, residua, or sediment.

Cracking: The process by which an organic compound is split into two or more compounds of lower molecular weight. The cracking process may be carried out with heat and pressure (Thermal Cracking) or in the presence of a catalyst (Catalytic Cracking).

Chargestocks (charge-stocks or feedstocks, Feedstock): Any stream which can be used as feed to a process unit.

Cutterstocks (cutter–stocks, cutter): Any low viscosity material, which can reduce the viscosity, density or other property. of Marine Fuel Oil.

Deasphalter bottom: A stream drawn from the bottom of the Solvent extraction unit. This is referred to as TAR or PD-TAR.

Feedstock, Feedstocks, Charge or Chargestock: Primary feed for a process unit.

Gain (volume gain) : increases in volume during cracking.

Gas oil or Light Gas oil (LGO) : Any stream which can be used to produce Diesel fuel.

Marine Fuel Oil (Bunker Fuel Oil, BFO) : A blend of various refinery streams used by seafaring vessels as fuel.

Medium Gas Oil (MGO) and Heavy Gas Oil (HGO) : These gas oils are an intermediate stream and usually have to be re-processed or can be routed to the fuel oil system.

Naphthenes: Cyclo-paraffin hydrocarbons in which all of the available bonds of the carbon atoms are saturated with hydrogen are called naphthenes.

Normal Pentane Insoluble (*n*-Pentane Insolubles): A test to measure Asphaltenes content of petroleum residue. It is expressed in weight percent of the materials not being dissolved in normal pentane.

Olefins: A class of unsaturated, i.e. hydrogen deficient, paraffinic hydrocarbons having one or more double bonds per molecule.

Paraffins: The paraffin series of hydrocarbons is characterised by the rule that the carbon atoms are connected by a single bond and the other bonds are saturated with hydrogen atoms.

Severity : Process plants mode of operation(s). This is often expressed in terms of pressure, temperature, or product yields.

Vacuum Residue (VR) : Crude tower bottom (bottoms) is the primary feed to the Vacuum distillation unit. The Vacuum tower bottom is often referred to as the VDU-bottom or short residue. It can be routed to the visbreaker unit, solvent extraction unit, and asphalt blending unit.

Visbreaker Residue : Visbreaker bottom (bottoms) or Visbreakate is the heavy and viscous material obtained from the visbreaking process. This product needs to be blended into Bunker Fuel Oil or burnt in a refinery as a fuel.

2.1 Product Blending

Almost all of the petroleum products are blends of the various streams mixed to meet a rigid specification. Blending allows the refiner to allocate the available blending stocks produced from the various refining process in such a way as to meet product demands and specification at the least cost. In other words, to optimise the use of the available raw materials (Grosdidier, 1997). The availability and quality of the blending stocks are directly related to the quality of the process unit's feedstock and the plant's mode of operations. Selection of blend components and their proportions in the product blend is one of the most complex problems facing the refiner (White, 1995).

The physical process of blending is relatively simple and may be carried out in a number of ways, for example, by mixing the blend components in an agitated storage tank on a batch-based operation. To ensure that the blended

products meet the desired specifications, stream analysers may be installed to provide feedback to the computerised control systems.

Since the blending operations offer such an enormous number of options, most refiners use linear programming (LP) techniques to aid them in their blending decisions (Bradley, 1976 and Winston, 1991).

Most refinery products are a blend of two or more streams, each having different physical and chemical properties. A property is additive when the blend quality can be expressed as the average quality of the blend components. That is, it will blend linearly. In other words, ***one*** of the following equations must be satisfied:

$$P_b = \sum_i W_i P_i \qquad \textbf{(2.1)}$$

$$P_b = \sum_i V_i P_i \qquad \textbf{(2.2)}$$

$$P_b = \sum_i X_i P_i \qquad \textbf{(2.3)}$$

where

P_b = property of total blend.

P_i = property of component i.

W_i = weight fraction of component i.

V_i = volume fraction of component i.

X_i = mole fraction of component i.

Some properties are additive on either a volume, weight, or molal basis, for example specific gravity and sulphur content; whereas others such as viscosity, flash point and pour point do not blend linearly on any basis. To handle those properties which do not blend linearly, one must convert these properties into functions which behave in a linear fashion. These functions, which are referred

to as blending numbers, blending indices, or blending factors, must satisfy *one* of the following equations:

$$I_b = \sum_i w_i I_i \qquad \textbf{(2.4)}$$

$$I_b = \sum_i v_i I_i \qquad \textbf{(2.5)}$$

$$I_b = \sum_i x_i I_i \qquad \textbf{(2.6)}$$

where

I_b = blending index for total blend.

I_i = blending index for component ***i***.

The blending constraints are written using the blending index value instead of the true property value of components. The product blending index in any stage of the optimisation process has to be transformed back to the actual product quality to meet the specification required (Baker *et al*, 1996). Because of the simplicity and universality of LP techniques, there are advantages in transforming non-linearities into approximate linear equivalents, rather than in using non-linear methods which have to be tailored to the specific problem (Frank, 1995).

The qualities blended in the refinery LP model must be based on the same units, that is weight, volume, or molal. In the USA, most refinery LP models and blending calculations are based on volume units since these are the common units for the domestic petroleum business. However, in Europe and elsewhere, weight units are most often used. In South Africa, for example; blending of Marine Fuel Oil (MFO) is volumetric, but the final product is sold in weight units of metric tonnes.

2.2 Visbreaking Process

The understanding of the visbreaking process requires firstly, a clear definition of the process objective and the process variables, and secondly, a detailed discussion of

- Process Description & Kinetics
- Process Performance
- Process Configuration
- Fuel Oil Blending

The following section attempts to define the process objective and the process variables. This is followed by a detailed discussion on other aspects of the visbreaking operations.

Process Objective is:

To reduce the viscosity and pour point of residua and use less cutter-stock;

To produce stable Marine Fuel Oil (MFO), which meets the required specification;

To produce gasoline;

To produce light gas oil (diesel) and heavy gas oil (feed for catalytic cracker).

Process Variables are:

Temperature

Pressure

Time of reaction (residence time)

Characteristics of the charge stock (quality of feedstocks).

Process Description & Kinetics

Visbreaking is a relatively mild noncatalytic thermal cracking operation. It is mainly used to reduce the viscosities and pour points of the refinery heavy residua such as crude tower bottoms, vacuum tower bottoms, and deasphalter

bottoms to meet the Marine Fuel Oil (MFO) specification. It is also used to reduce the amount of light materials (cutterstock) required to dilute these residua to meet the MFO's specification. Visbreaking can reduce a refinery's production of fuel oil by 20-35% and cutter stock requirements by 20-30%. Visbreaking is also used to increase the gasoline and gas oil yields and to produce feedstocks for the Fluid Catalytic Cracker unit.

The conversion of the refinery heavy residue is accomplished by heating the residue material to high temperatures in a furnace. The material is passed through a soaking zone, located either in the heater or in an external drum, under proper temperature and pressure constraints so as to produce the desired products. The heater effluent is then quenched with a quenching medium to stop the reaction. With refineries today processing heavier crudes and having greater demand for distillate products, visbreaking offers a low-cost conversion capability to produce incremental gasoline and distillate products while simultaneously reducing fuel oil viscosity.

Long paraffinic side chains attached to aromatic rings are the primary cause of high pour points and viscosities for paraffinic base residua. Visbreaking is carried out at conditions to optimise the breaking off of these long side-chains and their subsequent cracking to shorter molecules with lower viscosities and pour points. The amount of cracking is limited, however, because if the operation is too severe the resulting product becomes unstable. The oil then forms polymerisation products during storage causing filter plugging and sludge formation.

The extent of residue conversion is limited by a number of feedstock characteristics, such as asphaltenes, sulphur, sodium, and Conradson carbon content. A feedstock with high asphaltenes will result in an overall lower conversion than normal asphaltene feedstocks, while maintaining production of a stable fuel oil from visbreaker bottoms. Also the presence of sodium, as well as higher levels of feed Conradson Carbon, can increase the rate of coking in the heater tubes. Minimising the sodium content to almost negligible amount and

minimising the conradson carbon weight percent will result in a longer cycle run length.

In summary, the principal reactions that occur during the visbreaking operations are:

1- Cracking of the side-chains attached to cycloparaffin and aromatic rings at or close to the ring, so the chains are either removed or shortened to methyl (CH_3^+) or ethyl groups ($C_2H_5^+$).

2- Cracking of resins to light hydrocarbons (primary olefins) and compounds which convert to asphaltenes.

3- At temperatures above 900°F(483°C), some cracking of naphthenic rings occurs. There is little cracking of naphthenic rings below 900° F.

4- Chain radical reactions (dominant mechanism in visbreaking process).

Although certain processes, such as polymerisation, are exothermic, the visbreaking reaction essentially remains endothermic, meaning that high temperature is required to achieve the target conversion in order to maximise the yield of white oil.

From the aforementioned discussion, we conclude that in the absence of a catalyst, the process of thermal decomposition of mixed-hydrocarbons, such as the crude residue, is difficult to understand and almost impossible to control. On account of the visbreaking reaction's complex nature, the extent and number of process variables is unknown. However, the fundamental variables in all types of cracking operations (namely; temperature, pressure, time, and feedstocks quality) influence the visbreaking operations.

Process Performance

The visbreaking process performance has historically been a controversial issue. The yardstick used to measure the unit's performance is "*Conversion*"; the ratio of the quantity of feed converted to other products in the process. Traditionally, conversion is defined as the yield of gas plus gasoline. Some researchers however, use the combination of the gas, gasoline, and distillate yields. Others have related the conversion to the severity of the visbreaking process.

The severity of the visbreaking operation can be expressed in several ways: the yield of materials boiling below 330°F(165°C) , the reduction in product viscosity, and the amount of standard cutter stock needed to blend the visbreaker bottom products to Marine Fuel Oil's specification compared to the amount needed for the feedstocks (Cooper *et al*, 1962).

Although the term used throughout this project is "*conversion*"; its definition greatly varies from the traditional definition(s) already explained above. In line with the modern visbreaking process configuration and economics, this project re-defines the term visbreaking conversion as:

> Volume percentage of the visbreaker's white oils, obtained from the visbreaking of the heavy residue(s). These products are; gasoline or naphtha, kerosene, and the visbreaker's diesel, which are usually collected from the atmospheric tower of the visbreaker unit.

Mathematically this can be shown as follows:

$$\textit{Conversion} = \left(\sum_{i=1}^{n} x_i * 100\right) / V_f \qquad (2.7)$$

where

x_i = Volume of white products *i.* Produced by the visbreaker and n is the number of products.

V_f = Total volume of feed to the unit.

This definition of the visbreaking conversion is also consistent with the fundamentals of the visbreaking process variables and fuel oil blending operations. Clearly, the objective is to find an optimal solution to the complex problem of an integrated system that combines the visbreaking and fuel oil blending operations.

The importance of the conversion, and its effect on the overall system's optimality is shown in the following diagram.

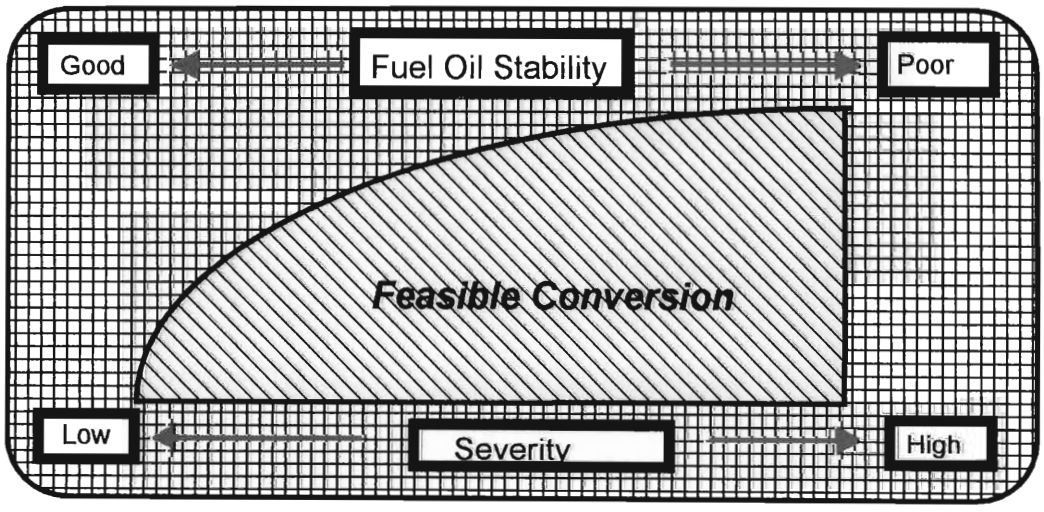


Figure 2-2 Feasibility of the visbreaking operations. The higher severity result in a higher profit but the fuel oil becomes unstable.

It can be seen from Figure 2.2 that higher visbreaking severity results in higher conversion, that in turn increases the white oil yield, which improves the visbreaking performance. The drawback is the stability of the fuel oil, which is adversely affected by an increase in the process conversion. In order to understand this conflicting statement, a few words should be said about the structure of a typical petroleum residuum and its transformations during the process of visbreaking. A typical petroleum residuum, as obtained after a simple distillation operation, consists of three classes of compounds, loosely defined as; hydrocarbons, resins and asphaltenes (Siewert *et al*, 1985).

As discussed earlier, the asphaltenes are high molecular weight agglomerates held together by physical forces and they can be precipitated from a residue by paraffinic solvents. The resins are thought of as very high molecular compounds, which can be separated from a deasphalted residue by adsorption. The typical petroleum residuum is a colloidal solution in which the asphaltenes are held in a colloidal suspension in the hydrocarbon phase, the resins and aromatic hydrocarbons acting as peptising agents (Sane *et al*, 1992).

According to Dominici *et al* (1995,1) feedstock with low *n*-pentane insolubles (low asphaltenes) show good susceptibility to visbreaking while those having high values of *n*-pentane insoluble respond poorly. The following figure shows the capability of greater conversion at lower *n*-pentane insoluble for a 900 ^{o}F (482 ^{o}C) vacuum residue.

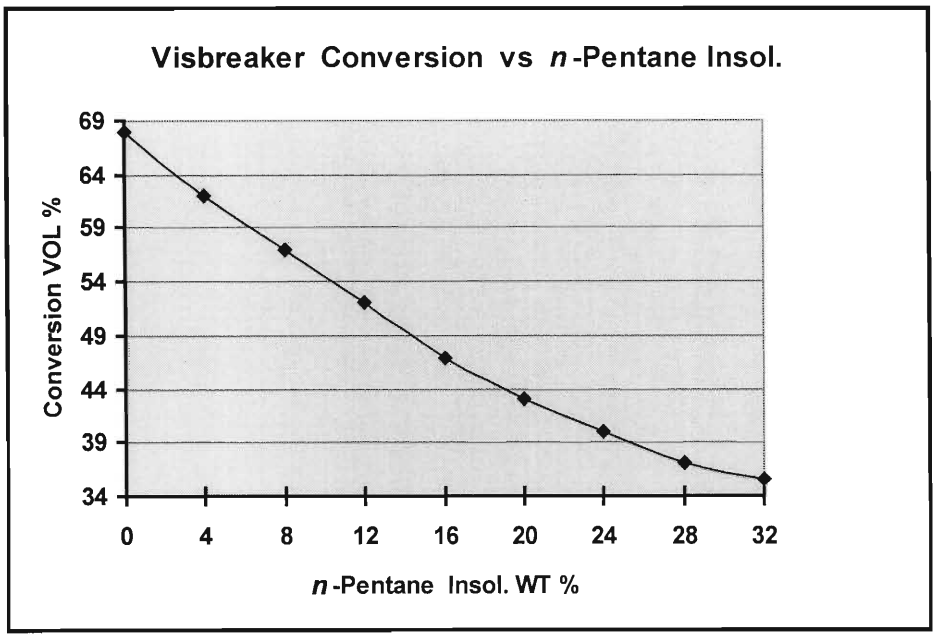


Figure 2-3 Visbreaking susceptibility (900 $^{o}F^{+}$ charge converted)

From "*Handbook of Petroleum Refining Processes by Meyers*".

Undoubtedly, the *n*-Pentane insoluble of the feedstocks is one of the many parameters affecting the visbreaker's conversion. The visbreaker's conversion is also dependent on the process reaction. During the thermal process of visbreaking, two processes take place. The hydrocarbons are partly cracked, producing lighter products which can be distilled out and, at the same time, carboids and coke are formed through polymerisation, condensation, dehydrogenation and de-alkylation reactions.

These carboids and coke, as well as the asphaltenes, continue to be held in a stable colloidal solution or suspension up to a certain limit of conversion. Past this limit they tend to separate and to form deposits, either in storage tanks, or in the equipment used for heating and burning the residual fuel oils. Additionally, at the limit, operational difficulties can be experienced in the visbreaking unit itself. This means that the visbreaker unit has to be temporarily shut down for a coke clean up, a process often called a "de-coke". This phenomenon generally sets the upper limit of conversion in a typical visbreaking process.

Several analytical methods are used to determine the stability of the residual fuel oil. These are:

- Sedimentation
- Navy Boiler and Turbine Tests.
- Hot filtration test
- Shell filtration test
- Institute of Petroleum test(s)

Although all of them represent certain aspects of the stability of the visbreaker's residue, they ***are not*** equivalent. Some of them are only qualitative measures of this stability.

To forecast the fuel oil stability, intensive experimental studies have been performed on the characteristics of the visbroken residua. Janis and Carlo (1992) have used the Nuclear Magnetic Resonance (NMR) technology to study the nature and characteristics of the residuum and asphaltenes of the crude atmospheric bottom. Using data from a visbreaker pilot plant, they have further developed an empirical equation to estimate the maximum volume of a paraffinic solvent (cetane) that can cause precipitation of asphaltenes. An arbitrary term, "stability index" has been developed using the following equation:

$$SX = 1 + X_{max} \qquad \textbf{(2.8)}$$

where

X_{max} is the maximum volume of cetane in millilitres that can be added to a gram of product without causing sedimentation.

In summary, so far, no satisfactory mathematical relationships exist that can produce a meaningful and reliable forecast of the quality of the visbreaker's products.

Process configuration

There are many types of visbreaker operations. The soaker cracker developed by Shell Petroleum (Geelen and Akabr, 1981) is known to be one of the popular types used by many refiners. Foster Wheeler, UOP of USA and IFP of France have engineered a number of these types of visbreakers as well.

In this configuration, a soaker drum is added to increase the residence time and thus achieve a high volume conversion at longer de-coke cycles. In general, the soaker process achieves some conversion within the heater, but the majority of the conversion occurs in a reaction vessel or soaker which holds the two-phase effluent at an elevated temperature for a predetermined length of time. By providing the residence time required to achieve the desired reaction, the soaker drum design allows the heater to operate at a lower outlet temperature. This outlet temperature of the lower heater results in a lower fuel cost. Although there is an apparent fuel saving advantage experienced by the soaker-drum type design, there are also some disadvantages. The main disadvantage is the de-coking operation of the heater and soaker drum. Although de-coking requirements of the soaker design are not as frequent as those of the conventional (coil-type) design, a visbreaker with the soaker configuration requires more equipment for coke removal and handling.

A simplified flow scheme of a soaker visbreaker is shown in Figure 2.4

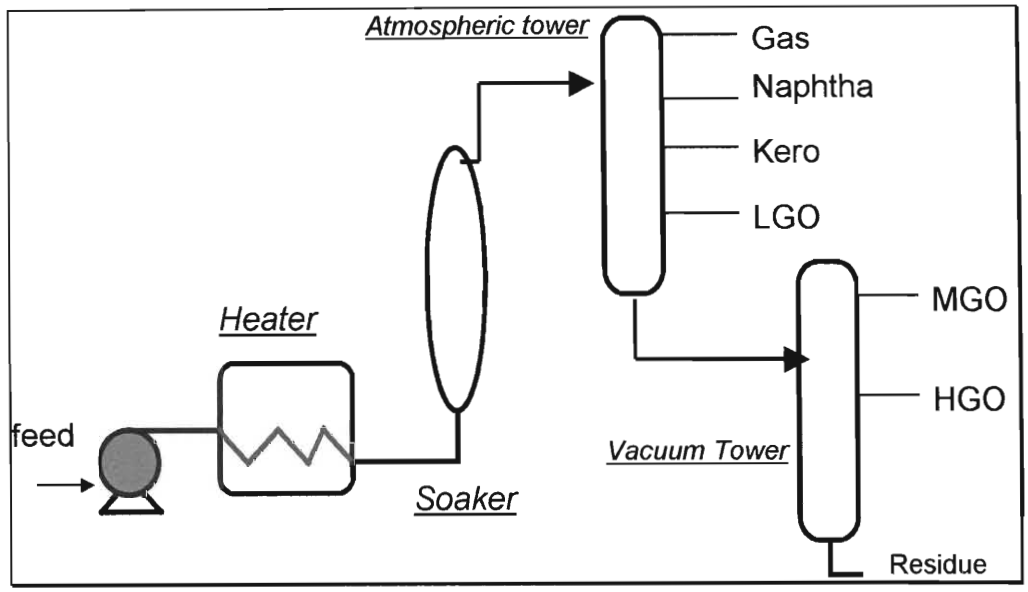


Figure 2-4 Typical Soaker Visbreaker with the Atmospheric and Vacuum Towers.

The visbreaking operation occurs in the heater along a curve of increasing temperature and decreasing pressure. Obviously, the rate of reaction increases with the process temperature. In practice a so-called "soaking factor" is often used to assess the total operating severity both for design purposes and for following the operation of industrial plants. The soaking factor is calculated as follows:

$$\boldsymbol{F} = \frac{1}{D}\int_{0}^{v}\frac{Pt}{P0}\frac{Kt}{K0}dV \qquad \textbf{(2.9)}$$

where:

$\boldsymbol{F}$ = soaking factor is defined as the equivalent coil volume in cubic feet per daily barrel of charge to unit.

V = coil volume in cu ft per bbl of daily throughput

D = feedstocks flow rate in bbl/day

P_t = pressure at a given point in the coil in PSIG.

K_t = reaction rate constant at a given temperature in Fahrenheit.

P_0, K_0 = standard reference values for P_t , K_t (relative cracking reaction velocity at temperature Fahrenheit)

Such an equation permits the calculation of the conversion to be expected in a given volume of heater coil, for a given feedstock and at given heater outlet conditions. The use of the soaking factor must be combined with the correct heat transfer characteristics of the coil, since a correct soaking factor does not in itself guarantee either long cycles or a stable fuel oil (Gearhart *et al* , 1992). This is mainly a function of feed quality and process kinetics. In essence, the soaking factor is not strictly comparable with conversions for naphthas and gas oil since each stock has a different equivalent datum temperature for initial conversion due to thermodynamic consideration.

The unit under study is a soaker visbreaker with a vacuum flasher. In this configuration, the visbreaker atmospheric tower bottom is sent to a vacuum tower flash zone. The liquid portion of the feed falls to the bottom section of the tower, where it is steam-stripped. The vapour portion rises through the tower wash section and then is partially condensed into distillate products. Usually, there are 2 to 3 side draws. On the lower drawoff, heavy visbroken vacuum gas oil product and pumparound along with wash oil are withdrawn. On the upper drawoff, light and medium gas oils and reflux are withdrawn. Linear programming is used to determine the visbroken gas oil disposition (e.g. catalytic cracker, thermal cracker, refinery residual fuel oil pool,…etc.).

The overhead vapours from the vacuum tower flow to a multi-stage vacuum ejector system. Condensed vapour and steam are collected in a condensate accumulator.

Although the usual feed (chargestock) is a vacuum residuum, other stocks that are occasionally visbroken are de-asphalter bottoms (TAR) and crude atmospheric residua. Visbreaking produces a small quantity of gas and a fair

amount of low octane gasoline often referred to as wild naphtha. The kerosene stream is rich in olefins and in most cases it is used as the cutterstock (a product used to dilute the bottom residue to the fuel oil viscosity limit). Depending on the visbreaker's operation, and fuel oil blending, the light gas oil is either used as cutterstock, or can be blended into diesel. The medium and heavy gas oils (MGO and HGO) are often routed to the Fluid Catalytic Cracker Unit (FCCU) for further processing.

A typical visbreaker's products and their possible disposition is presented in the Figure 2-5 below.

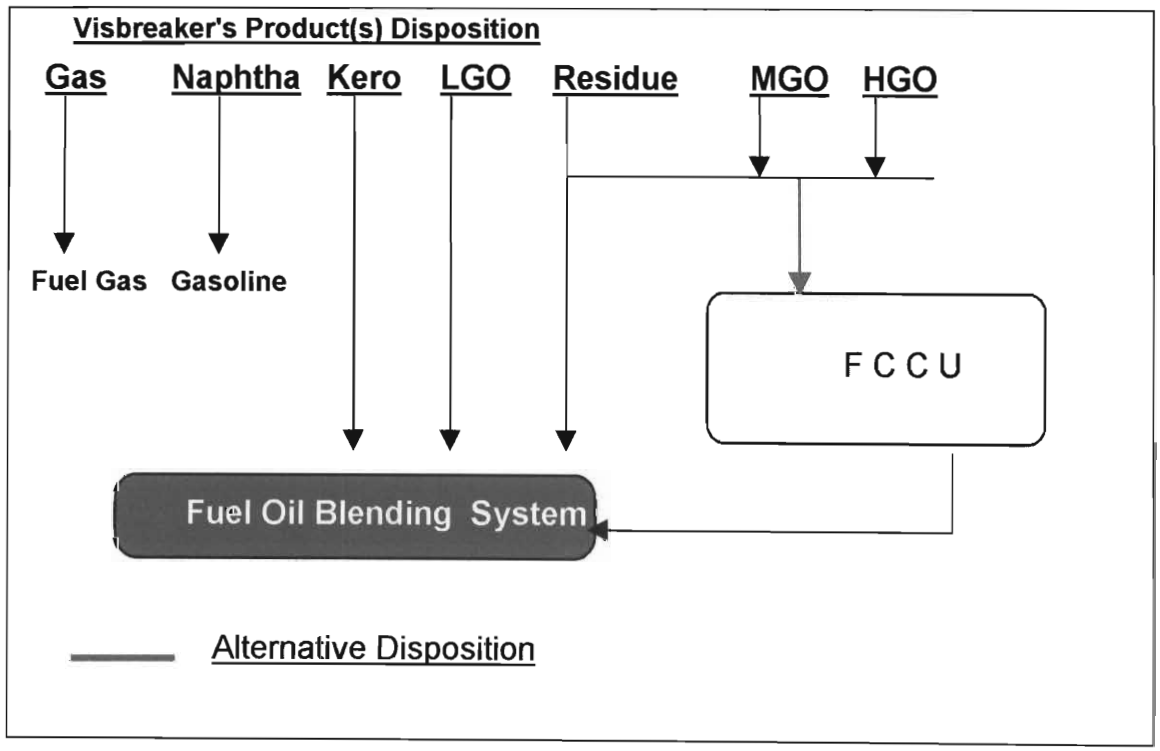


Figure 2-5 Typical visbreaker's product disposition.

It is evident from the Figure 2.5 that, the visbreaker's products have many possible dispositions (destinations), either as a feed to other units (FCCU) or, as a component in product blending (various pools).

In summary, the main operating variables in visbreaking are temperature, pressure, and residence time. The severity of the plant changes with a change in

any one of these three variables. To achieve a certain severity, these variables can be interchanged within limits. For a given severity, as measured by conversion, product distribution and quality are virtually unchanged (Dominici *et al*, 1995, 2).

An increase in yields of distillate and gaseous hydrocarbons can be achieved by increasing visbreaking severity. For example, by raising the heater outlet temperature. Increasing visbreaking severity will also result in a reduction of cutter stock required to meet fuel oil specifications. However, the higher severity will cause the heavy distillate oils to break down and crack to lighter components. These heavy distillate oils act to solubilize (peptise) the asphaltic constituents. The asphaltic constituents will then tend to separate out of oil and form coke deposits in the furnace. Visbreaker operation at this level can cause premature unit shutdowns. There is also a tendency to produce unstable fuel oils at these more severe conditions.

Fuel Oil blending

Increased operating flexibility and profits result when refinery operations produce basic intermediate streams that can be blended to produce a variety of on-specification finished products. The objective of fuel oil blending is to allocate the available blending components in such a way as to meet the end product's specification at the least cost (Wenzel, 1992).

The refiner blends fuel oils for two reasons; first, to meet certain specifications and second, to make the oil easier to handle. When blending the heavy residual oils, the viscous nature of these residuals, as well as the wide spread in gravity between the heavy oil and distillate, make mixing more difficult. Complete mixing of these blends is not always satisfactorily accomplished.

If a refinery is situated near a major waterway or port, then the fuel oil is usually blended to meet the required bunker, or marine fuel oil specification.

Sophisticated linear programming models are often used to generate the blending recipe. However, blending components to meet all critical specifications most economically is a trial-and-error procedure.

In most refineries, fuel oil blending is a batch process (Schmidt, 1985), where the visbreaker's bottom residue is blended into marine fuel oil (MFO).

The finished fuel oil should also comply with international and local limitations and requirements that may be stipulated by the customers, or environmentally related laws and regulations.

Typical components available to the residual fuel blending system are shown below:

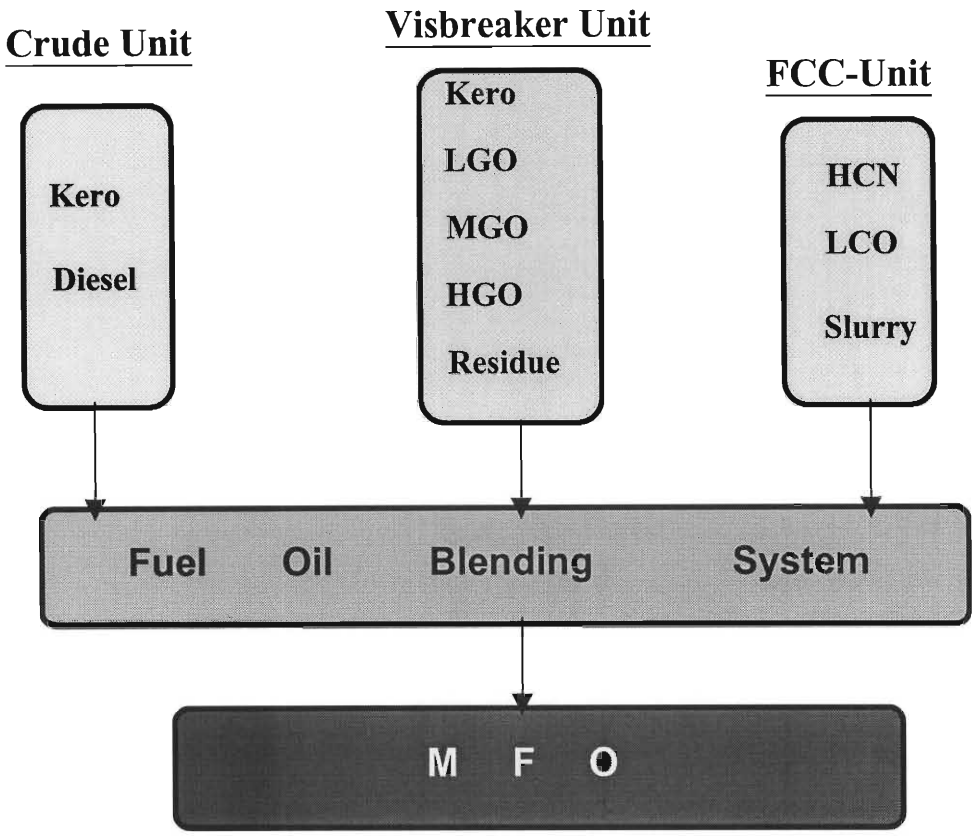


Figure 2-6 Typical components used in Fuel Oil Blending System.

As stated earlier, the refinery LP model is employed to generate the blend's recipe as well as to determine the alternative routing of the other components. The economics of the refinery is highly sensitive to the fuel oil recipe, blending procedure, and the finished product's pricing structure.

In concluding this section, the review of the visbreaking operation reveals that, because of the many contributing factors, the process of upgrading the refinery residua is in fact complex in nature. As yet, no simple, generic solution

can be identified which can fully describe the mechanism of the thermal decomposition of the petroleum residues. Consequently, the practical plant experience in many respects can provide a better understanding of the visbreaking process.

CHAPTER 3

MODELLING & METHODOLOGY

The purpose of this chapter is, firstly, to formulate the problem associated with predicting the yields of the visbreaking process and, secondly, to propose a computerised solution strategy using the principles of artificial neural networks and other mathematical modelling techniques.

3.1 Model formulation

In the beginning of this thesis, we stated that a mathematical model based on the principles of the artificial neural network can be utilised to predict the yields of the visbreaking process. From a practical standpoint, this is because the process of thermo-decomposition of hydrocarbon residue cannot satisfactorily be described by the theory of the thermo-kinetics. What is required is an amalgamation of physical modelling with that of the neural network systems. In their recent survey Thompson & Martin (1996) have demonstrated that the methods of large-scale neural network modelling are complementary with those of physical modelling widely used in the refining and petrochemical process industries.

Since the introduction of the visbreaking process, engineers and scientists have been eager to find a way of estimating the product yields and properties of the said unit. As stated previously, the complexity of the problem is

compounded by the uncontrollable and often unknown reactions resulting in asphaltenes formation, change of yield's pattern, or properties of the bottom residue. In this respect, the important criteria in modelling the visbreaker unit can be classified as follows:

Input

- Feed flow rate (velocity and resident time)
- Feed quality
- Unit's operating condition (temperature and pressure)

Output

- Product yields
- Quality of the visbreaker's products

As noted before, we will be using an artificial neural network system to model the visbreaker unit. The neural network is an information processing system that learns from the historical events and predicts the future trend. In this context any neurally based system requires an input and an output layer. Accordingly, in the remaining of this section, we present and describe the methodology employed to prepare the system's input and output data sets.

System's Input: Feedstock Quality, and Unit Operating Conditions.

The system's input consists of two major parts; feedstock quality, and the unit's operating condition, shown as follows:

$$\text{System Input } I = \begin{bmatrix} f_q \\ U_c \end{bmatrix} \qquad \textbf{(3.1)}$$

where;

f_q = feedstock quality

U_c = unit's operating conditions

Feedstock Quality

The quality of the feed charged to the visbreaker unit is represented by the vector $\boldsymbol{f_q} = \begin{bmatrix} f_1 \\ \\ f_n \end{bmatrix}$

This relationship can be shown as

$$f_j = \sum_{i=1}^{n} V_i \begin{bmatrix} q_{i,1} \\ \\ q_{i,n} \end{bmatrix} \qquad \textbf{(3.2)}$$

where V_i is the volume fraction of the stream i. ($i=1...,n$) and $q_{i,j}$. ($j=1...,n$) represent various quality components of stream i. Obviously, this equation is only valid if the blending relationships are linear. As discussed in section 2.2 of chapter 2, the blending indices are used to form the non-linear relationships.

In this research work, the feed to the visbreaker unit consists of the following refinery streams :

VR = Vacuum Residue

AR = Atmospheric Residue

TAR = De-asphalter Residue

HDON = Hydrogen Donor, often high aromatic diesel stock

The important properties of the feedstock are (as defined in Appendix-1):

VBI = Viscosity Blending Index at 122 °F (50 °C)

CCR= Conradson Carbon Residue in weight percent

API = API degrees

KFC= K-factor (UOP K-factor or Watson K-factor, expressed as an index or a factor defined in Appendix -1).

SUL = Sulphur content in weight percent

Using the above terms, we define the relationships between the input vectors and the feedstocks quality. This is shown below:

$$f_q = \left(V_{VR} * \begin{bmatrix} \text{VBI} \\ \text{CCR} \\ \text{API} \\ \text{KFC} \\ \text{SUL} \end{bmatrix}_{VR} + V_{AR} * \begin{bmatrix} \text{VBI} \\ \text{CCR} \\ \text{API} \\ \text{KFC} \\ \text{SUL} \end{bmatrix}_{AR} + V_{TAR} * \begin{bmatrix} \text{VBI} \\ \text{CCR} \\ \text{API} \\ \text{KFC} \\ \text{SUL} \end{bmatrix}_{TAR} + V_{HDON} * \begin{bmatrix} \text{VBI} \\ \text{CCR} \\ \text{API} \\ \text{KFC} \\ \text{SUL} \end{bmatrix}_{HDON} \right) / V_{Total} \quad (3.3)$$

It can be clearly seen that quality of the feed to the unit changes with a change in the quality or volume fraction of the components contained in it.

Next, we have to define the total volume of the feed (per day of operation) to the unit as the sum of the individual components of the feed. This is shown below:

$$V_{Total} = V_{VR} + V_{AR} + V_{TAR} + V_{HDON} \quad (3.4)$$

Expressed in cubic meter per day of visbreaker operation.

Unit's Operating Condition

The unit's operating condition u_c is dependent on the temperature, pressure, and flow rate. It should be noted that the overall process of visbreaking and fuel oil blending are in fact extremely complex and dynamic. In this case, since the possible effect of the equipment's ageing, cannot accurately be measured, or ascertained, it will not count as an independent variable.

The plant monitoring system is programmed to update the material flow every 60 seconds, then calculate and report the consolidated data for every 24

hours of visbreaking operations. The volume of feed to the visbreaker unit is a volatile variable that needs to be defined. In this respect, refinery planners often introduce some empirical terms that can assist them in their estimation. For the sake of clarity, let us introduce a term called the Transit Period, **TRP** , which represents the time in seconds for one cubic meter (m^3) of feed to travel through the visbreaker unit comprising of the soaker drum, the atmospheric tower, and the vacuum tower. This is calculated as follows:

$$\mathbf{TRP} = \frac{(24*60*60)}{V_{Total}} \qquad (s.m^{-3}) \qquad \textbf{(3.5)}$$

Where V_{Total} is the total volume of feed per day.

It should be noted that this is a ***convenient*** way of representing the volume of feed charged to the visbreaker unit, therefore, this term should not be mistaken with the cracking residence time, a term not applicable to this study.

As discussed earlier, the theory of thermo-kinetics cannot satisfactorily provide a scientific correlation between all the pre-defined elements of the input data and the process conversion. It does however provide some rules that can be used as a yardstick to establish the validity of the input data. According to the laws of thermo-kinetics, an increase in the system's temperature should result in a higher cracking rate for the heavy hydrocarbon residue. Inversely, the lowering of the system pressure at a constant temperature results in an increase in the process conversion. As a result, along with the TRP, it is necessary to include both pressure and temperature in the proposed model.

Since the severity of the visbreaking process is time and temperature dependent, the term TRP can be used to define the effect of the process severity on one cubic meter of the mixed feed at temperature interval Δ_t. In this respect, along with the variations in the feedstock quality, the relationships between the TRP and temperature are extremely sensitive to the system's output. In other words, the temperature at the Soaker drum should be adjusted to correspond to the variation in the TRP. However, no pre-defined rules exist that can satisfactorily be used to adjust the temperature with the variation in the TRP.

Another advantage of the TRP is that unlike the total feed V_{Total} its value is in line with the scale of the values applied to the other elements of the feed's quality vector, as given in the equation (3.3).

The following schematic provides a complete picture of the paradigm's input variables:

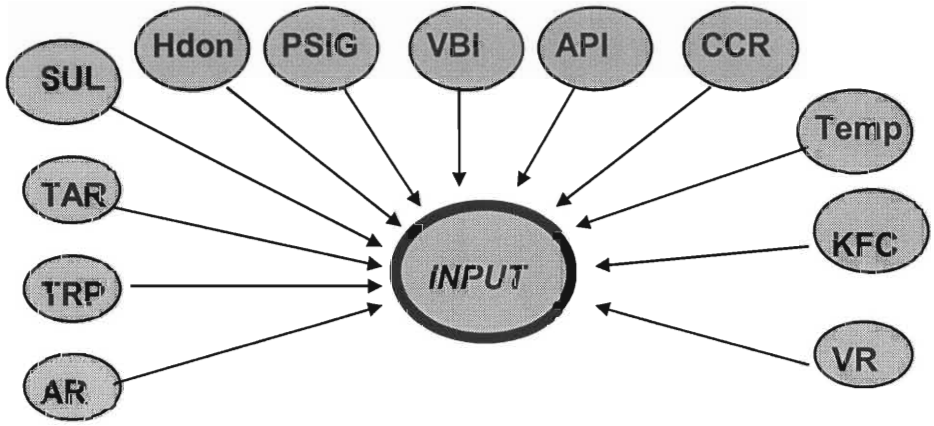


Figure 3-1 Illustration of an Individual Data set. (A total of 141 data sets, each having 12 data elements. (the input nodes are defined under Feedstock Quality in chapter 3. pp.54 . Further information on neural network model formulation is presented in Appendix-3).

System's Output: Product Yields and Quality.

At this stage, we define the system's output as a single response to a stimulus. In other words, any change in the value of any element of the input data-set generates ***a*** response. In line with the modern visbreaking process configuration and economics, we define the system's response as the process *conversion*. Furthermore, as explained earlier, the term conversion is defined as :

> The volume percentage of visbreaker products obtained from the thermal cracking of heavy residua. These products are; gasoline or naphtha, kerosene, and visbreaker diesel, which are usually collected from the atmospheric fractionation tower of the visbreaker unit.

In modelling the visbreaking operations, we have assumed that the neural network has to learn from the real world examples. The real world inputs are observations (measurements of data), obtained by means of sensors designed to probe the environment in which the neural network is supposed to operate. Ordinarily, these observations are inherently noisy, being subject to errors due to sensor noise and system imperfections. In any event, the observations so obtained provide the pool of information from which the examples used to train the neural networks are drawn. Needless to say, the predictability of the paradigms trained with real world observations is often poor. This of course is not a modelling fault. It is for these reasons that we base our proposed model on a single response to the input stimulus; namely the visbreaker's volume conversion. Accordingly, at the initial stage of model making, we introduce a prototype paradigm of the visbreaking operation. The rationale behind prototype fabrication, rather than a full-scale paradigm, will be discussed in the following section.

Accordingly, the prototype neuronal model of the visbreaker unit needs to learn from the historical data, concerning feed flow rate, feed quality, plant's operating condition(s), and conversion achieved under these circumstances. In

return, the model is expected to produce a single response to the given input; and predict the percent volume conversion across the process unit. To determine the quality of the response, the network results should be closely examined. If the quality of the response is satisfactory, then a multi-response model can be developed.

In summary, the proposed neural network model is a multi-layer system with the following characteristics:

Input nodes: 12 input nodes related to the feed quality, feed rate, and unit's operating condition.

Output nodes: Initially a single node (unit's volume percent conversion), expanding to a multi-response neural system that has to be linked to the heavy fuel oil blending module to optimise the blending operations.

3.2 Proposed Approach – Solution Technique

This section begins with formulating a prototype paradigm to predict the visbreaker's percent volume conversion. The rationale behind the prototype fabrication, rather than full scale paradigm, is that we have no prior knowledge regarding the complexity of the model nor the noisiness of the input data. Hence, instead of developing a large network and then prune out the non-contributing connections, we opted to build a prototype paradigm that, if satisfactory, can later be extended to a full scale multi-response neural network system. Accordingly, the process of the network formation is divided into the following phases:

Prototype Fabrication Phase: Formation of the Many-To-One network, where the objective is to produce a multi-layer neural system that is capable of predicting the volume percent conversion of the visbreaker unit.
The development of the idea of the prototype paradigm, was influenced by the work of Stephen Grossberg printed in the book "Neural Networks and Natural Intelligence" (1989).

Full Scale Paradigm Fabrication Phase: Evolution of the Many-To-One topology to the Many-To-Many network by extending the number of the output nodes to accommodate the full spectrum of the visbreaker's products and the quality of the visbreaker's residue.

Fuel Oil Blending Phase: Where the Many-To-Many paradigm interacts with the fuel oil blending and optimisation operations.

Prototype Paradigm Fabrication Phase

The input to this network consists of several data sets, each having 12 data elements. The prototype paradigm is called "Many-to-One", since there is a single system output, namely; volume percent conversion of the visbreaker unit.

The next step is to select an architecture and the learning algorithm. This research work uses the Cascade method of network construction together with the adaptive gradient back propagation learning rule. Back propagation is one of the earlier learning algorithm used in neural systems. Back propagation iteratively reduces the error of fit to learning samples by fine tuning the weights in the network. Each iteration consists of two stages: forward propagation and reverse propagation. Forward propagation computes the output of the network using the input vector. The total error is derived in forward propagation by comparing desired and actual outputs. Reverse propagation computes the error derivative with respect to all the weights in the network. The error derivative assigned to each weight estimates the effect of each weight on the total error.

Due to its simplicity, Cascade architecture is selected as the means to develop the many-to-one paradigm. In this respect, the constructive approach in paradigm building (developed by Scott Fahlman (1990) of Carnegie Mellon University) is adopted. In its original form, this technique is referred to as the Cascade Correlation. The "Cascade" part of this title refers to the architecture and its mode of construction. This entails adding hidden units (network nodes lying between input and output) one at a time, and always connecting all the previous units to the current unit. The "Correlation" part of the title refers to the way hidden units are trained by trying to maximise the correlation between the output of the hidden unit and the desired output of the network across the training data.

In general, the Cascade Correlation is a supervised learning architecture that builds a near-minimal, multi-layer network topology in the course of training. This single layer of connections is trained to minimise the error. When no further improvement is seen in the level of error, the network's performance is evaluated. If the error is small enough, the process is terminated. Otherwise a new hidden unit is added to the network in an attempt to reduce the residual error.

The major benefit of using the Cascade Correlation algorithm is that there is no need for the user to guess in advance the network's size, and topology. The schematic of the Cascade architecture is shown below:

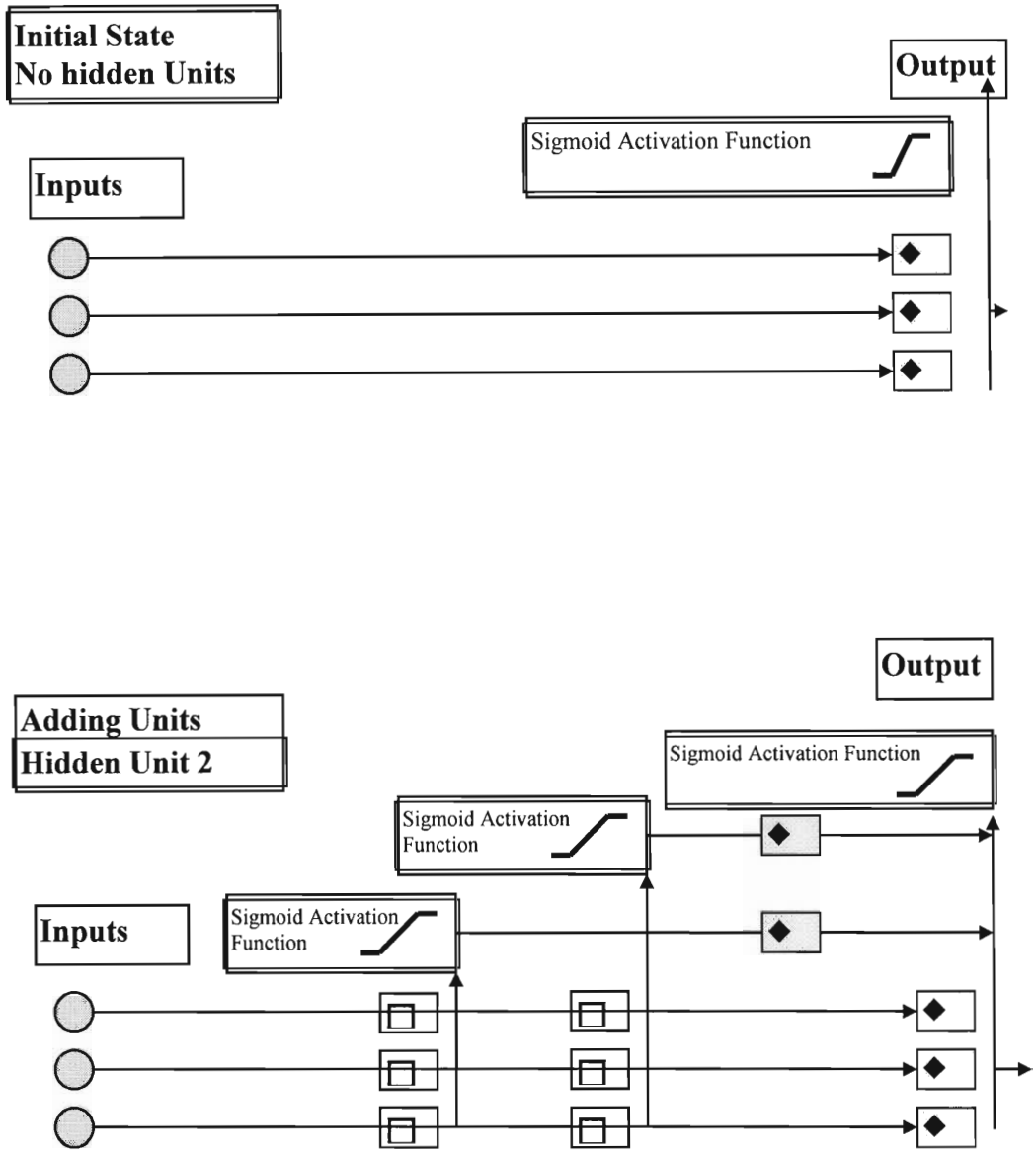


Figure 3-3. The Cascade architecture, initial state and after adding two hidden units. The vertical lines sum all incoming activation. Boxed connections are frozen, ◆ connections are trained repeatedly.
Sigmoid activation function is defined in Appendix –3.

As stated earlier, the cascade correlation network consists of input units, hidden units, and output units. Input units are connected directly to output units

with adjustable weighted connections. Connections from inputs to a hidden unit are trained when the hidden unit is added to the network and are then frozen. Connections from the hidden units to the output units are adjustable. It can be seen from the above figure the second hidden unit receives an input signal both from the *input units* and from the previous *hidden unit*. All weights on these connections are adjusted and then frozen. The connections to the output units are then trained. The process of adding a new unit, training its weight from the input units and previously added hidden units, and then freezing the weights, followed by training all connections to the output units, is continued until the error reaches an acceptable level of the maximum number of epoch's (or hidden units) is reached. An epoch is defined as one pass through the entire training set, followed by a weight update (Zupan, 1993). Here, the objective is to construct and train a network that is capable of producing an output, namely, "*conversion*".

The training of the output units, that is, volume percent visbreaker conversion (defined as the sum of products that boil at a temperature less than 900 degrees F), starts by minimising the sum-squared error function of $\boldsymbol{E}$, as given by:

$$\boldsymbol{E} = \frac{1}{2} \sum_{o,p} (\boldsymbol{Y_{op}} - \boldsymbol{T_{op}})^2 \qquad \textbf{(3.6)}$$

where $\boldsymbol{Y_{op}}$ is the observed value of output $\boldsymbol{o}$ from training pattern $\boldsymbol{p}$, and $\boldsymbol{T_{op}}$ is the predicted. Although any optimisation algorithm can be used to minimise $\boldsymbol{E}$ cascade correlation employs the gradient descent method using

$$\boldsymbol{e_{op}} = (\boldsymbol{Y_{op}} - \boldsymbol{T_{op}}) \boldsymbol{f'_p} \qquad \text{and} \qquad \textbf{(3.7)}$$

$$\frac{\partial E}{\partial W_{oi}} = \sum_{p} \boldsymbol{e_{op}} \boldsymbol{I_{ip}} \qquad \textbf{(3.8)}$$

where f'_p is the derivative of the sigmoid activation function of the output unit for pattern p , I_{ip} is the value of the input (or hidden unit) i and W_{oi} is the weight connecting input i to output 0.

Candidate units are trained to maximise C, the correlation between the candidate unit's output Y and the residual errors e_o still observed at the outputs of the active network. This correlation is computed over all the training patterns p. The correlation between the candidate unit's, C is defined as

$$C = \sum_o \sum_p (Y_p - \bar{y}) (e_{op} - \bar{e}_o) \qquad (3.9)$$

where $\bar{y}$ and $\bar{e}_o$ are average of y and e_o over all patterns p. The maximisation of C proceeds by gradient ascent using

$$\delta p = \sum_o \sigma_o (e_{op} - \bar{e}_o) f'_p \text{ and} \qquad (3.10)$$

$$\frac{\partial C}{\partial W_i} = \sum_p \delta p I_{ip} \qquad (3.11)$$

where σ_o is the sign of the correlation between the candidate unit's value and the residual error at output o . Each candidate unit in the pool starts from a different set of initial weights and independently tries to maximise its own C value.

Given the gradient values computed above, we could in principle minimise E and maximise C by steepest gradient descent (or ascent). Instead, to get good convergence in a reasonable number of cycles, we can use the quickprop algorithm (Fahlman, 1990) to compute the updates. Abbreviating the slopes

$\frac{\partial E}{\partial W}$ and $-\frac{\partial C}{\partial W}$ by S and t, respectively, the weight change Δw is computed by

$$\Delta Wt = \begin{cases} \varepsilon S(t), & \text{if } \Delta W_{t-1} = 0 \\ \frac{S(t)}{S(t-1)-S(t)} \Delta W_{t-1}, & \text{if } \Delta W_{t-1} \neq 0 \text{ and } \frac{S(t)}{S(t-1)-S(t)} < \mu \\ \mu \Delta W_{t-1}, & \text{otherwise.} \end{cases} \quad \textbf{(3.12)}$$

Here, ε is a parameter that controls the linear steps used to get the algorithm started. The parameter μ controls the maximum step-size compared to the previous step. Weights are now updated using

$$W(t-1) = W(t) + \Delta W(t) \quad \textbf{(3.13)}$$

This description of the cascade correlation and quickprop algorithm is slightly over-simplified, but it is sufficient to demonstrate how the topology of the many-to-one paradigm is formed. In this case, our multi-layer paradigm consists of three layers; one input layer, one output layer, and an intermediate or hidden layer. The number of the units per input and output layer is 12 and 1 respectively. The cascade correlation algorithm should determine the number of nodes or units in the hidden layer. The process of node addition and learning stops, when for every system patience (defined as 2 iterations) there is no improvement to the objective function by the tolerance value of 0.002. In this case the training is terminated and the network is preserved.

Since the optimal number of hidden units depends on the complexity of the network, as well as the chosen representation of the input and output nodes, the author feels it is not safe to rely exclusively on the given algorithm. It is better to scan a range of possibilities. Accordingly, we impose some arbitrary error tolerance to the learning process to see how the network behaves with the

addition of a node (or nodes) to the hidden layer. Theoretically, the performance of a network increases with an increase in the number of the hidden units. If more hidden units are taken, the performance increases slightly to a limiting value and often decreases again (Mukesh, 1997).

Another problem seen occasionally in practice is that the system will end up in a local minima. Gradient descent, and almost all other optimisation techniques can become stuck in the local minima of an objective or cost function. The effect is that the network appears to stop learning: that is, the error does not continue to decrease with the addition of a node or further system training.

As stated previously, the visbreaker's conversion is often a yardstick used to measure the performance of the visbreaking process. Additional information is required in order to measure the overall profitability of the visbreaking and fuel oil blending operations. This can be achieved by expanding the network's output nodes to accommodate all the relevant data affecting the visbreaking operations. This will lead us to expand the Many-To-One paradigm.

Full Scale Paradigm Fabrication Phase

A neural network system with an output node has already been defined, namely the visbreaker's volume conversion. The objective is, however, to study the visbreaking operation. This implies that the full spectrum of the visbreaker's products must be available to the fuel oil blending pool. Accordingly, there is a need to fabricate a neural system with the ability to:

- Predict the yield of the visbreaker product(s)
- Predict the quality of the bottom residue

To achieve this, the topology of the many-to-one network has to be expanded by extending the number of the output nodes to accommodate the visbreaker's product yields and quality. In this thesis, this is called the Many-To-Many visbreaker paradigm, as the output layer of the network contains many nodes.

The question arises as to what these additional nodes are and how they should be represented. The answer lies in the fuel oil blending pool, where the system's objective is a function of the following parameters:

Volume of the product to be blended;
Quality of the product to be blended;
Cost of the product to be blended.

The additional nodes, therefore, should provide necessary information needed by the fuel oil blending pool. In other words, the neural system should predict the yield as well as the quality of the following:

- Visbreaker Naphtha (gasoline) = Gasol
- Visbreaker Kerosene = Kero
- Visbreaker Diesel = Diesel
- Visbroken Medium Density Gas oil = MGO
- Visbroken Heavy Gas oil = HGO
- Visbreaker bottom, or residue = Residue

Here, the objective is to produce an integrated prediction/optimisation system. This is done by linking the prediction results of the full-scale visbreaker paradigm to that of the marine fuel oil blending pool. Hence, along with the visbreaker's product, the blending properties of the visbreaker's residue need to be included in the output vector of the many-to-many paradigm.

The following nodes represent the quality of the visbreaker's residue:

RCCR = the Conradson Carbon Residue content, in weight percent of the visbreaker's residue
RSUL = the sulphur content, in weight percent of the visbreaker's residue

RAPI = the API gravity of the visbreaker's residue

RVBI = the Viscosity Blending Index of the visbreaker's residue

For the sake of clarity, let us summarise the aforementioned assumptions. In the process of converting the many-to-one to many-to-many paradigm, the 12 nodes forming the input vector are essentially unchanged. The ultimate goal is to link the paradigm's response to the optimisation process of fuel oil blending. To account for the economic evaluation of the visbreaking operation, the presence of the visbreaker's products in the output vector is needed. Accordingly, we may produce the volume conversion by simply summing up the predicted yields of Gasoline, Kerosene, and Gas oils. When required, the conversion can also be included in the model.

Fuel Oil Blending Phase

The physical process of blending is relatively simple. The mathematical program to optimise the fuel oil blending pool, on the other hand, is highly complex. Since the main ingredient of marine fuel oil is the visbreaker's residue, the quality of this stream is extremely important. Essentially, the properties of the visbreaker's residue are a function of the feed quality and the unit's operating condition. The quality of the feed in turn is characterised by the type of petroleum crude bought by the refinery.

This is shown in the following figure:

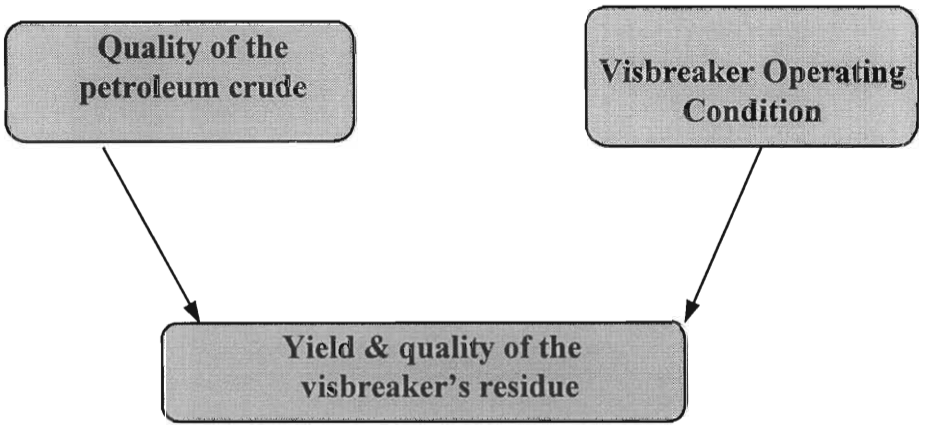


Figure 3-4 Yield & Quality of visbreaker product(s)

In contrast to the visbreaker's residue, many of the qualities of other visbreaker's products 1) do not play a great role in the fuel oil blending system and 2) do not violently change with changes in the feedstocks or operating conditions. Consequently, for simplification purposes, we assume that the variation in the feed quality and operating conditions only affects the quality of the visbreaker's residue.

As stated earlier, beside the gas and gasoline, all other visbreaker's products can be routed to the fuel oil blending pool. These products are listed below:

- Visbreaker Kerosene
- Visbreaker Diesel
- Visbroken Medium Gas oil
- Visbroken Heavy Gas oil
- Visbreaker bottom, or residue

Here, the final product (Marine Fuel Oil, or Bunker Fuel Oil) is a blend of various refinery streams. The equations to blend the necessary components are

given below. These equations are used by the visbreaker adaptive paradigm (and Global Refinery LP) to blend visbreaker bottoms into Bunker Fuel Oil.

$$P_b = \sum_i W_i P_i \qquad \textbf{(3.14)}$$

$$P_b = \sum_i V_i P_i \qquad \textbf{(3.15)}$$

where

P_b = Blend Property.

P_i = Property of component i.

W_i = Weight fraction of component i.

V_i = Volume fraction of component i.

The blending optimisation system should be capable of estimating the optimum values of V_i in order to meet the stipulated specification imposed on the final product. A linear programming technique is employed to generate the most economical recipe. Any non-linear relationship is addressed by converting the property into an appropriate blending index for linear calculation. The computed result is transformed into its original unit of measure. Generally speaking, most chemical processes are non-linear systems. Consequently, non-linear mathematical models would describe their behaviour more accurately. Non-linear models can be developed by utilising either first principles (such as material and energy balances), or process input and output information. The advantages of first principle models include the ability to incorporate the scientist's view of the process into the model, the capacity to describe the internal dynamics of the process, and the capability to explain the behaviour of the process. Their disadvantages are the high cost of model development, the bias that they may have because of the model developer's choices, and the limitations due to a lack of information about specific model parameters. As details are added to the model, it may become too complex and too large to run the model on the computer within an acceptable amount of time. However, this constraint has a moving upper limit, since new developments in computer

hardware and software technologies permit faster execution times. Often, some physical or chemical parameters are computed by using empirical relations, or they are derived from experimental data. In either case, there is some uncertainty about the actual parameter. The blending indices used in this research work are based on practical experiments, and are thus empirical in nature. However, these indices are widely used in the petroleum industry (Maxwell, 1950).

In summary, the steps required to form the proposed integrated knowledge-based model are presented below:

Table 3-1 Overview of the modelling tools and proposed solution

Model	Modelling Tool	Solution Technique
Prototype Paradigm To produce Conversion	Neural Networks	ANNS-Genetic Algorithm
Full Scale Paradigm To produce Product yields and quality	Neural Networks	ANNS-Genetic Algorithm / Integer Programming
Fuel Oil Blending To produce Recipe	Mathematical Programming	Linear Programming / GRG2 Code
Integration of simulation and the optimisation phases	Visual Basic	ANNS-Genetic Algorithm / Mixed Programming / GRG2 Code

The application of the above mentioned tools and techniques to construct a paradigm that learns from the historical case, and predicts the visbreaking yield will be discussed in the following chapter.

CHAPTER 4

IMPLEMENTATION

So far, the motives for building a mathematical model of the visbreaking operation have been presented. Essentially, such a model should be able to predict the visbreaking yields, and to optimise the fuel oil blending operation. The framework and methodology to be used in building the model were presented in the chapter 3.

In keeping with the above objective, this chapter discuss the implementation of the neuroengineering technique in forming the "adaptive visbreaker paradigm". Here, neuroengineering is defined as a series of steps required to fabricate an artificial intelligence system. In this context, the neuroengineering method is employed to classify and link the physicochemical parameters of the visbreaking process to form a neural network paradigm. Having defined the chapters' objectives, the required stages in the model building are given below:

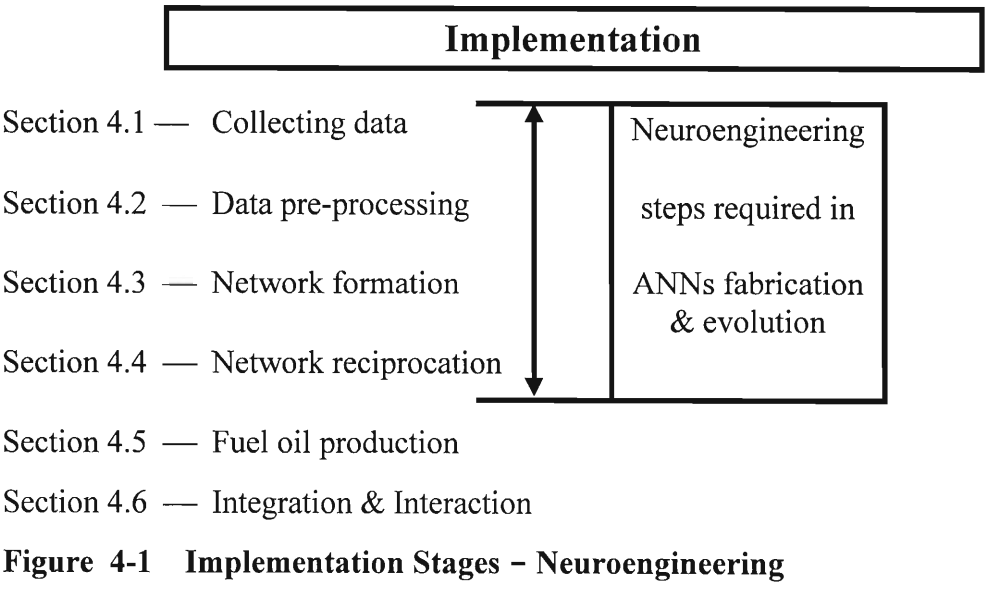


Figure 4-1 Implementation Stages - Neuroengineering

4.1 Collecting Data

The first step toward the building of a neural network is to identify and classify the type and the format of data required by the neural systems. Ultimately, the adaptive visbreaker's paradigm should predict the quality and product-yields of the visbreaking process. Undoubtedly, the accuracy of the final prediction depends on the quality of the raw data used. To fulfil this objective, two types of data are required:

Plant Process Data

This is the data related to the thermodynamics of the process, for example, temperature, pressure, flow rate, time. The process control computers often manage these.

Stream Property Data.

This is the data related to the physical and chemical properties, or quality of a refinery stream or product. These are usually the results of laboratory tests. Alternatively, on-line process analysers can provide the data.

At Engen Refinery, the plant process data is available from the Honeywell™ TDC-3000 process control computer. The TDC controller contains several computational slots each of which is capable of being configured to perform a specific computation called an algorithm. The main data sheet is designed to convert the in-coming signals into the characteristics to be used by each algorithm in each of its operating nodes (process variables). After proper configuration, the system is capable of measuring the properties of a stream and the process kinetics (temperature, pressure) in real-time format.

The PI™ Systems' Plants Information database is the medium to collect, regulate, and store the plants' real-time data. The PI system is a set of software modules for plant-wide monitoring and analysis. The Data Archive is the

foundation of this system. It handles the collection, storage, and retrieval of numerical and string data. The display system provides access to those data for the system operator.

The PI system runs on Digital Equipment's VAX computers (Digital, 1991). The real-time data is updated every 60 seconds. The PI system can be programmed to extract, record and amend the database whenever the variation in the data set is greater than an expected range, in our case, when the variation in range exceeds ± 5% of the statistical mean. Moreover, in line with the plant's statistical input/output report, the PI system is capable of producing consolidated data for every 24 hour of the operation.

Data on the properties of the streams on the other hand, are collected from the Laboratory Computer Database, where the test results on the physical samples of the visbreakers' feedstock, and products are stored.

The PI systems consolidated data, and the laboratory-based stream property data, then enters the PC-based computers hosted by the VAX-based local area network, or LANVAX. These data are often referred to as the coarse or raw data that need to be further refined.

Our investigation to find a suitable data manipulation software package with a programming interface resulted in selecting the Excel™ 5C package, widely used in scientific and industrial applications.

The schematic of the integrated plant and laboratory data acquisition system is shown in the Figure 4.2.

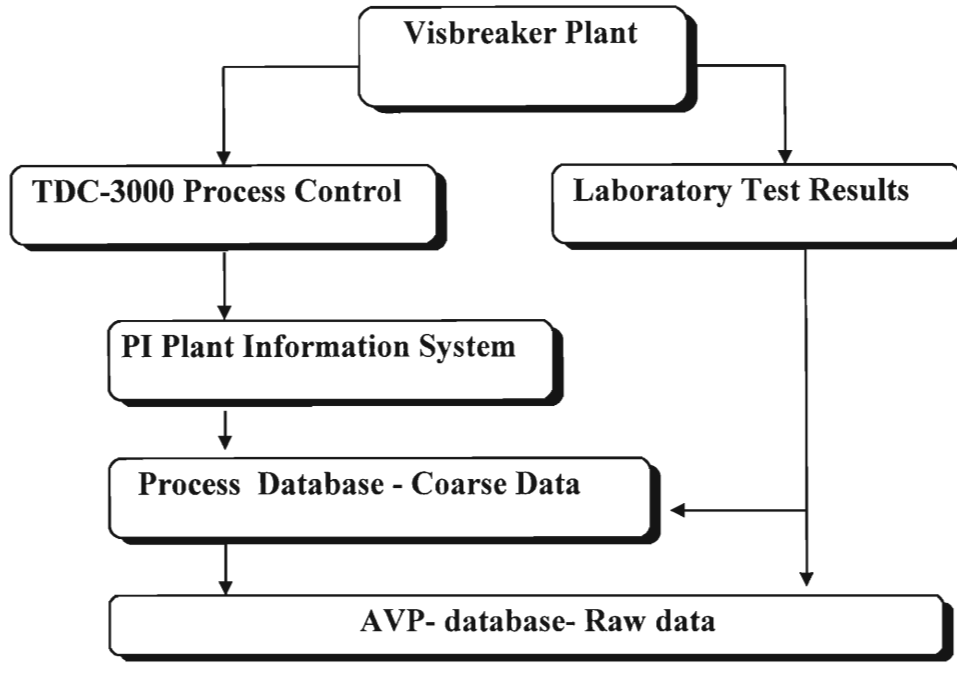


Figure 4-2 Process and Laboratory Data flow

The MS Excel5C™ data sheet is designed to extract the data required for this project (AVP-database). The PI System™ is programmed to deal with the data magnitude. This is to produce a daily consolidated report from the 356 process data tags that are automatically updated every 60 seconds. Additionally, the daily test data from the laboratory consists of 29 test results on the visbreaker's products, plus 6 test results on the final blend of the marine fuel oil. In other words, the AVP database must be able to handle a total of 391 raw data entries per day of the visbreaking operation.

In this research work, we have opted to use the plant data from a continuous visbreaker cycle of 168 days operation. The total raw data in the AVP database is therefore $168 \times 391 = 65688$ items.

Input Data — Analysis

Here, the basic idea is to examine data range available to form the proposed model. This will provide an insight into the model's limitations concerning the data range employed. As discussed in the chapter 3, in modelling the visbreaking operations, we have assumed that the neural network has to learn from the real world examples. Accordingly, the model needs to learn from the historical data, concerning feed flow rate, feed quality, plant's operating condition, and conversion achieved under these circumstances. The available data are categorised as the data sets that form the neural network nodes and layer. It is worthwhile to mention that the proposed network can be formed using fewer nodes. Obviously, this could improve the predictability and reduce the processing time. Several extra nodes were employed. This was done for the sake of completeness and to accommodate future research projects,. This is to cover both the feedstock's quality and to account for the change in operating condition. The following graphs show the range of various data obtained from processing various refinery feedstocks. Where applicable, comments are provided under the graph headings. Obviously, the prediction accuracy of the model reduces, when data fall towards the boundaries or outside the range used to train the AVP.

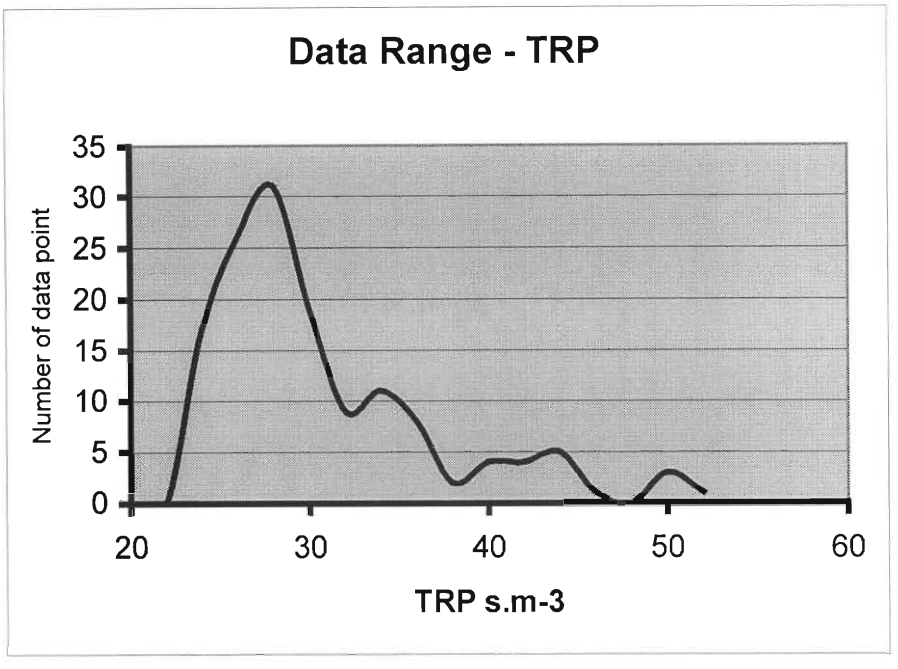


Figure 4-3 Recorded Data Range – TRP represent the fluctuations in feed volume to soaker drum

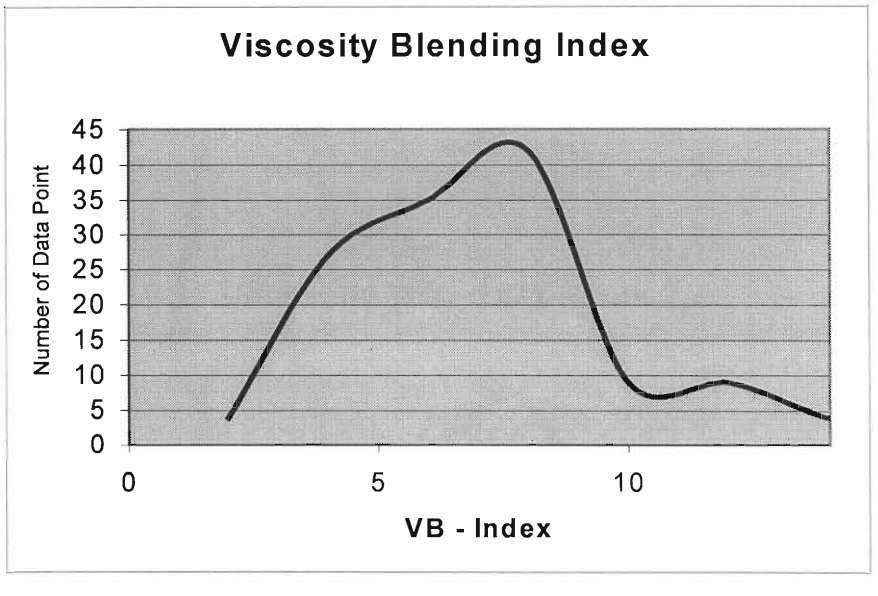


Figure 4-4 Recorded Data Range on viscosity Blending Index of feed. This value is influenced by the addition of light materials such as H-Donors to the crude vacuum residue.

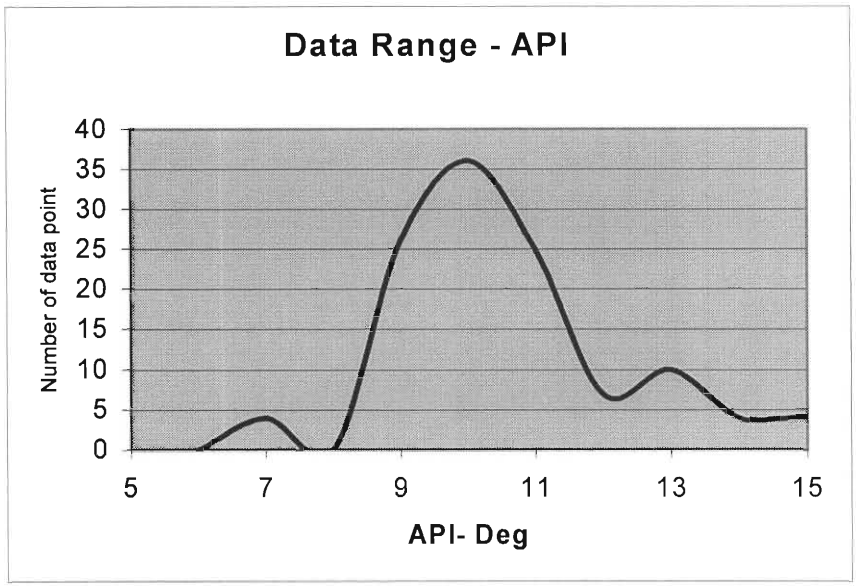


Figure 4-5 Data Range – Using the API of the Feed.

Similar to the viscosity blending index, This value is influenced by the addition of light materials such as H-Donors to the crude vacuum residue

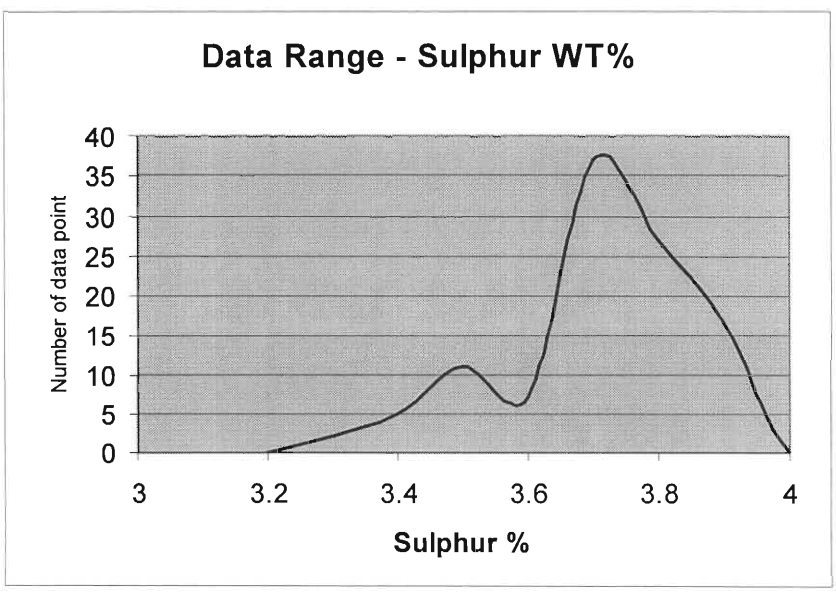


Figure 4-6 Variation in Sulphur Content of the Feed. It is known that operations severity decrease with an increase in the feed's sulphur content.

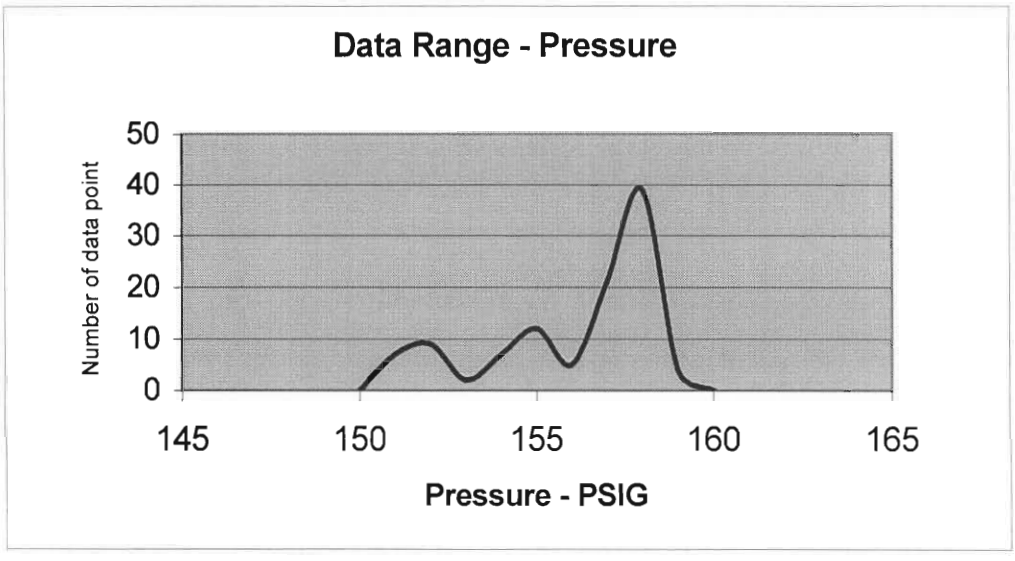


Figure 4-7 Variation in average Soaker Pressure. In practice, the effect of soaker pressure on visbreaking yields find to be insignificant.

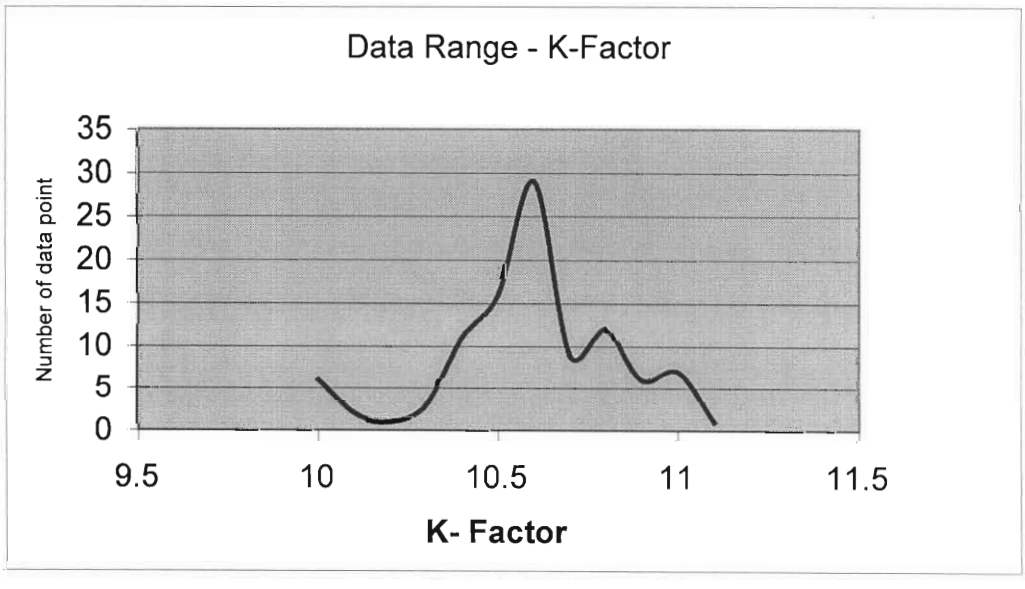


Figure 4-8 Variation in the K-Factor of the Feed. Feeds with the high Kfactor are preferred. Although waxy feed may adversely affect the fuel oil stability.

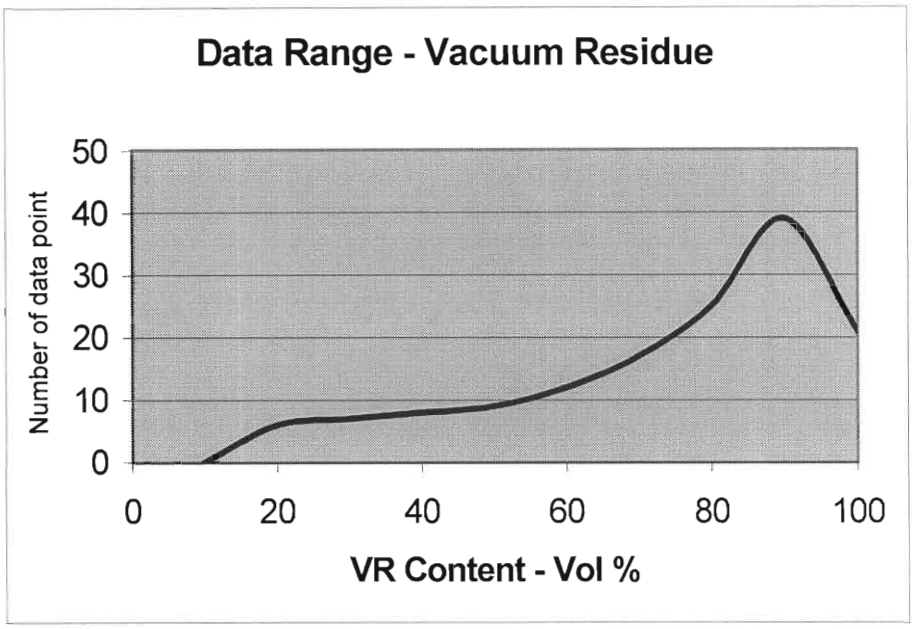


Figure 4-9 Variation in the visbreaker Feed. Vacuum Residue Content of the visbreaker feed.

The feed to the visbreaker process unit is vacuum residue drawn from the bottom of vacuum distillation unit. There is however, other refinery stream that can be routed to the visbreaker unit. Some materials such as catalytic gas oils from FCC units (often classified as the H-Donors) are added to improve the visbreaking yields. Others, such as the long residue (materials obtained from the bottom of the crude atmospheric distillation unit) are also potential feed for visbreaking. The economics of routing various streams to different destinations is estimated by the proposed decision support system.

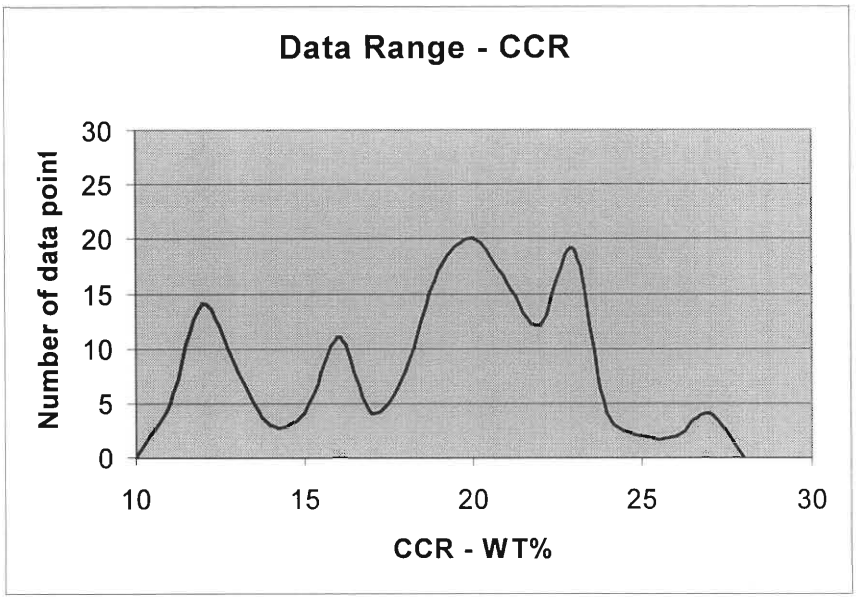


Figure 4-10 Variation in the quality of the Feed – Conradson Carbon Content adversely affects the visbreaking yields. This is an important variable.

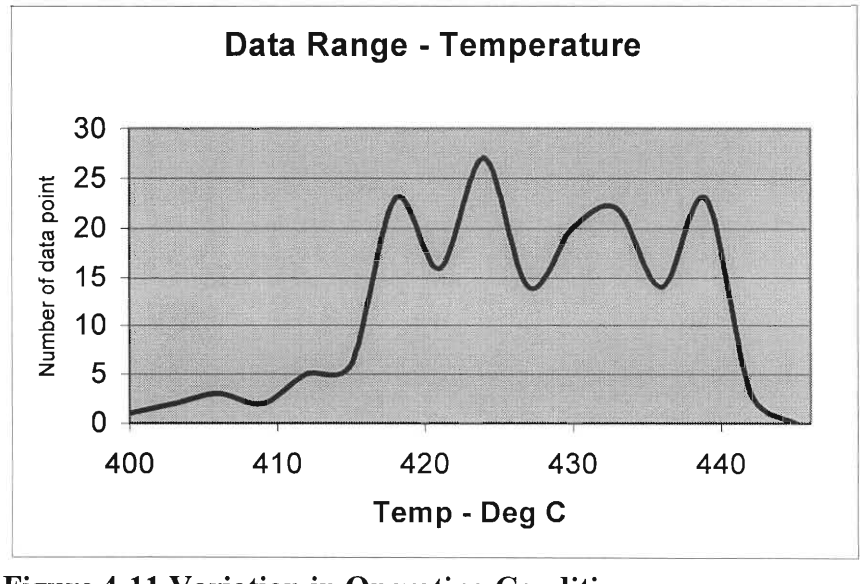


Figure 4-11 Variation in Operating Condition

Average Soaker Temperature expressed as the operations severity. This is an important variable.

4.2 Data Pre-Processing

The next step after data acquisition is data pre-processing, where the objective is to convert the coarse or raw data into meaningful data set that eventually are used to train the neural networks system. Since the AVP is trained under supervision, examples (historical plant data) have to be available. As stated in the previous section, data for 168 days of visbreaking operation have already been recorded by the AVPs' main data-sheet. Another important decision that must be made is the classification and subdivision of the data, which is necessary to form the relevant data sets. This is required for network training and testing. Data pre-processing is therefore concerned with information science. In other words, along with data classification, the relationship between the elements of each data set is subject to examination.

The PI system also records the temperature and pressure variations at the top, middle, and the bottom level of the visbreaker's Soaker drum. To reduce the amount of input data, we have opted to accept an average Soaker temperature and pressure. To achieve this, we have used the programming capability of Visual Basic to calculate and record the arithmetic mean of the temperature and pressure across the Soaker drum. To be in line with the other value scale, the PI's reported pressure units of kPa is converted to PSI(G) (Himmelblau, 1989).

Moreover, we are concerned with data intensity, which along with data validity and the inter-variable correlations among the selected system parameters may deceive the paradigm's learning process. In other words, we should not overload the neural networks with types of data that could result in the system's confusion. To reduce the data intensity we have to rely on *a priori* knowledge of the visbreaking operations. In this respect, we have used the programming capability of Visual Basic to search for and to discard any data sets when 1) the unit's feed rate is less then 2000 cubic metres per day of operation 2) the average Soaker temperature is less than 410 degrees C.

The above assumption is based on our understanding that firstly, the plant's performance at a feed rate below the 2000 cubic metres per day (12580 bbl) of operation may become erratic, thus not representing the real operation. Secondly, there is little chance of performing a proper visbreaking at a temperature as low as 770F°(410C°). Consequently, the data pre-processing is employed to eliminate any data set that relates to an unstable unit operation.

The implication of applying the above rule results in reducing the number of the data sets from 168 to 141. In other words, the data from 141 days (daily averages of 24 hours of continuos operation) of the stable visbreaking operations are available to the model.

In the following section, we use the processed data to fabricate and train the adaptive visbreaker's paradigm.

4.3 Network Formation

At the beginning of this chapter, we presented a work flow, illustrating the sequences of the neuroengineering process. The network formation is an important building block in our endeavour to fabricate a neural network paradigm.

As a new step in our neuroengineering technique, we introduce two different but simultaneous approaches to this problem. First, we use a genetic algorithm to search the network's weight and minimise the degree of the error. Genetic algorithms perform a global search and are thus not easily fooled by the local minima. A detailed discussion on the performance and limitation of the genetic algorithm, will be presented in Appendix 4.

Second, we impose some arbitrary error tolerance to the learning process to see how the network behaves with the addition of a node (or nodes) to the hidden layer. We then measure the system's learning effectiveness in pre-defined intervals. Whether or not this situation is acceptable depends on the value of the error when the minimum is reached. If the error of the paradigm in predicting the volume conversion is acceptable, then it does not matter whether or not the minimum is global. If the error of prediction is unacceptable, then, the process of training must continue.

It is imperative for our understanding of this approach to distinguish between the error evaluation algorithm used by the cascade correlation and our external error tolerance limit that is defined below:

$$\textbf{Error Tolerance} = ET = \left(\sum_{o,p} \left(\frac{Yop - Top}{Yop} * 100\right)^2\right)^{1/2} \qquad (4.1)$$

where

where Y_{op} is the observed value of output o from training pattern p, and T_{op} is the predicted output.

The ET is a percentage deviation from the original observed value during the learning process. As training continues, an improvement in the system's recognition is expected. In other words, when

$$ET \rightarrow 0$$

Finally, we introduce a system profile table, where we record our assumptions and impose some arbitrary tolerance limits on the network's learning process.

Table 4-1 System Profile

Error Tolerance	Max Limit %	RUN #	Action to be taken
ET-1	≤ ±20	RUN-1	Report on the networks' status, then continue
ET-2	≤ ±15	RUN-2	Report on the networks' status, then continue
ET-3	≤ ±10	RUN-3	Report on the networks' status, then continue
ET-4	≤ ±5	RUN-4	Report on the networks' status, then terminate

At this stage, using the common neural network heuristics described in chapter 3 of this thesis, we initiate the process of network fabrication. Briefly, the process starts with analysing and transforming the input data (12 variables in

141 datasets). The steps to follow (after the data transformations) are initial network formation and training, where the objective is to maximise the correlation between the desired output and the predicted output. Accordingly, this results in minimising the degrees of the error between the predicted output and the desired value. The overall process, however, is interrupted at the intervals when the error tolerance approaches the limits stipulated in the profile table. In other words, the process of learning is repeated until the prediction error reaches the acceptable tolerance level. It should be noted that the purpose of this paradigm is to predict the visbreaker's conversion as defined in chapter 2. The following results were obtained from the "Many-To-One" paradigm runs, using various error tolerance limits.

Table 4-2 Networks' Results

Status	**RUN-1**	**RUN-2**	**RUN-3**	**RUN-4**
Max *ET* limit %	**±20**	**±15**	**±10**	**±5**
Error reported %	**15.2**	**13.6**	**10.5**	**0.46**
No. Of hidden nodes	**3**	**4**	**6**	**9**

It is evident from the above table that the addition of hidden nodes results in an increase in the accuracy of the prediction. However, there is no point in increasing the number of the hidden nodes beyond 9 units because the system's error (0.46) is much lower than our required value of ±5% (from the profile table).

The following chart illustrates, how the increase in the number of hidden nodes can decrease the system's learning error.

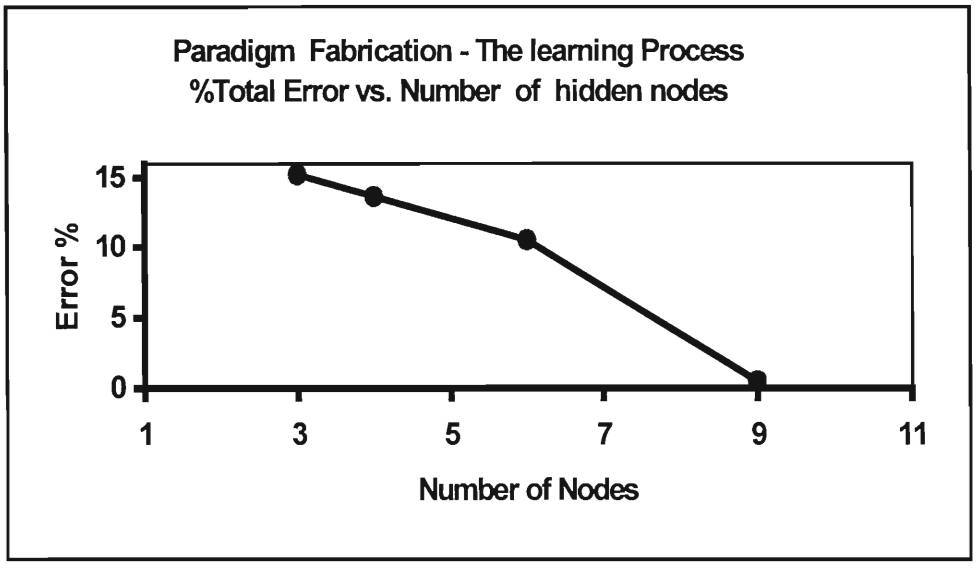


Figure 4-12 Comparison of the results produced by the "Many-To-One" paradigm, predicting the visbreaker's volume percent conversion.

In summary, in this section, we have formulated an artificial neural network system that is capable of forecasting the volume percent conversion of the visbreaking process. Furthermore, this system is able to recognise the patterns that were originally used in its training process. The theoretical results presented above show that one hidden layer is sufficient for cascade correlation networks to approximate any continuous mapping from the input pattern to the output pattern to an arbitrary degree of accuracy.

Next, we have to measure the performance of the system.

The performance of the Many-To-One Paradigm

Developing a neural network system is said to be an art. Many parameters have to be set and this is often done based, to some extent, on neural network heuristics. The spatial relationships between the networks' objects or nodes cannot be shown schematically. However, in the following diagram, we attempt to illustrate the topology of the many-to-one paradigm (RUN-4) of the visbreaker unit.

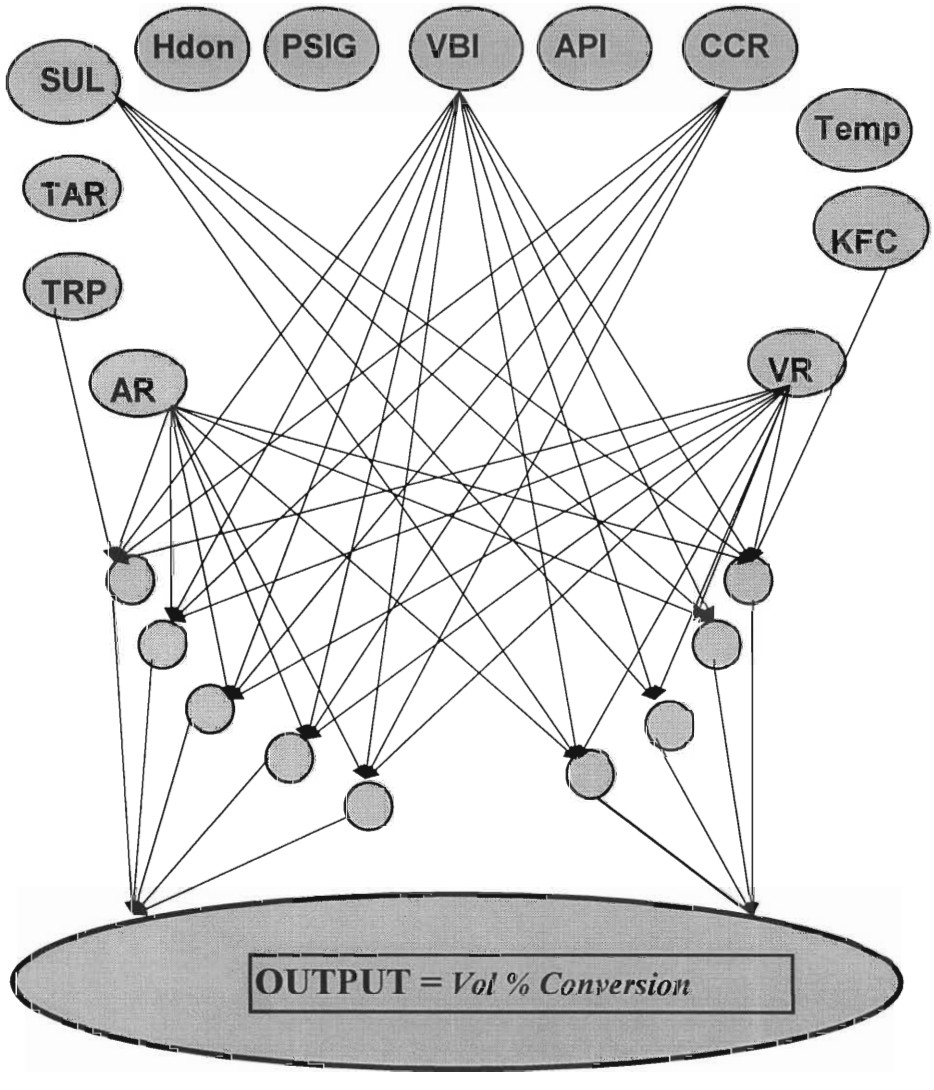


Figure 4-13 The Topology of the Many-To-One Paradigm
(the input nodes are defined under Feedstock Quality in chapter 3)

For clarity, we have not shown a complete picture of the nodes' interconnections.

The purpose of developing a neural model is to produce a formula that captures essential relationships in data. Once developed, this formula is used to interpolate from a new set of inputs to corresponding outputs. In neural network terminology, this is called generalisation. The training set is the set of points that are used to fit the parameters of the paradigm. The test sets measures how well the model interpolates. It is used as a part of the paradigm fabrication process to prevent over-fitting. The validation set is used to estimate model performance in a deployed environment.

The training data set used in the training of the many-to-one paradigm is extracted from a continuous run of the visbreaker unit. This set contained no missing data elements. Often the performance of a network is measured using the *test set*, rather then the training data set. The test set consists of examples other than the one used in the training of the neural network. The methodology is somewhat different from that of the jack-knife method used in statistics. The jack-knife computes the variance of the estimates by omitting each of the observations in turn (Kennedy, 1994). However, in neural network computation, it has been customary to divide the original input data into two sets. One set is used for network training and the other for cross-validation testing.

In the testing phase, the input patterns are fed to the network and the desired output patterns are compared with those given by the neural network paradigm. The (dis)agreement of the two output sets gives an indication of the performance of the trained network. When the performance meets the requirements specified in advance, the network is ready for real analysis purposes.

There are many statistical methods to test the performance of a neural network paradigm. Statistical models often use the T-test confidence intervals at the 90% or 95% certainly level. Just as the T-test is applied to linear models, it can be applied as well to *some* neural paradigms. The only requirement is that the residual errors are approximately normally distributed. If the residual meets

this requirement, the T-test can be validly applied to either neural or linear models. When performing this test, it is essential that the data selected for the validation has the same distribution as the main population.

Another way to measure the performance of the prediction paradigm is to calculate a near-match index. This is done by first, selecting the number of the correct output patterns, and then to divide by the total number of pattern pairs present in the final set (Wasserman, 1993).

In our case, the question arises regarding the type of data that could be used as the test set, and how the network's performance should be judged ?

To account for a test set, we may use the data acquisition procedure (explained at the beginning of this chapter) to retrieve the operational data obtained from *another* visbreaking cycle. Like any other refinery unit, the visbreaker operation is cyclic. Thus, at the end of each cycle, the unit has to be shut down, either for maintenance, or to clear the coke formed from cracking of the residue (a process called de-coking). Obviously, after start up, the overall unit's operating parameters have changed.

Using the data from another visbreaker cycle results in exposing our paradigm to a new test set belonging to a different environment. Obviously, the data distributions of these new data sets (test sets) are very different from the original data used in the training of the many-to-one paradigm.

However, at this stage, the main objective is to fabricate a prototype paradigm that is capable of recognising an unseen test pattern. Consequently, for the purpose of testing the model's validity, we prepare a new test set, using the data from another visbreaker operational cycle.

Using the PI systems and Excel database, we managed to retrieve and prepare a data set that represents 48 days of continuous visbreaker operations. This we call the test set from cycle 2 of the visbreaking operations.

Next, we measure the performance of the many-to-one visbreaker paradigm using the following steps:

- Recall or Recognition process: measures the network's capability to remember the training data patterns (data that is used in the training process).
- Prediction process: measures the system's response to the test data (data that is not used in the training process).

In summary, the many-to-one visbreaker paradigm was tested, using both training and test data sets. The test sets were obtained from the second visbreaker's cycle. In this respect, we have exposed the paradigm to a new stimulus. This is a new data set, unseen by the network. The new data set contain 48 × 12 rows of plant data. The responses from running the paradigm with the data and test sets are presented in the following figures.

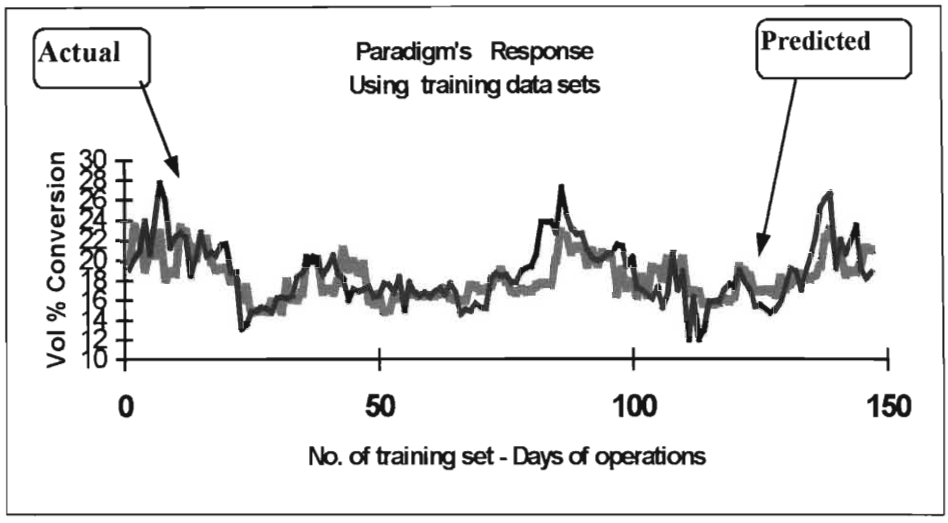


Figure 4-14 Paradigm's Response to training sets obtained from 141 days of the continuous visbreaking operation (cycle-1)

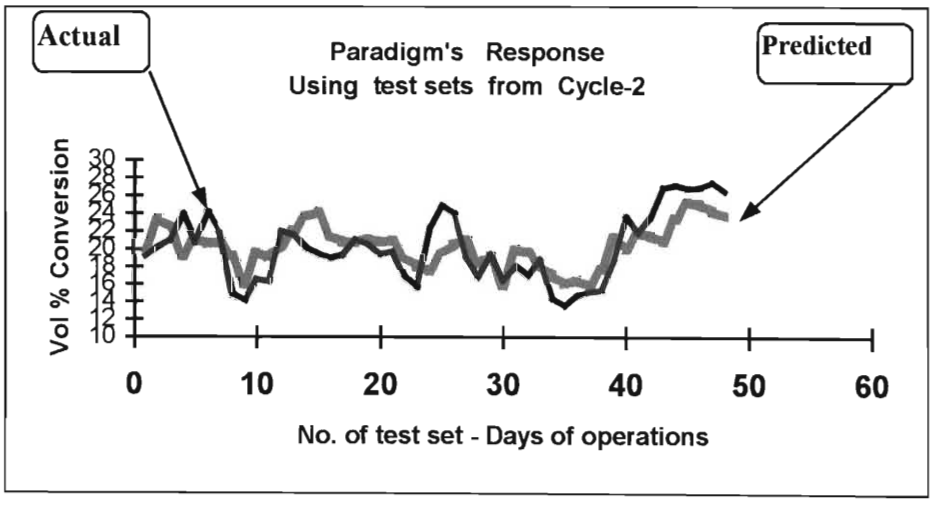


Figure 4-15 Paradigm's Response to test sets prepared from cycle-2 of the visbreaking operation.

It is evident from the first chart (Figure 4-5) that the paradigm is capable of remembering the pattern(s), originally used in the learning process. By this, we mean the 141 data sets that we used in training of the many-to-one visbreaker paradigm. Figure 4-6 suggests that the network cannot produce a perfect match for each of the 48 days of the visbreaker's operation. This is because of exposing the network to the unseen test sets, obtained from cycle-2 of the visbreaking operation. Nevertheless, the many-to-one paradigm exhibits a strong pattern recognition ability.

Again, the question arises of how to measure the performance of a neural network system and how reliable the results are? (taking into account that the purpose of this model is to predict the yield of a refinery process unit). Several different methods have been applied. Our investigation indicates that there is not a universally agreed-upon method to measure the neural systems' performance. Most researchers, however, are using root mean square (RMS) or mean absolute deviation (MAD) to evaluate the efficiency of neural networks (Freeman, *et al*, 1991).

The prediction capability of the many-to-one paradigm is an indication of the correlation between the desired output and predicted one. In other words, how well the paradigm's interpolation and extrapolation mechanism works.

At this stage, we only need to define a simple but practical statistical method to measure and express the paradigm's accuracy of prediction. The mean absolute deviation (MAD) is a simple, but accurate yardstick to judge the network's performance.

$$\text{Mean Absolute Deviation} = \frac{\sum |Yop - Top|}{Np} \qquad (4.2)$$

where

Y_{op} is the observed value of output ***o*** from training pattern ***p*** , and T_{op} is the predicted output and N_p is the number of test sets or patterns to be predicted (Winston, 1991).

The result of running the many-to-one visbreaker paradigm with the training and test sets is given in the following table.

Table 4-3 ANNs paradigm's response -Training set vs. Test set

Data Type	Training Set	Test set
Visbreaker cycle	1	2
Number of data set	141	48
Data dimension	141 × 12 = 1692	48 × 12 = 570
Data Range Volume conversion %	10 - 30	10 – 30
Mean Absolute Deviation of volume conversion %	1.78	2.28

The results are indicative of an artificial neural network system with the capability to recognise the input patterns and producing desired responses. The degree of the error of prediction is also estimated.

At this point, the process of generalisation of the many-to-one paradigm is complete. To further improve the prediction accuracy, we have to modify the network's topology. The next step is to expand the existing network and fabricate the visbreaker's final paradigm.

Evolution of the Many To One visbreaker paradigm into a full scale visbreaker-paradigm

Let us recap the work done so far. In the previous chapter of this thesis, we fabricated and trained (under supervision) a multi-layer neural network that learns by rules stipulated by cascade correlation architecture. Additionally, we imposed on this network, some external error tolerance to ensure that the system learns didactically. Since its topology requires only an output node, this fully interconnected network is called a many-to-one paradigm. Furthermore, beside the training data set, the network was also exposed to a set of stimuli that was generated in a different environment. The system's response to the unseen data set was monitored. Under these conditions, the performance of the many-to-one visbreaker-paradigm, although not highly desirable, is satisfactory. Consequently, we may now proceed to the next phase of the neuroengineering process, that is, to evolve the existing network into a full-scale prediction apparatus.

According to our pre-defined solution approach described in chapter 3 , up to this point, we have been using a network with an output node, namely the visbreaker's volume conversion. Our objective is to study the visbreaking operations. As a result, the full spectrum of the visbreaker's products must be available to the fuel oil blending pool. The full scale neural system is in fact an evolution of the many-to-one paradigm to a multi-layer, multi-response network containing output nodes, representing the visbreaker's product and residue quality.

The visbreaker's product yields and the associated quality are available from the PI System and the Laboratory Information computers respectively. These data can easily be retrieved and made available to the neural system. The visbreaker's residue cannot be sold on its own. This is because of its high density, viscosity, carbon residue, and sulphur content. Therefore, the objective of the fuel oil blending operation is to convert the visbreaker's residue into a saleable product that meets the marine fuel oil's specification.

The next step in this phase of the neuroengineering process is to fabricate the many-to-many paradigm by evolving, re-building, and re-training the existing paradigm. The necessary steps are as follows:

- Keep the input layer unchanged (12 nodes)
- Modify and expand the output layer (11 nodes)
- Re-build the network using the Cascade Correlation algorithm
- Re-train the network using the training data set (141 days)

At this stage, the process of forming the system's input and output nodes is complete. In what follows, we present a schematic of the many-to-many topology.

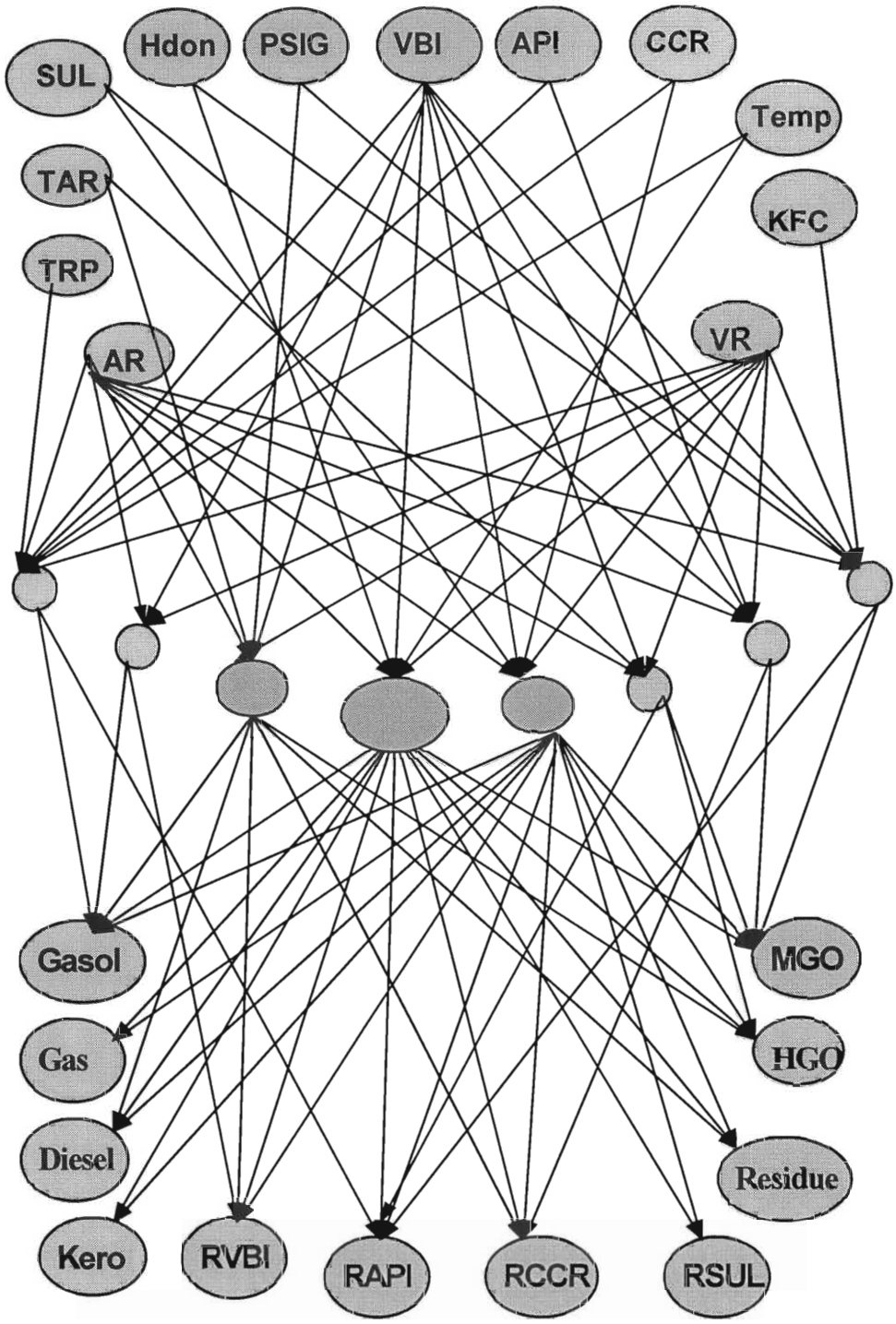


Figure 4-16 The Topology of the Many-To-Many Paradigm
(input and output nodes are defined in chapter 3, pp 54 and pp. 67)

As stated before, the spatial relationships between the networks' objects or nodes cannot be shown schematically. However, in figure 4-16, we attempt to illustrate the topology of the many-to-many paradigm of the visbreaker unit. For clarity, the complete picture of the node connections is not shown.

Compared to the many-to-one paradigm, the above neural network system is more representative of the modern visbreaking process. In this respect, the process is a combination of cracking, atmospheric, and vacuum distillation. Additionally, our ANNs is able to predict the quality of the visbreaker's residue (collected from the bottom of the vacuum tower). This information is vitally important in our endeavour to link the ANNs responses to the fuel oil pool, and to evaluate the economics of the visbreaking and blending operations.

In retaining the consistency of measuring the performance of the paradigm, we will continue using:

1) Volume percent conversion as the measure of the visbreaking process performance. As defined earlier, gasoline and distillate (the most valuable visbreaker products) are the major constituents of the visbreaker's volume conversion.

2) Mean absolute deviation (MAD) as the measure of the accuracy of the ANNs prediction.

Moreover, for a better understanding of the networks' behaviour, in the following paragraph, we introduce two additional performance-related criteria. First, the percentage visbreaker residue, as an indication of the volume of the residue that has to be converted (blended) into marine or bunker fuel oil.

Secondly, we introduce the Root Mean Square (RMS) as an additional measure of the accuracy of the ANNs prediction. The RMS is defined by the following equation:

$$\textbf{Root Mean Square} = \sqrt{\frac{\sum (Yop - Top)^2}{Np}} \qquad \textbf{(4.3)}$$

where

Yop is the observed value of output ***o*** from training pattern p , and Top is the predicted output and ***Np*** is the number of the test sets or samples used in the training test. The RMS error often provides a good insight into the noisiness of the input data. Also, it is in the same unit of measurement as the original data. As a result, RMS is preferred by many researchers (Diederich *et al*, 1997). Obviously, the lower RMS of error, the higher the accuracy of prediction.

The characteristics of the many-to-many paradigm and the responses obtained from running both training and test sets are shown in Table 4-4

Table 4-4 Network – Topology

Number of the input nodes	12
Number of the hidden layers	1
Number of the final hidden nodes	8
Number of the output nodes	11
Mode of operation	Prediction

To assess the paradigm's performance, the network is trained using the data from the first visbreaking cycle. The data set in the second cycle of visbreaking operation is used to measure the networks performance. The results are shown in the following table.

Table 4-5 Network performance

Testing the network performance with regards to the Conversion and Residue Yield

Description	**Recall**	**Prediction**
Data set used	Training set	Test set
Number of the data sets	141	48
1) Conversion in volume %		
Data Range Volume conversion - %	10 - 30	10 – 30
Mean absolute deviation of volume conversion %	1.6364	3.5942
Root mean square of the volume conversion %	2.1262	4.3145
2) Visbreaker residue make in volume %		
Data Range Visbreaker residue make %	50 - 90	50 – 90
Mean absolute deviation of Visbreaker residue make %	3.6767	9.9613
Root mean square of Visbreaker residue make %	4.8851	12.4818

The predictive results of the network shown in the above table are not overwhelmingly impressive. With respect to the visbreaker's residue make, the predictive figure is a function of the residue upgrading process through hydrocarbon decomposition, and the stream separation through distillation. In this research work, we regard the unit's yield as a measure of the visbreakability of the heavy petroleum residue. Hence, due to the overlay in boiling range of

gas oils, separation of the bottom residue from the vacuum gas oils is not accurately measured. This problem has resulted in the RMS error of 12.48 percent in Visbreaker residue make.

Upon closer examination of the visbreaking process data, we realise that the process of gas oil recovery from the vacuum tower of the visbreaker has not been consistent. This is purely an operational problem that is inherent in some plants. The root of the problem resides in the separatability of the vacuum gas oils, and not the crackability of the visbreaker's feed. Accordingly, using the visbreaker's residue as a measure of the accuracy of the neural network's prediction appears to produce some misleading values. Hence, it seems reasonable to substitute the visbreaker's residue content with the combined residue plus vacuum gas oils streams (this is essentially the product driven from the bottom of visbreaker's atmospheric tower as seen in Figure 2-4).

The logic behind this proposition is that both the visbroken vacuum gas oils and visbreaker's residue are represented in the model. Hence, by combining their volumes we can account for the combined yield of the visbreaker bottom and visbroken gas oils. This is to address the deficiency of the gas oil recovery at the vacuum distillation tower. This stream is the bottom of the atmospheric tower of the visbreaker unit (as shown in Figure 2-4). The procedure suggested above should essentially assist us to calibrate the network. Once the network is trained and calibrated, the volume of visbroken gas oils can be included into the output nodes. This many to many paradigm is called a *Standard Network.*

Moreover, our suggestion is consistent with the process illustrated in Figure 2-4, where the combined stream from the bottom of the atmospheric tower is routed into the vacuum distillation column for gas oil(s) recovery. Having this in mind, we compute the network's measure of accuracy of prediction, using the effect of the combined residue/gas oil's stream.

The results obtained from re-computing the MAD and RMS error of the combined streams are presented in the Table 4-6.

Table 4-6 Network performance

(Combining the visbreaker's bottom residue and medium and heavy vacuum gas oils as one stream).

Description	**Recall**	**Prediction**
Data set used	Training set	Test set
Number of the data sets	141	48
1) Conversion in volume %		
Mean absolute deviation of the volume conversion%	1.6364	3.5942
Root mean square of the volume conversion%	2.1262	4.3145
2) Visbreaker Residue make in volume %		
Mean absolute deviation of the combined stream(vol%)	2.2237	3.5095
Root mean square of the combined stream (vol%)	2.8977	5.0544

Our suggestion has resulted in a significant improvement in the network's performance indicators. This can be viewed from Table 4-6, where the results of measuring the networks' accuracy of prediction are illustrated. As a result, using the combined stream of the visbreaker's bottom plus gas oils is a preferred method of calibrating the above network.

Table 4-7 Networks performance – Comparison of the results

Description	Recall	Prediction
Mean absolute deviation of the bottom residue make vol%	3.6767 MAD	9.9613 MAD
Mean absolute deviation of the combined stream vol%	2.2237 MAD	3.5095 MAD
Root mean square of the bottom residue yield, vol%	4.8851 RMS	12.4818 RMS
Root mean square of the combined stream, vol%	2.8977 RMS	5.0544 RMS

The degree of the improvement(s) made to the statistical performance indicators is self-evident, having reduced the RMS error of bottom yield % from 4.8 to 2.8 in recall, and 12.4 to almost 5 in the prediction mode. As noted earlier, the data set used in the prediction mode are derived from the second visbreaking cycle.

The reduction in the RMS error improves the networks performance (or paradigms predictability). The significance of this however, needs to be quantified. In this respect, since visbreaker bottoms is the main product of the visbreaking process, its effect on the refinery's profit can effectively be measured. Accordingly, the sensitivity of the refinery's profit with the variation in the visbreaker bottoms can be established.

Using the refinery's Global LP model, the effect of varying the visbreaker bottoms' product on the refinery's gross margin can be measured. The refinery's gross margin is calculated as follows:

Gross Margin in $/ barrel = (Sales – Purchases – Operating Expenses) / (Volume of crude in barrel used on that LP run). **(4.4)**

This is presented in the following graph, where the effects of varying residue make (at constant quality) on the refinery margin are depicted.

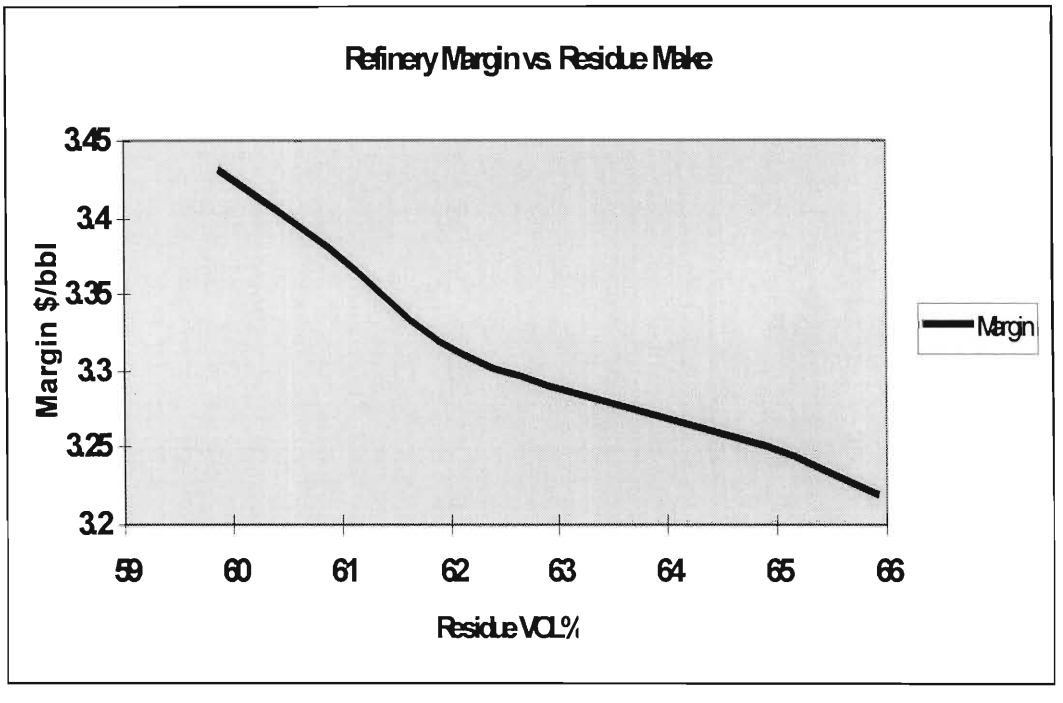


Figure 4-17 The Sensitivity of gross marine with the residue make

It is shown in the above graph that the refinery's gross profit is highly sensitive to the visbreaker's residue make. This can be further demonstrated by the following example:

In order to calculate the refinery's gross margin, a crude charge of 100,000 barrels per calendar day of Arab crude yielding a visbreaker residue make of

59.6 volume percent is assumed. Using the above graph, the corresponding drop in the margin for a 2% error in residue make is calculated as follows:

Drop in Margin = (3.32 – 3.43) = 0.11 $/bbl

For 100,000 bbl per calendar day : 100,000 * (– 0.11) = – 11000 $/day

For Annual loss 365 * (– 11000) * (4.5 exchange rate)

= – 18.6 Million Rand.

In calculating the loss reported above, we have assumed that the refinery's operation can be re-optimised with a change in the quantity or quality of the visbreaker's residue. Obviously, additional loss will occur, if such re-optimisation can not be achieved.

Clearly, the magnitude of the loss reported above, justifies further investigation into methods that can result in a lower degree of error in the paradigm's output. It should be noted that the shift in profit is in fact the result of downgrading some white oil into black oil. Moreover, reducing the prediction error will assist the refinery planners with the feedstock evaluation and selection process.

In summary, by evolutionary means, we have fabricated the many-to-many visbreaker paradigm. This fully connected neural network paradigm can be used as the forecasting apparatus to predict the yields of the visbreaking process. The predictability of the paradigm is judged by the computed value of the visbreaker's white oil. The performance of the neural system is measured using statistical methods. It was also demonstrated that the profit of the refinery is sensitive to the degree of error produced by the visbreaker adaptive paradigm.

However, before proceeding to the next stage, that is, to present the fuel oil blending operation, the author feels that, in spite of its encouraging predictability characteristics, the performance of the paradigm can stand further improvement. Accordingly, we shall investigate ways and means of improving the network's current performance.

To test the potential of this proposition, in the next section we re-examine the structure of the existing paradigm, and propose a computational methodology to enhance the recognition capability of the network.

4.4 Network Reciprocation

In the previous section, using statistical performance indicators we analysed the network's output. Furthermore, by re-defining (and subsequently re-computing) the performance criteria, the predictive quality of the paradigm was greatly improved.

The question, however, arises as to what degree of variability between the network's actual and predicted output should be tolerated?. The obvious difficulty is that neural systems have *no* judgmental sense, meaning that the predictive quality of the paradigm is an external parameter that needs to be included in the systems' objective. That, of course, requires quantification.

Consequently, in this section, we attempt to examine the validity of the paradigm's response to both seen and unseen inputs. To achieve this task, we need to clarify the system's objective. In this respect, we shall employ the aspiration-level criterion, often practised in decision theory (Taha, 1989). Accordingly, we state that the aspiration-level criterion does not yield an optimal decision in the sense of maximising profit or minimising cost. Rather, it is a means of determining an acceptable course of action. In this context, the aspiration-level theory requires firstly *a priori* knowledge of the process that needs to be examined. Secondly, it requires an understanding of the degree of tolerance that is acceptable as the upper and lower limits of the decision frame.

The application of the aspiration-level criterion enables us to define and pre-set the limits of error that can be expected from neural network systems.

The implementation of the above theory requires further clarification regarding the variability of the systems structure. In this respect, we have *borrowed* the term "reciprocation", applied to electro-mechanical systems (Walker, 1991). This is described as follows:

In electrical engineering terminology, the reciprocity theorem is defined as the interchange of the electromotive forces at any point in a network and the current produced at any other point, resulting in the same current for the same electromotive force. For the sake of clarity, in this thesis, the term reciprocation is further defined as the continuous evaluation of input data, to ascertain that the allocated data set can in fact improve the predictability of the network. This definition is consistent with the proposed adaptive neural network model of the visbreaking process, where frequent training is provided. As stated earlier, the process of petroleum refining is of a continuous nature and therefore a PI monitoring system is employed to provide continuous plant data.

By analogy, the quantitative validation of the response should be independent of the network's input and output nodes. In other words, the system's requirements with regard to the network's processing elements (stimulus and response) are essentially unchanged. The paradigm's topology, however, may or may not change. That is, there are no changes to the input and output nodes.

Hence, in the last stage of the neuroengineering process, we employ the network reciprocation theorem to find a practical procedure that can improve the neural network's predictive quality by the aspiration-level criterion. Here, the goal is to improve the network's predictability. This is done by removing the data sets whose contribution result in an increase in the neural prediction error. The network reciprocation procedure therefore prevents the formation of data outliers. Essentially, the technique is more suitable in a continuous operation scheme, where there is no limit to the number of process data available to produce an accurate pattern. It should be noted that the network's prediction results are updated regularly. This is because the process control computers

continuously generate the process data. In this respect, Pass (1997) writes, it is highly likely that not all data is appropriate for data mining. When seeking to uncover patterns it only makes sense to seek out those that will have meaningful impact on the business.

To illustrate the orderly application of network reciprocation we provide, in the following format, a full explanation regarding the succeeding steps required to develop our proposed procedure. We emphasise that at each stage the form of the reciprocated network (regarding the stimulus and response) is equivalent to that of the original paradigm. The paradigm's topology (and the number of hidden nodes), however, may or may not change.

The network reciprocation sequences are presented in the following pages:

Proposition: Improve the predictive quality of the visbreaker paradigm employed by the neuroengineering process.

Procedure: Apply network reciprocation

Step 1: Fabrication and generalisation of a multi-layer, multi-response neural network of the visbreaker unit. (Completion of the data processing stage is assumed)

Comment: For the purpose of consistency, and in line with the work done in the previous section, the cascade correlation architecture will be used in the neuronal learning process.

Execution: Using all the available data from cycle-1 of the visbreaking operation, proceed with topology formation and network training.

Step 2 This phase addresses network calibration, where the network is exposed to the previously-seen data (the input data set used in the learning process). The network's response to this stimulus is to produce a set of data that is essentially

the neural network's prediction of visbreaking yields and residue quality. It is recalled that the visbreaker's conversion is calculated by summation of the gasoline, kerosene, and diesel streams flows. On the other hand, the volume of the visbreaker's residue and the vacuum gas oils has to be combined to paint a more accurate picture of their respective production volumes. As a result, for every input vector, our neural system generates an output vector. This is shown below:

Conversion = Volumetric sum of products boiling at less than 900 F (in percent).

Conversion	input vector ⇒ in our case 141 actual data
	output vector ⇒ in our case 141 predicted values
Residue make	input vector ⇒ in our case 141 actual data
	output vector ⇒ in our case 141 predicted values

Step 3: In the optimisation step, we need to devise a mathematical programme to minimise the RMS error between the actual and predicted results obtained in the previous step. Based on the aspiration-level criterion, we can define the system's objective, which is to minimise the prediction error subject to some constraints that set upper and lower limits for the desired target (conversion, or residue make). That is, we strive to search for the lowest possible value of the objective function, provided that our target result is within a set boundary. In this instance, the system's optimality criterion has been satisfied. Accordingly, the system's constraints can be formed using the mean value of the predicted output within a range, derived from the formula that is measuring the variability in the given data sets. Mathematically speaking, this is essentially a constrained optimisation problem that can be formulated as follows (Azizi, 1997):

Minimise the following fitness or cost function:

$$Z = \sqrt{\frac{\sum (L(Yop - Top)^2)}{Np}} \quad \textbf{(4.5)}$$

For Y_{op} and T_{op} and L that is defined as the load factor, that can *only* accept an integer value of $L = 0$ or $L = 1$.

Subject to the following constraints

$$M_P > (M_A - C_d) \quad \textbf{(4.6)}$$

$$M_P < (M_A + C_d) \quad \textbf{(4.7)}$$

Where

Y_{op} is the observed value of output o from training pattern p, and T_{op} is the predicted output and N_p is the number of active data sets used in the minimisation process.

and

M_P is the mean of the predicted value in a given data set

$$M_P = \frac{\sum Top}{Np} \quad \textbf{(4.8)}$$

M_A is mean of the actual value in a given data set

$$M_A = \frac{\sum Yop}{Np} \quad \textbf{(4.9)}$$

C_d is the coefficient of the data variability

$$C_d = \frac{\sum (Top - M_A)}{Np} \quad \textbf{(4.10)}$$

This is a binary integer minimisation problem. The generalised reduced gradient solver based on Lasdon and Smith (1992) GRG2 code is widely used in product blending problems. Therefore, initially, this code was used to minimise

the degree of error associated with accepting a data set for the learning process. As expected, this method found to be problematic, since a GRG2 solver often converged to local minima. The experimental result indicates that a solver based on genetic algorithm is more suitable for the given binary integer and sparse problem. Accordingly, Genehunter™ a solver based on the genetic algorithm is used to minimise the fitness function. The fundamental of Genetic Algorithms (Gas) and the method to calculate L is explained in Appendix 4 of this thesis. Here, L is an integer chromosome whose value should be estimated by the genetic algorithm. If the value of L is zero, the chromosome is not biologically fit to live. Accordingly, the data set represented by an unfit chromosome is a passive set. In this case, the entire data set is removed from further data processing. On the other hand, if the value of L is 1, then the chromosome is fit to live and the relevant data set is classified as the active set. Subsequently, the minimisation process continues with the surviving chromosomes. That is, only the data sets with a load factor of 1 will be used in further computation. In a neurological context, the load factor role is somewhat similar to that of the brain's thalamic unit. The purpose of thalamic unit is to compare the computed output with the target value and evaluate the outcome. If they do not match, the thalamic unit sends an error signal to the output synaptic unit of the brain for further processing.

Step 4 At this point, the neural network needs to be re-trained with the surviving data sets. The number of visible neurons remains unchanged, but the cascade correlation algorithm is free to increment the hidden node(s) dynamically, until no further improvement is seen in the level of error. At this point, the network's performance is evaluated. If the error is small enough (in our case the maximum tolerance is 1% from the previous result), the process is terminated. Otherwise, a new hidden element is added to the network in an attempt to reduce the residual error. This concludes the reformation and re-training step.

Step 5 By removing the data sets whose contribution may result in an increase in the neural prediction error, the network reciprocation procedure should essentially improve the quality of the paradigm response. At this step, the reciprocated network is exposed to the previously unseen data set(s). The responses are recorded and compared with that of an original network fabricated in the Step-1.

The process of the network reciprocation procedure is depicted in the following diagram.

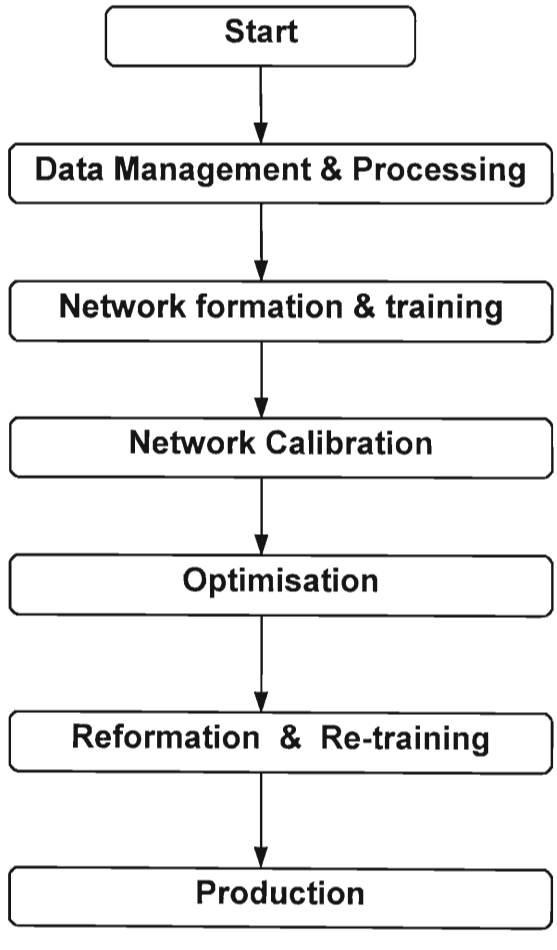


Figure 4-18 Network Reciprocation Procedure

It is evident from the above figure that a reciprocated network needs to be re-trained. In this case, the process of reciprocation and re-training may be achieved by a back-to back run of the Predict (neural network) and Genehunter (Genetic Algorithm) modules.

The following table compares the outcome of the reciprocation of the visbreaker's neural network with that of the many-to-many paradigm, already presented in the tables' 4-5 and 4-6.

Table 4-8 Reciprocated Neural Network

Conversion and Residue +gasoils make are expressed in volume %.

	Standard Neural Network		**Reciprocated Network**	
Description	**Recall**	**Prediction**	**Recall**	**Prediction**
Visible nodes	12 , 11	12 , 11	12 , 11	12 , 11
Hidden nodes	8	8	14	14
Data set	141	48	56	48
Data Type	Seen	Unseen	Seen	Unseen
RMS *Conversion*	2.12	4.31	1.55	3.41
RMS *Residue+gasoils*	2.89	5.05	1.84	4.03
corresponding Visbreaker residue %		60		61.2

Using the refinery's Global LP (GLP) the economics of using the reciprocated network versus standard network can be measured. In this example, the objective function value of GLP indicates that using the visbreaking yields derived from the standard network result in over estimation of annual profit of approximately $1,534,815 (6.9 million Rand). This information assists the refinery planners in their evaluation of various refinery feedstock. To achieve the same level of profit, other feedstock needs to be identified. Accordingly, the plant's operating condition has to be reviewed. Consequently, a revised production slate should be forwarded to the Marketing division. Against this

background, it may be said that firstly, network reciprocation procedure improves the accuracy of the planning system and secondly, its effect on the refinery profitability is significant.

It can be argued that network reciprocation is a valuable procedure when the quality of the visbreaker feed varies frequently. In other words, there is very little use for this procedure if a refiner continuously uses a particular crude oil (with no change in the physicochemical properties of visbreaker feed). This option of course is neither practical nor economical. As discussed in chapter 1 of this thesis, the world reserves of the more desirable crude's decline, while the reserves of the less desirable and inevitably more viscous crudes grow. Moreover, anticipated changes in crude quality and the product slate are expected to result in a wider price differential between heavy and light crudes. As a result, refiners have to continuously evaluate various feedstock (cost and quality), and select a crude or mix of crudes which can improve their profitability.

It should be noted that a neural network model could only learn from the examples (historical plant data). If a new crude is introduced, and if the properties of this new crude are vastly different from the historical plant data, then the system needs to be re-trained using the data pertained to the new crude. Obviously, in a multi-crude environment, the process of learning needs to be done more frequently.

The results presented in the above table prove that network reciprocation improves the predicting quality of the visbreaker's neural systems. In this respect the overall decrease in the RMS error between the actual plant data and the predicted response from an unseen stimulus is significant. Again, we have to remember that our unseen data are derived from cycle-2 of the visbreaking operation. As stated earlier, in addition to the variation in the quality of the feedstocks, the plant's operating condition surely differs in each of the visbreaking cycles.

Another impressive characteristic of the network reciprocation procedure is that it does not result in the over-training of the neural system. This is evident from the above table, where the RMS errors of *both* the recall and predicted responses have simultaneously been reduced. It should be emphasised that the refinery operation is of a continuous nature. Therefore, there is no limit to the number of process data available to produce an accurate pattern. Moreover, network reciprocation is not just a data or outlier eliminator, but a procedure to continuously evaluate the available data sets. Accordingly, it can be stated that, any data set originating from an unreliable or unstable unit operation should be detected and deleted during the data pre-processing stage of the neuroengineering procedure.

At this stage, we can conclude that our proposition regarding the application of the network reciprocation procedure to improve the predicting quality of the many-to-many visbreaker's paradigm has successfully been implemented.

In summary, in the first three sections of this chapter we have used the neuroengineering technique to fabricate an empirical neural network system. The system is capable of processing some unseen data and producing patterns that are related to the visbreaking yields and residue quality. In the fourth section of this chapter, we proposed a network reciprocation procedure with the intention of improving the predicting quality of the artificial neural network of the visbreaking process. Note that the reciprocated data (yields, quality) enter the fuel oil blending pool, where essentially the visbreaker's bottom residue is blended into a product that is marketed on its own, namely bunker fuel oil used by seafaring vessels as fuel. Since the economics of the visbreaker's operations are closely related to that of the fuel oil production, in the next section a mathematical model to optimise the blending operations will be presented.

4.5 Fuel Oil Production

In the previous chapter, we commented that the objective of fuel oil blending is to allocate the available blending components in such a way as to meet the product's specification at the least cost and to produce incremental products that maximise the overall profit. It was further explained that a refiner blends fuel oils for two reasons first, to meet certain specifications and second, to make the oil easier to handle.

Along with the above statements, there are, however, other points to observe. The first point is the objective of the visbreaking process, that is, to reduce the fuel oil make and save the expensive cutterstock that must be added to reduce the viscosity of the visbreaker's bottom residue. The other pertinent point is that most refiners have no alternative disposition for the visbreaker's residue. In old days this material was burned as the source of the energy in the refinery. Because of the environmental hazards, this of course is no longer an option. Consequently, a refiner must find an outlet for the visbreaker's bottom residue. Fuel oil blending provides an opportunity to produce a saleable product when the refinery is close to a port. The visbreaker's product constitutes almost 70% of the final blend. This includes visbreaker's bottom plus other products drawn from the atmospheric tower of this plant. Along with other environmental limits, the sulphur content of the blend is controlled to meet an international specification. This provides sufficient reasons to state that the economics of the visbreaking operations should essentially include the fuel oil blending.

The blending operation is in fact an optimisation process that needs to be mathematically modelled. In this respect, section 4-5 attempts to present a mathematical model to blend the visbreaker's products into a marine fuel oil.

In essence, we have an optimisation problem that can be formulated as follows:

Maximise $\boldsymbol{Z}$ = Profit

$$Z = C_1X_1+C_2X_2+.....+ C_nX_n$$

subject to the constraints

$$a_{11}X_1+a_{12}X_2+.....+ a_{1n}X_n \leq b_1$$

$$a_{21}X_1+a_{22}X_2+.....+ a_{2n}X_n \leq b_2$$

.....

$$a_{m1}X_1+a_{m2}X_2+.....+ a_{mn}X_n \leq b_m$$

$$X_1 \ , \quad X_2 \ ,....., \ X_n \quad \geq 0$$

To formulate the model, we begin by defining the profit as the objective:

Objective: Maximise the profit of selling marine fuel oil by blending various components for:

$$Z = W_f \ P_f - \sum_i^n V_i . d_i . C_i \qquad \textbf{(4.11)}$$

Decision variable is V_i = Volume of the component i in cubic meter that will produce the fuel oil blend.

where

Z = Profit in US $

W_f = Weight of fuel sold in ton

P_f = Price of the fuel sold in $/ton

d_i = Specific gravity of the component i at 60/60 °F (15/15 °C)

C_i = Cost of the component i in $/ton.

Constraints are

$$\text{Subject to } \sum_{i}^{n} V_i \cdot d_i \cdot Q_i \quad = \quad Q_b \qquad \textbf{(4.12)}$$

Where $Q_b \leq Q_s$

Q_i = Quality of the component i in the blend

Q_b = Quality of the final blend b

Q_s= Specified quality of the final blend b, in accordance with the manufacturing specification requirements presented in the following table:

Table 4-9 Typical CKS specification for the Marine Fuel Oil

Property	Test Method	Unit	Minimum	Maximum
Viscosity	D 445	cSt at 122 °F	90	180
Specific Gravity	D 1298	@ 60/60 °F		0.992
Flash Point	D 93	Degree °F	147	
Pour Point	D 97	Degree °F		75
Sulphur	LABA-242	Percent WT		4
CCR	D 189	Percent WT		20
Total Sediment	IP 375	Percent WT		Report
Stability	IP 390	Percent WT		0.2

Source: International Standards Organisation using standard: ISO 8217 RMF 25 for Marine and Bunker Fuel Oil.

Each component of the blend has its own distinctive quality that could greatly affect the quality of the final product. Some qualities (such as the Viscosity, Flash and Pour point) do not blend linearly. To account for the above-mentioned non- linearities, blending indices and a property transformation method is used. The procedure to transform the non-linear properties into

blending indices have been explained in section 2.1. The blending indices are given in Appendix-1.

We recall that property transformation consists of the following steps:

Transform the property to the appropriate blending index

Blend linearly, using the relevant blending index

Convert the final value to the unit's stipulated in the Table 4-9.

In the remainder of this section, we present an overview of the proposed fuel oil blending model.

With the exception of gas and gasoline, all the visbreaker's products can be blended into fuel oil. In order to meet the prescribed fuel oil specification, however, we need to expand our fuel oil recipe and include other refinery streams whose inclusion could result in a higher profit margin. In this respect, the structure of the proposed blending model is essentially a matrix of rows to represent the volume of various components of the blend, and columns to account for the specific gravity, cost, and associated qualities of each component.

Historically linear programming has been used to blend marine fuel oil. The LP model developed for this thesis uses the component's weight to blend the final product, since it is sold by weight unit (Azizi, 1993).

Furthermore, for simplicity, we have introduced a new column in the blending matrix. This new column should essentially account for an arbitrary variable ϕ, that we define as the fraction factor. The fraction factor may accept any value within the limits specified below:

$$0 \leq \quad \phi \quad \leq 1$$

Each component of the blend can have a fraction factor value within the above range (for $\phi_1 \ldots\ldots \phi_n$). In this case, a fraction factor of 1 means that the

full available volume of the specific stream is blended into the fuel oil. Conversely, when $\phi = 0$, that specific stream is removed from the blending pool. Obviously, the optimal values of the variable ϕ is computed by the system's optimiser.

The structure of the fuel oil blending matrix is shown below:

Table 4-10 Fuel Oil Blending Matrix

Stock	**Volume Barrel**	**Specific Gravity**	**Cost $/ton**	**Quality Q_1.....Q_n**	**Fraction Factor**
	V	d	C	Q	ϕ
Kerosene	V_1	d_1	C_1	Q_1.....Q_{1n}	ϕ_1
Diesel	V_2	d_2	C_2	Q_2.....Q_{2n}	ϕ_2
M-gasoil	V_3	d_3	C_3	Q_3.....Q_{3n}	ϕ_3
H-gasoil	V_4	d_4	C_4	Q_4.....Q_{4n}	ϕ_4
Visb-bottom	V_5	d_5	C_5	Q_5.....Q_{5n}	ϕ_5
Crude Kero	V_6	d_6	C_6	Q_6.....Q_{6n}	ϕ_6
Crude Diesel	V_7	d_7	C_7	Q_7.....Q_{7n}	ϕ_7
FCC LOC	V_8	d_8	C_8	Q_8.....Q_{8n}	ϕ_8
FCC-HCN	V_9	d_9	C_9	Q_9....Q_{9n}	ϕ_9
FCC-bottom	V_{10}	d_{10}	C_{10}	Q_{10}...Q_{10n}	ϕ_{10}
Others	V_i	d_i	C_i	Q_i .....Q_{in}	ϕ_i

The column "Quality" represents the related properties of the components of the fuel oil blend. In its simplest form, the fuel oil blending is a 4 × 12 matrix whose dimension increases with the number of desired properties to be included in the model's constraints.

The sources of data to initiate the above matrix are:

Table 4-11 Data sources

Data type	Source
Available volume to blend	Global refinery LP
Properties (stream's qualities)	Global refinery LP
Cost of streams	Global refinery LP
Price of products	Global refinery LP
Visbreaker's products	Adaptive visbreaker paradigm
Quality of the visbreaker bottom	Adaptive visbreaker paradigm

We recall that equation (4.11) represents the model's objective whose value needs to be maximised.

$$Z = W_f \; P_f - \sum_{i}^{n} V_i \cdot d_i \cdot C_i \qquad \textbf{(4.13)}$$

In this respect the Fuel Oil Blending model (FOB) is in fact an optimisation model whose solution produces a recipe for blending a marine fuel oil that meets the required specification. Since the model's interface is through Excel™, we use an Excel compatible solver from FrontLine™ Systems to solve this model. In contrast to the Genetic Algorithms solvers, the Premium solver is fast to converge and employs the Reduced Gradient algorithm applied to linear optimisation problems. In this respect, the Premium solver will replace the standard solver bundled with MS Excel™ software.

It is worthwhile to mention that to start the process of optimisation, some initial values for the variable ϕ are needed. These initial values should essentially produce a feasible solution. Setting a suitable value for the variable ϕ is often an educated guess often initiated by the refinery planners.

4.6 Model Integration

In the previous sections, using neural networks we constructed a model that is capable of predicting the yields and the quality of a refinery process unit called a visbreaker. In order to explain the performance of the visbreaking process, one must look very closely at the fuel oil blending operation, where the system's economic equilibrium is produced by the blending optimisation program. Consequently, due to the complex interactions among the parameters determining the economics of the visbreaking process (in terms of AVP and FOB), an Integrated system to represent the real-world problem is highly desirable. The schematic of the proposed system is shown below:

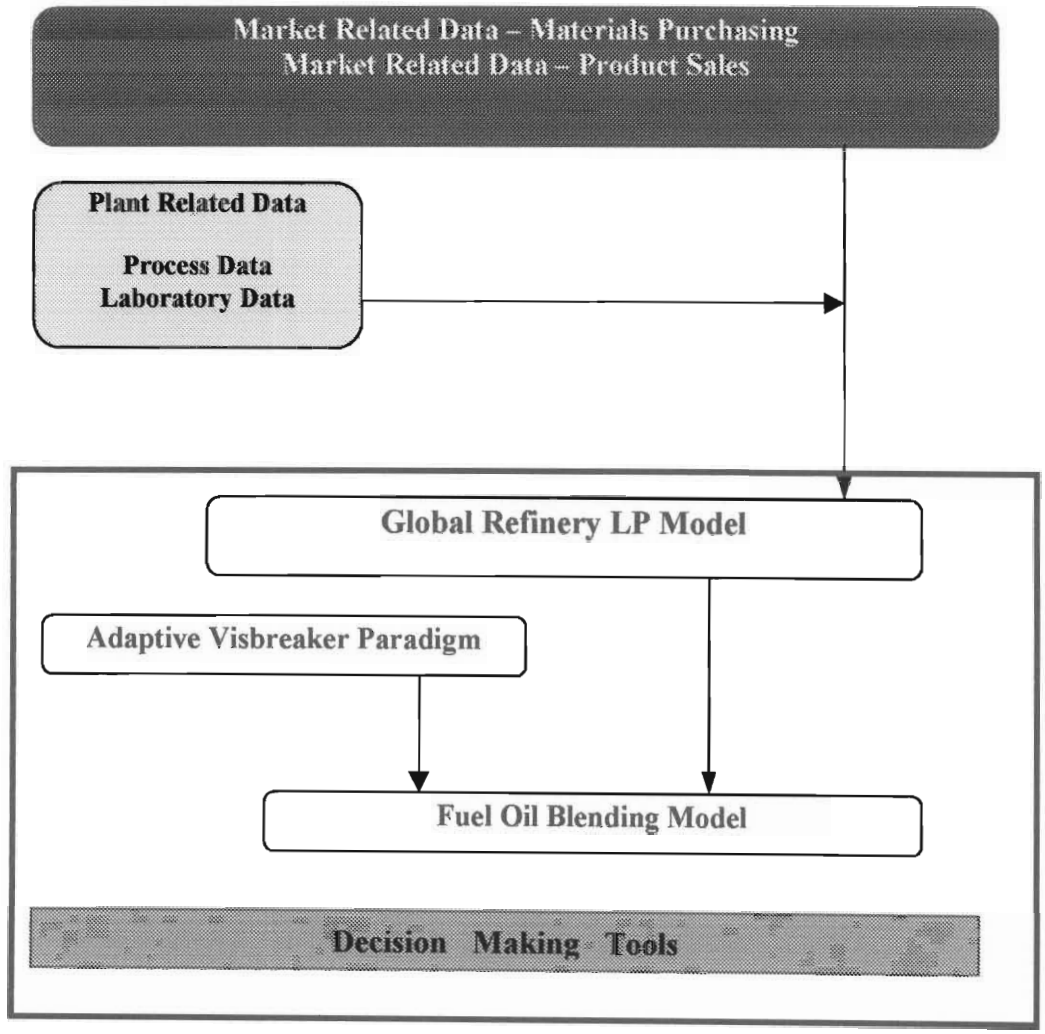


Figure 4-19 Model Integration and data flow chart in an integrated decision support system

In the "Roots of Backpropagation", P. J. Werbos (1994) writes:
"Within the brain, we know that there are subsystems and phenomena such as memory and pattern recognition. But we cannot really hope to understand the functions of a subsystem until we know how it fits in to the design of the whole system; therefore, once again an understanding of neuro-control is a prerequisite."

Our task, therefore, is to study the profitability of the visbreaking process based on the value of the objective function equation obtained from the optimisation of the fuel oil blending system. Accordingly, it is imperative for our understanding of the overall economics to examine the effect of parameter changes in an Integrated simulation / optimisation system.

In this respect, the full connectivity between the visbreaker's paradigm and the fuel oil blending model is highly desirable. Using the Excel and the Visual Basic programming tools (Webb *et al*, 1994), it is possible to produce an automated computer program to update the coefficient of the blending matrix, whenever the neural network's outcome has changed.

At this stage, we may add that, in an integrated system, it is possible to quantify the value of a changing parameter in statistical format as well as in monetary terms (Diaz *et al*, 1997). In our case, this is the value of the objective function equation expressed in US Dollars. This implies that the sensitivity of the *error* in predicting the visbreaker's yields or quality can be monetarily quantified.

In the next chapter, the financial impact of changing the major coefficients of the neural network system, as well as those relevant to the fuel oil blending matrix will be explored.

CHAPTER 5

RESULTS & ANALYSIS

The recent developments in artificial intelligence and software engineering promise a more complete programming environment for simulation /optimisation studies in the refining industry than has transpired in the traditional kinetically-based models. In a broader sense, any equation related to the physicochemical properties of the hydrocarbons can be incorporated into an artificially intelligent model. At the same time, such knowledge-based models may be trained to provide some valuable information about the problem area.

Such models, although invaluable for observing behaviour of a complex system in the closely replicated artificial setting, are, however, seriously limited as a decision making tool for a multi-dimensional problem, where the decision incentive is often economical rather than operational. Addition of an optimisation module, however, improves the decision making process. This is where the application of an integrated decision support system can be particularly useful.

Accordingly, in this chapter, along with the presentation of results, we demonstrate the potential of using an integrated system of an artificial neural network and optimisation technique. This is to produce a business-oriented solutions to the problem of residue upgrading in an oil refinery.

This chapter is organised as follows:

Section 5.1 Computational Results: Discussion and analysis on the significance and meaningfulness of the results obtained.

Section 5.2 Sensitivity Analysis: An important step in many applications of simulation modelling is to perform a sensitivity analysis on the performance of the model. Accordingly, this section evaluates the performance and limitations of the AVP.

Section 5.3 Interaction with the global refinery LP model: This section explores the practicality of an integrated decision support system to produce operational as well as economical data of the visbreaking operations. Accordingly, this section demonstrates the various applications of the adaptive visbreaker paradigm when is used as a vehicle to provide the visbreaking yield of crude petroleum. This is to improve the accuracy of the global refinery LP model used in crude selection and refinery-wide optimisation.

Section 5.4 Practical Consideration & Future Research Direction: The fuel oil storage stability criteria can not mathematically be formulated. In this section, we present an overview of the fuel oil storage stability performance and the motivation for further research into the fuel oil stability phenomenon.

5.1 Computational Results

In previous chapters, we have defined, designed, and consequently developed an integrated data management, simulation, and optimisation system. We have also described the tools applied and demonstrated the results produced. However, thus far, we have not yet fully discussed the significance and meanings of our computational results. Accordingly, in this section, we present the computational results obtained and endeavour to examine the meaningfulness of these results.

To begin with, we consider the many-to-many visbreaker paradigm. This is a multi-response neurally fabricated network. To improve the predictive quality of the paradigm, we introduced "network reciprocation". The network's topology can be modified by removing the undesirable input data set(s) and increasing nodes in the hidden layer of the network. The network reciprocation procedure resulted in the evolution of the many-to-many paradigm into a new and fully interconnected topology that is used to integrate with the fuel oil blending model.

The above discussion leads us to confine our ANNs response to real-world expectations. We need firstly to show a picture of the reciprocated network and secondly, a demonstration of its performance.

Thus in the following pages we present the topology of the standard and reciprocated network of the visbreaker unit. A plastic overlay-sheet is employed to illustrate the changes resulted from the network reciprocation procedure.

Obviously, the spatial relationships between the network's objects or nodes cannot be shown schematically. Again, for the purpose of clarity, we have not shown a complete picture of the real connections of any node.

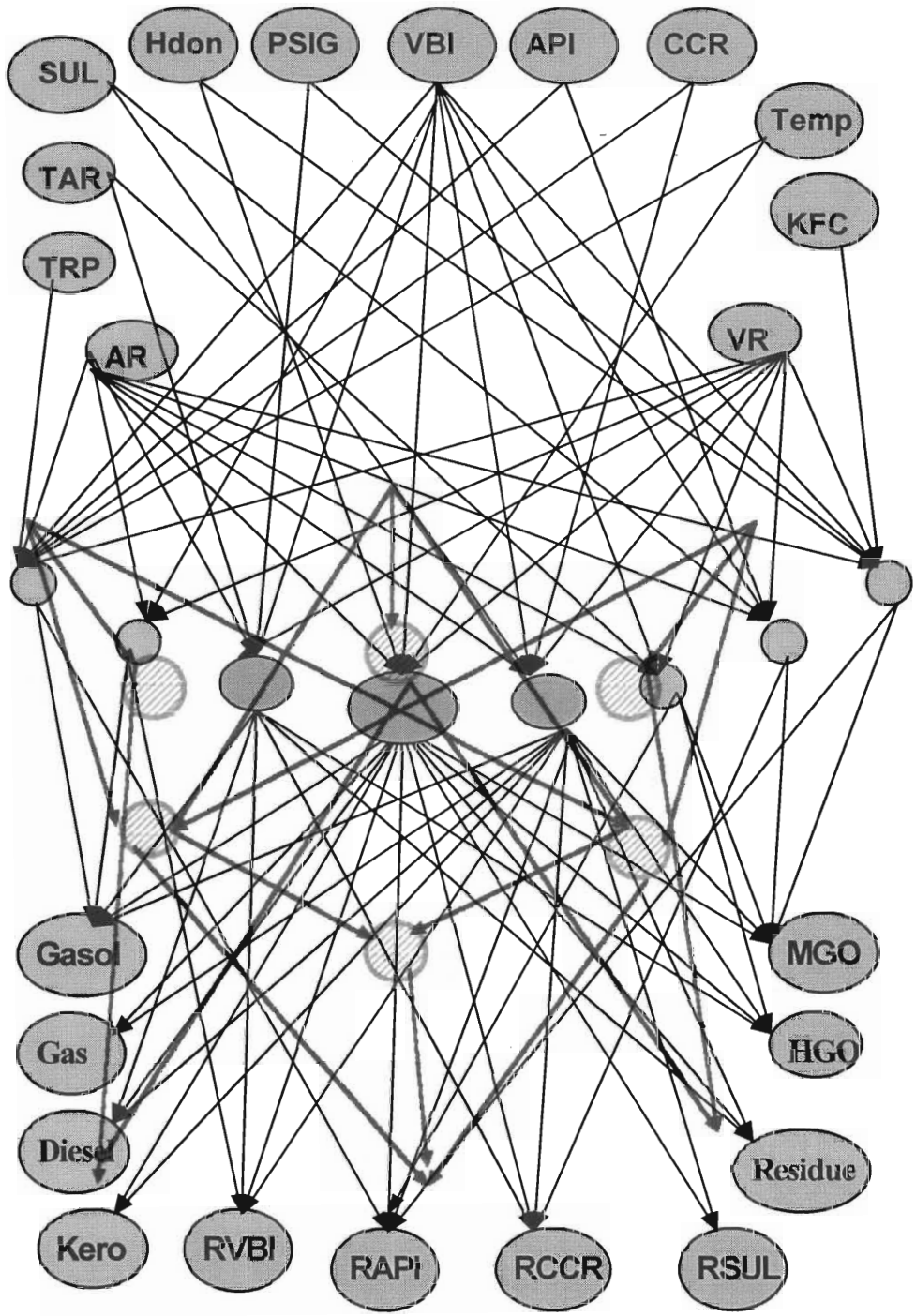


Figure 5-1 The Topology of the standard and Reciprocated Adaptive Visbreaker Paradigm

We observe that in a reciprocated network such as the visbreaker paradigm (shown above) the number and the properties of the input as well as the output units are essentially unchanged. The reciprocation procedure however, has resulted in the following changes:

- The number of data sets used in the training of the network has been reduced.

- The number of hidden units used in the training of the network has been increased.

We have already demonstrated that the implementation of the above change (using a reciprocation procedure) improves the predictive quality of the visbreaker paradigm. However, we have yet to demonstrate that our proposed procedure does not transform the given network into a parrot-like machine that captures the outgoing data from the neural network's memory field. This phenomenon often results in a discrepancy between the quality of the network output in respect of seen and unseen data. In other words, although the network produces an excellent match for the recall process, the predictive quality of the test set (unseen data) is often poor. One natural idea for dealing with this is to measure the RMS error of both seen and unseen input sets. If the RMS errors of both recall and test processes have been reduced, then the network is a reliable apparatus, otherwise the computational results are suspect and the given network has to be re-trained.

We have provided two additional charts. Figure 5-2A and 5-2B compares the actual visbreaker's conversion data with those predicted by the reciprocated network. The minimum and maximum conversion values of 13 to 28 volume percent are well within the historical data obtained from both cycle-1 and the cycle-2 of the visbreaking operations.

Figure 5-3A and 5-3B compares the actual versus predicted results of the combined residue plus gas oils make. In this case the minimum and maximum values of 75 and 90 percent reflect a realistic range for the residue plus gas oil recovery from the vacuum tower of the visbreaker unit.

The results obtained thus far are in line with the actual plant data reported by other researchers (Kuhn, 1979 and Maple, 1993). Furthermore, the following graphs attempt to demonstrate how the network reciprocation procedure has resulted in an improvement in the predicting quality of the adaptive visbreaker paradigm. Once again, we emphasise that the graphs are based on actual plant data obtained from the cycle-2 of the visbreaking operations.

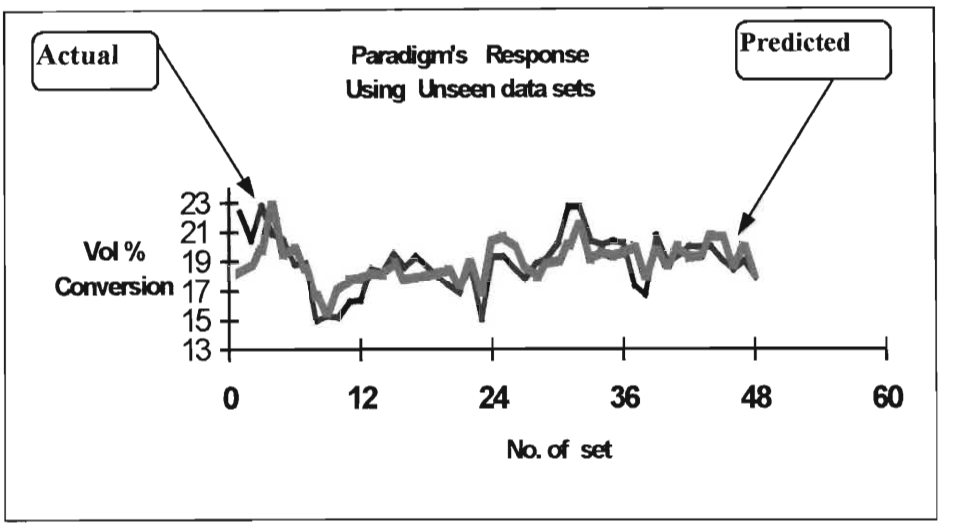


Figure 5-2A Reciprocated Paradigm's Response to Unseen data (cycle-2) Using 48 data set to represent 48 days of continuos operations. The mean absolute error of volume conversion is 1.10%.

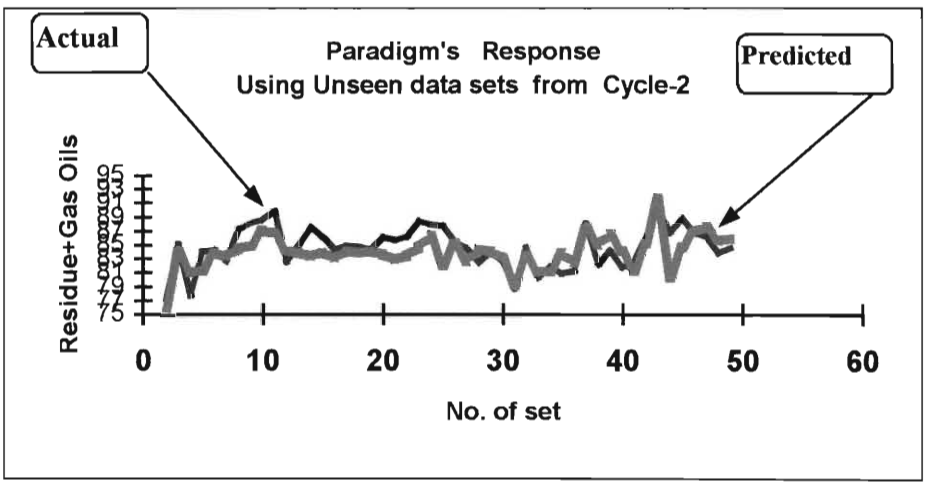


Figure 5-3A Reciprocated Paradigm's Response to Unseen data (cycle-2) Using 48 data set to represent 48 days of continuos operations. The mean absolute error of residue + gasoil is 1.86%.

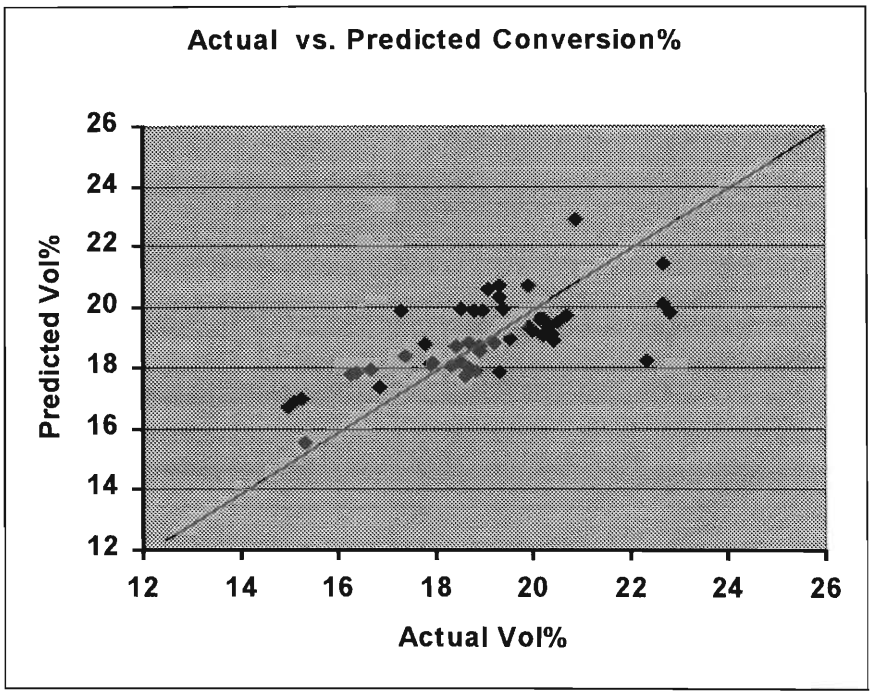


Figure 5-2 B- Reciprocated Paradigm's response to unseen data

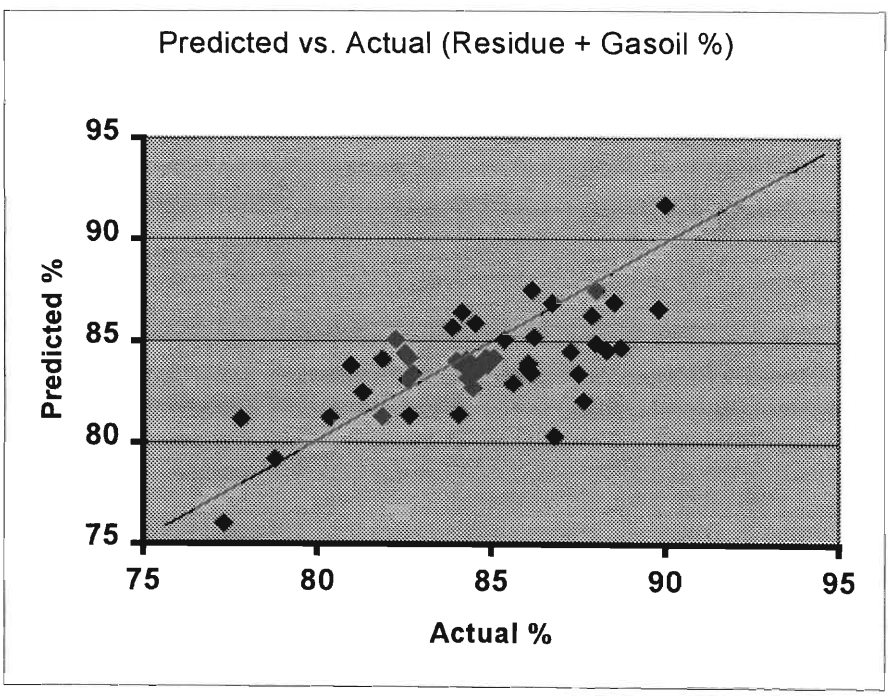


Figure 5-3 B Reciprocated Paradigm's response using actual versus predicted

Another important property of the reciprocation procedure is the preservation of the original data range. In other words, a data set that is removed from a training cycle may enter another training cycle, if its presence can contribute toward a reduction in prediction error. Thus, a reciprocated network should be capable of recognising a variety of data patterns. In this respect, it is desirable to widen the volume conversion range to account for the variation in the unit's severity. Given these complexities, it is not surprising that often the neural network system can not produce an exact match.

Lastly, in order to examine the validity of the paradigm's response, we have prepared the following graph:

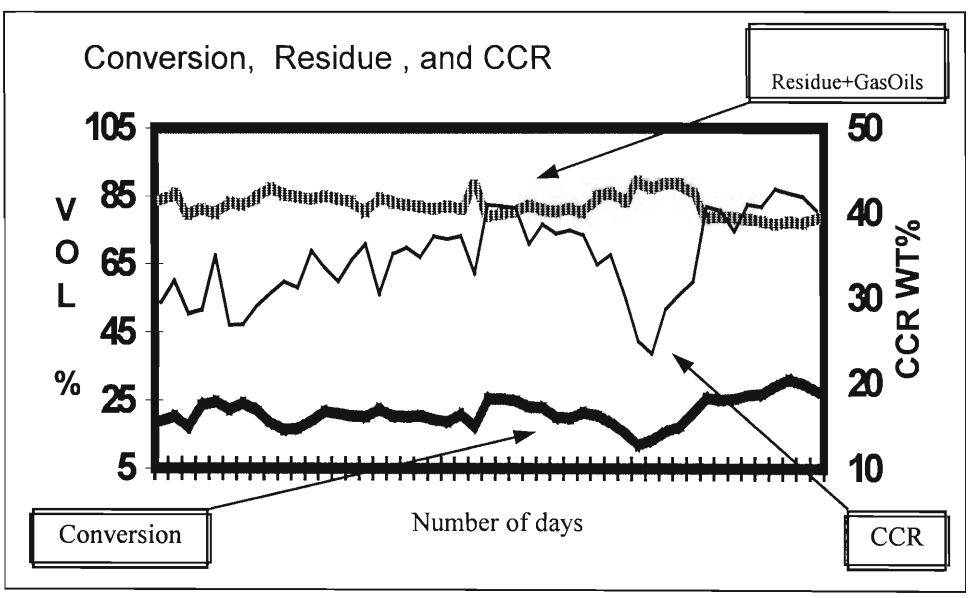


Figure 5-4 Reciprocated Paradigm's Response to Unseen data (cycle-2) for 48 days of continuos operation. Simultaneous prediction of Volume Conversion, Residue + Vacuum Gas oil make and Predicted CCR of the visbreaker bottom.

A multi-response paradigm is required to produce meaningful, accurate results. Here, the basic idea is to see if the predicted values are in line with the real world data. The above chart relates the adaptive visbreaker paradigm's prediction of the conversion, residue + gas oils to the CCR of the visbreaker bottom. It shows that using the actual data set properties, the predicted value of the CCR increases with an increase in volume conversion (and decreases when the residue + gas oil increase). Since the CCR content of the feed is expected to be concentrated in the visbreaker's bottom residue, the reported pattern in the above Figure is in fact an accurate account of the CCR disposition in the visbreaking process.

It is interesting to note that there are several contradicting theories regarding the CCR disposition (or asphaltenes formation) across the visbreaker unit (Giavarini *et al*, 1989). The increase in the CCR level can be as a result of:

Feed CCR

Feed Quality (Paraffinic, Aromatics, Metal Content, Sulphur,.....etc.)

Operating Conditions

and other unknown parameters.

Non the less, the most important issue remains to be the effect of asphaltenes content of the visbreaker feed. That is, an increase in asphaltenes in the feedstock reduces the yield of white products obtained from the visbreaking process.

In summary, from the materials presented in this section, we conclude that the computational results produced by the visbreaker paradigm correlates with experimental data obtained from the cycle-1 and cycle-2 of visbreaking operation..

5.2 Sensitivity Analysis

Modelling has always been a way of understanding the structure and function of a system. The purpose of model building is to explain, predict, or control a system. Businesses use different models for different reasons. The purpose of building a visbreaker model is to simulate the visbreaking process in order to understand the economics associated with its operations. Often, data in multi-criteria decision-making problems are imprecise and changeable. Therefore, an important step in many applications of simulation modelling is to perform a sensitivity analysis on the performance of the model. In this respect, the basic idea is to re-train and expose the model to various stimuli. This is to establish the limitations of the model in predicting the process yields. The method employed for this study consists of the following steps.

The sensitivity analysis concerns the re-training of the visbreaker model. This is to establish the limitations of the model in predicting the process yields. The visbreaker's process yield is of course dependent on the feed quality and unit's operating condition. The network stimuli are Conradson Carbon Residue (CCR) and the average soaker temperature, often expressed as the process severity. The visbreaker feed tank is regularly sampled and tested for the CCR content. This is because CCR is one the most important property of the visbreaker feed. CCR affects both the process yield and the quality of the visbreakate that need to be blended into the marine fuel oil. The sensitivity analysis on the adaptive visbreaker model consists of the several stages. The basic idea is, however, to re-train the network, expose the AVP to stimulus such as CCR and temperature, record and analysis the results.
This is explained below:

Stage1 - Data Preparation and Network Training

As stated previously, the pre-processed data from PI system represents 141 days for cycle-1 and 48 days for cycle-2 of the visbreaking operations. For the purpose of the sensitivity analysis, the model is re-trained twice. In the first re-training, only half of the data sets from the first cycle are used. For the second

training, all the data from the second cycle are used. The idea is to measure the network's prediction error when training data sets are vastly different. Essentially, the training process of AVP is similar to the method described in chapter 3. The nature and number of input and output nodes is also unchanged.

Stage2 – Network Testing Procedure

The model has been exposed to two stimuli: temperature, to represent the process severity, and Conradson Carbon Residue to represent the quality of feedstock. As stated above, the severity of the visbreaking process is often expressed as the average soaker temperature in degrees Celsius. The temperature range has been extended to measure the network's prediction error when the model is exposed to the data falling beyond the range previously seen by the AVP. The re-training and testing on each visbreaking cycle is carried out independently.

Stage3- Network Response

The response is defined as the visbreaker's conversion, expressed as the volume percent of the white oils obtained from the atmospheric tower of the visbreaker unit.

Stage4 - Presentation of Results

Results are shown in the following four graphs. The results are self-explanatory. For the sake of clarity, however, further explanations are given below:

4-1 : Network Response when Stimulus is reaction "Temperature"

Results are shown in Figure 5-5, Figure 5-6.

Figure 5-5 – Re-trained model using data from **cycle-1** of the visbreaking operations.

The model was tested by varying the unit's severity from 400 to 450 °C.

The network's response and conversion in volume percent, at the given temperature, have been calculated and recorded.

It is clearly shown that conversion increases with an increase in the reaction temperature. The straight line is the linear trend.

Figure 5-6 - Re-trained model using data from **cycle-2** of the visbreaker.
This is similar to the Figure 5-5, except that the data from the second cycle of visbreaking has been used. As before, the variations in the unit's severity and the model response to the change in the soaker temperature have been shown in this figure. It is clearly shown that conversion increases with an increase in the reaction temperature. The straight line is the linear trend.

The charts depicted on the transparency paper show the percent of absolute error of prediction calculated for each visbreaker cycle(s). This is to demonstrate how the error is distributed. It is clearly shown that the error increases at both side of the temperature range (where there is less data point). The straight line is the linear trend.

4-2 : Network Response when Stimulus is feed "CCR"

Similar work has been carried out to show the effect of varying the CCR of the visbreaker feed on the unit's volume conversion. In this respect, the model has been exposed to the variation in the feed's CCR. Results are shown in Figure 5-7 and Figure 5-8. As before, both visbreaking cycles has been used to demonstrate how the variation in the feed CCR will affect the volume conversion.

Figure 5-7 Re-trained model using data from **cycle-1**

The model was tested by varying the feed's CCR from 17 to 25 weigh percent (WT). The network's response and conversion in volume percent, at the given CCR, have been calculated and recorded.

Figure 5-87 Re-trained model using data from **cycle-2**

The variations in the feed's CCR in weight percent and the model response to this stimulus have been shown in this Figure. The charts depicted on the transparency paper show the percent of absolute error of prediction calculated for each visbreaker cycle.

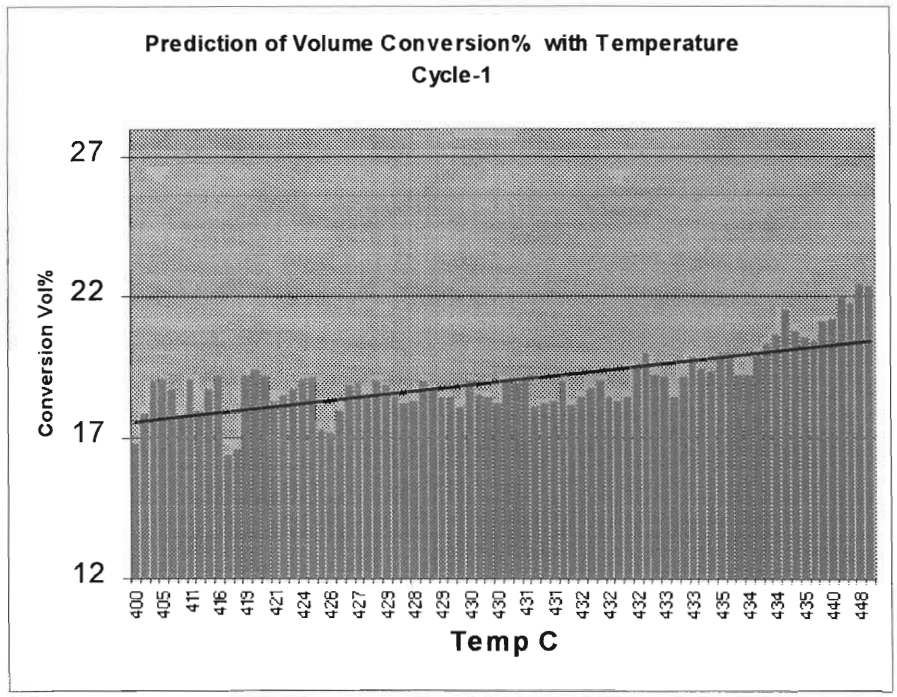


Figure 5-5 The effect of increasing severity on predicted conversion in cycle-1

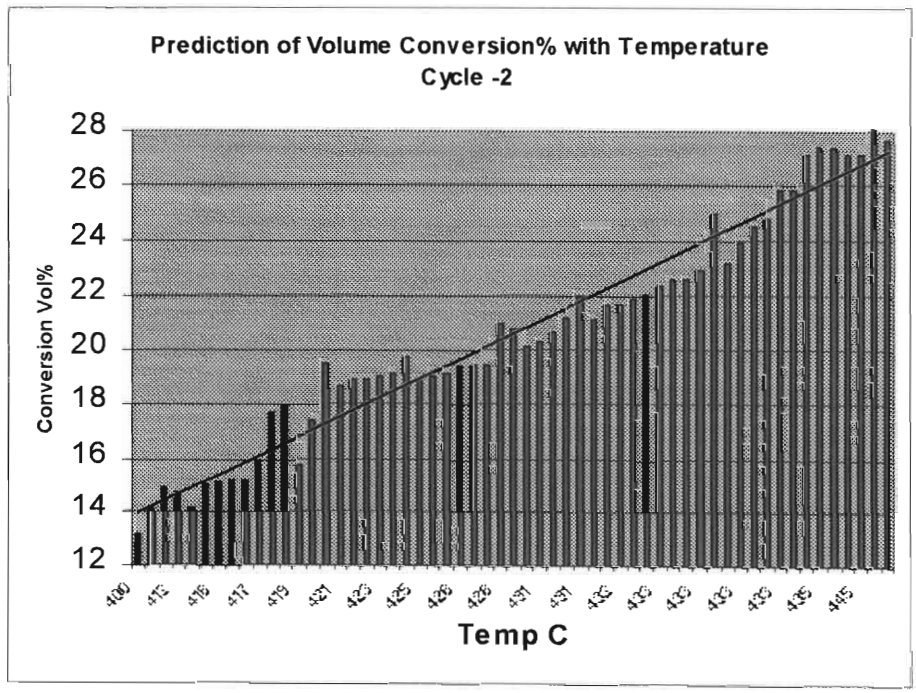
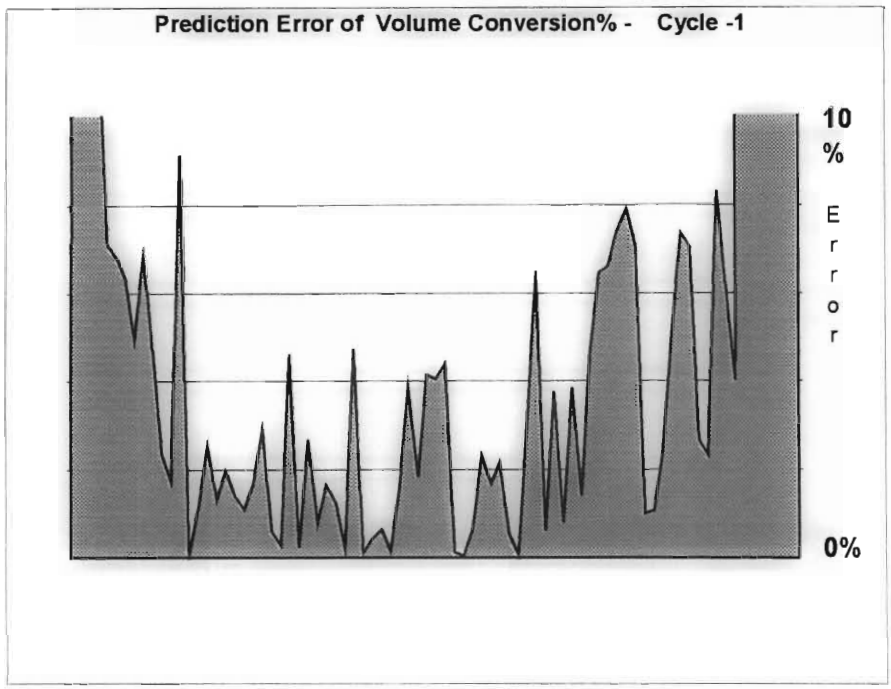


Figure 5-6 The effect of increasing severity on predicted conversion in cycle-2


Prediction Error of Volume Conversion% - Cycle -1
10
%
E
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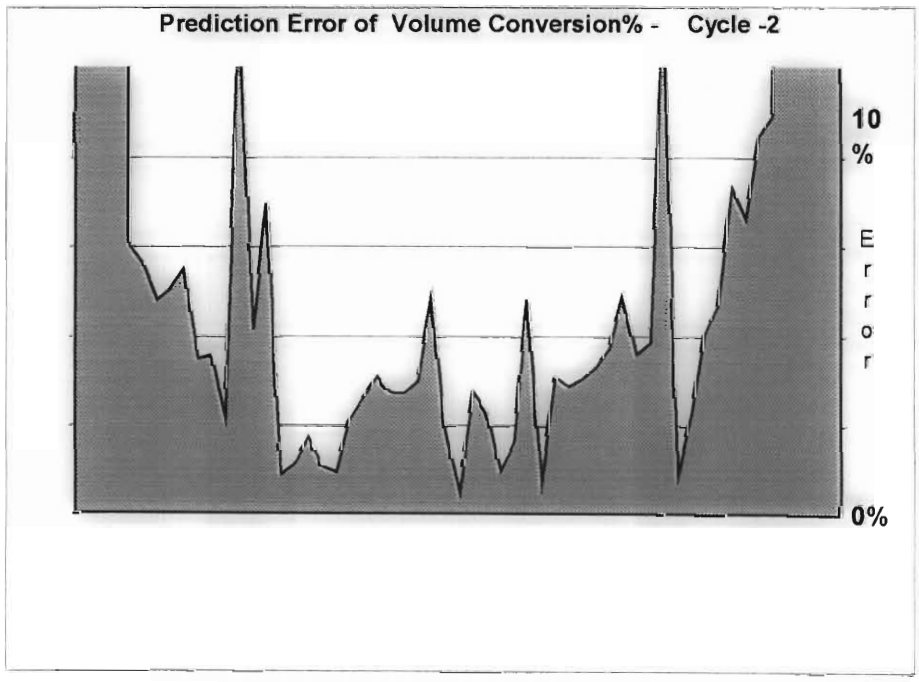
0%


Prediction Error of Volume Conversion% - Cycle -2
10
%
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r
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0%

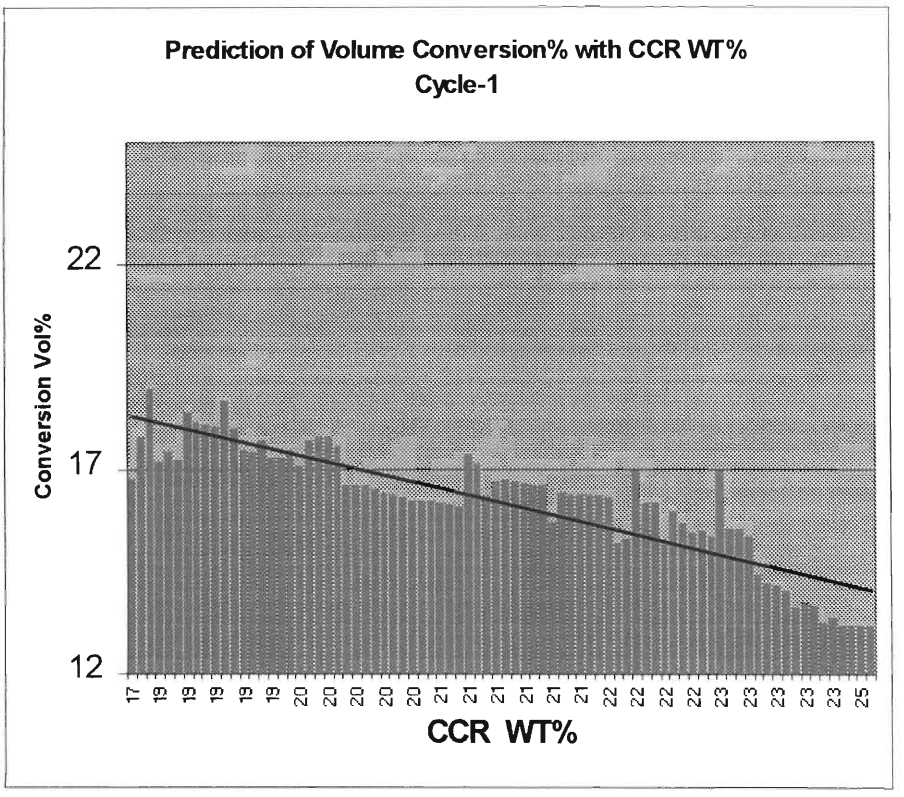


Figure 5-7 The effect of increasing feed CCR on predicted conversion in cycle-1

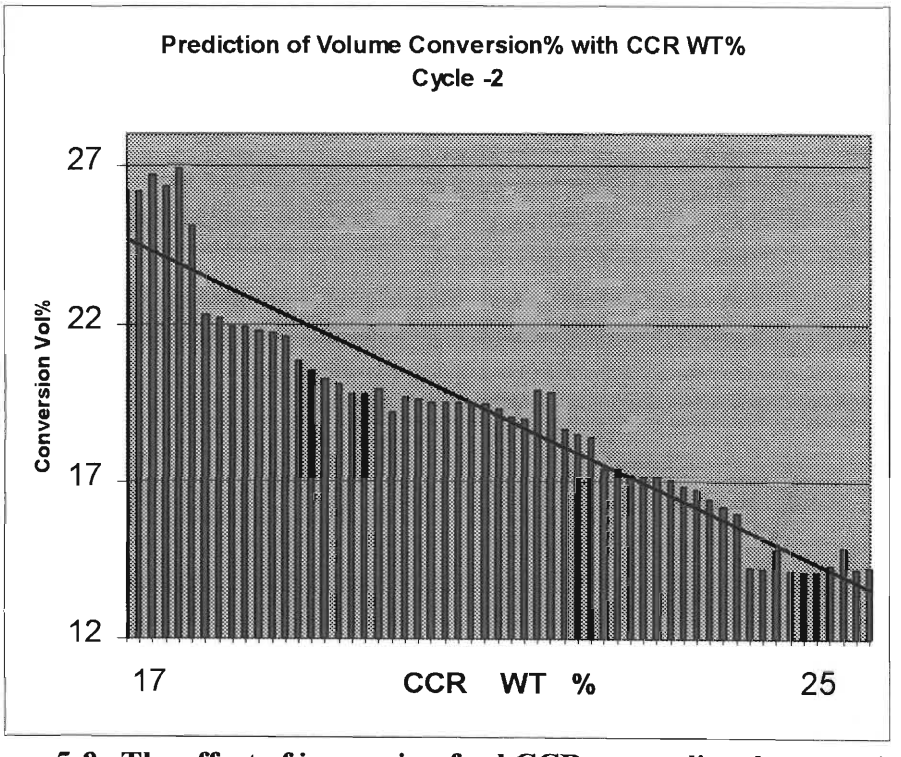
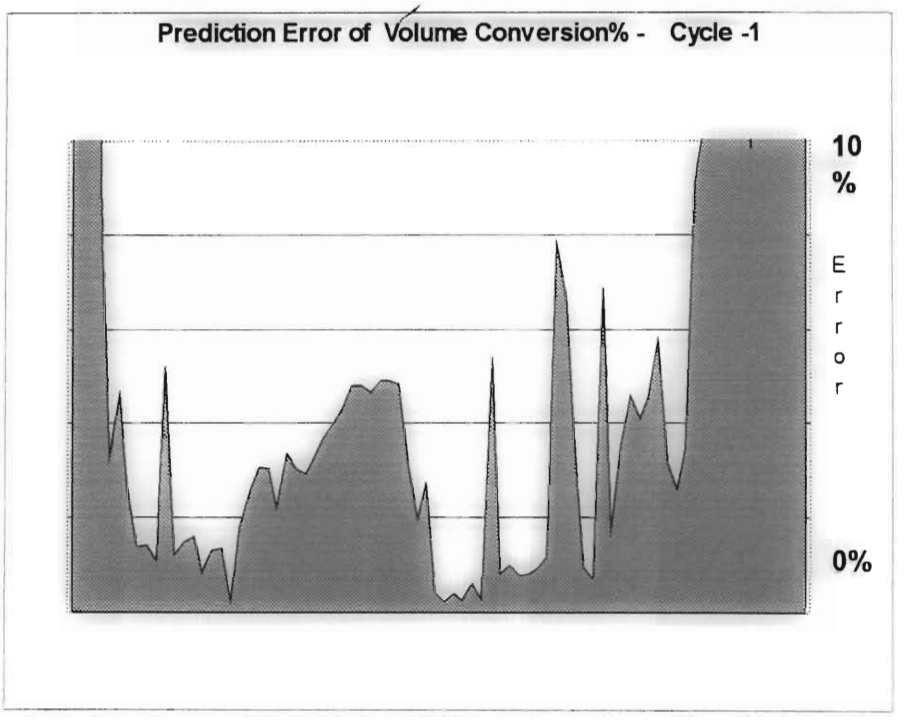
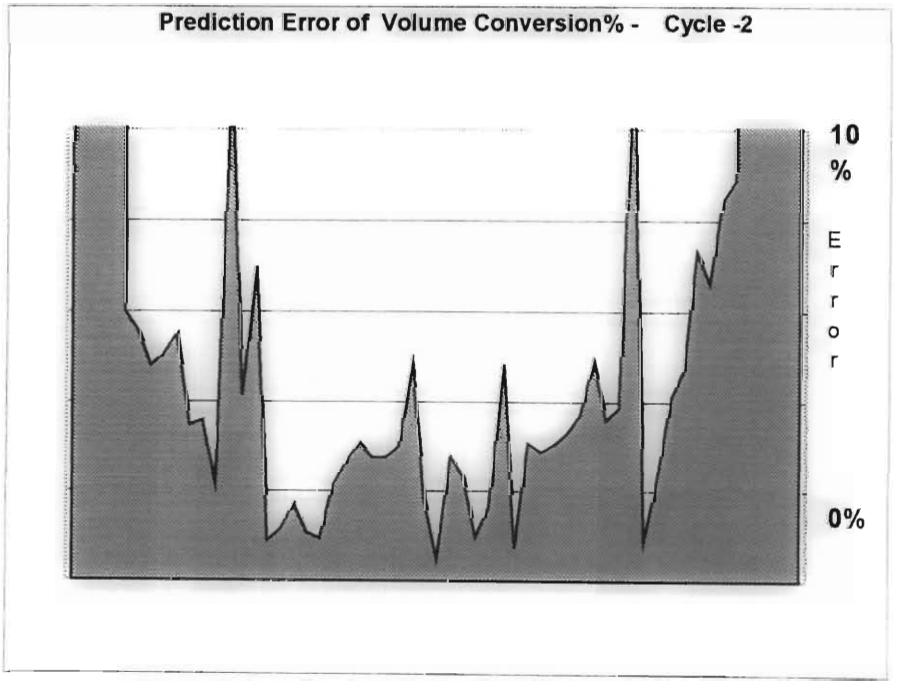


Figure 5-8 The effect of increasing feed CCR on predicted conversion in cycle-2


Prediction Error of Volume Conversion% - Cycle -1
10 %
Error
0%


Prediction Error of Volume Conversion% - Cycle -2
10 %
Error
0%

Stage5 - Analysis of Results

The results are summarised in the following Table.

Table 5-1 Error Summary

Source of test data	**Cycle - 1**		**Cycle - 2**	
No. of original data set	**71**		**48**	
A – Average of absolute error % in temperature range	**No. of data sets**	**Error %**	**No. of data set**	**Error %**
400-410 °C	6	54.3	4	100.0
410-420 °C	11	4.0	11	13.8
420-430 °C	27	1.9	14	2.3
430-440 °C	31	3.7	23	4.2
440-450 °C	8	88.8	6	84.8
Mean of vol% conversion		18.78		20.49
Confidence at 95%		0.27		0.81
B- Average of absolute error % in CCR range	**No. of data sets**	**Error %**	**No. of data sets**	**Error %**
17-19 WT%	6	52.0	4	75.0
19-21 WT%	37	3.0	16	7.3
21-23 WT%	32	3.9	33	2.3
23-25 WT%	8	74.2	5	78.0
Mean of vol% Conversion		16.82		19.51
Confidence at 95%		0.26		0.74

As expected, the above figures shows that the prediction error decreases with the increase in the number of data sets used in training of the network. This is

valid for both temperature and CCR stimulus. More importantly, the prediction becomes unreliable towards the outer limits of the range of the input data.

Another interesting observation is the limitation of the model to accurately predict the residue-cracking yield outside the temperature range seen during the training process. Using the statistical values shown above, the lower and the upper limit on the conversion with the confidence of 95% is 18.8 to 19.3 %. This corresponds to a severity of 429 to 433 °C, which is normally the temperature range, applied for this type of applications. Beyond this range, the prediction error increases radically. It is worthwhile to mention that severity of the visbreaking process is limited by over- cracking reactions, when the yield pattern changes violently. This of course affects the fuel oil stability; a phenomenon that will be fully discussed later in this chapter.

It should be noted that the primary objective of this exercise is to confirm the sensibility of the results produced by the model and whether the model's behaviour conform to the real world of visbreaking operations. From a practical standpoint, it is known that increasing the process severity produces more white oils. Conversely, feedstock with the high percentage of CCR will yield very little white oil. In other words, feedstocks with a low CCR are preferred.

In summary, it can be concluded that results produced by re-training the model conform to the real world of residue upgrading scheme presented in this thesis.

5.3 Interaction with the global refinery LP model

Since the interaction with the global LP model is one of the ***most*** important task of an integrated decision support system, let us to recap the work done so far. Using artificial neural networks and a genetic algorithm, we have custom-made a paradigm capable of predicting the yields of the visbreaking operations. As is seen earlier, the key issue in using the neuroengineering concept concerns the generalisation and the practicality of our decision support system. We have already discussed the validity of the model's findings and demonstrated that the paradigm's response and computational results are in line with the experimental data obtained from the plant. Accordingly, the roles or application of the adaptive visbreaker paradigm can be categorised as follows:

1- To be used as an integrated simulator/optimiser:

This is to predict the visbreaking yields and to measure the economics of visbreaking operations.

This application helps the refinery planners to simulate the visbreaking operation and fuel oil blending systems and thus set correct targets that affect production as well as scheduling, including tank capacity management.

2-To be used as a vehicle to improve the accuracy of the global refinery LP:

This is to produce yield patterns that can be used in the visbreaker sub-model of the global refinery LP.

This application improves the accuracy of the refinery LP model and thus helps the refinery planners with the crude evaluation and selection process as well as the global optimisation of the refinery.

Consequently, this section attempts to quantify the value of the system's decision parameters and to provide some insight into the real-world application (in the framework of the roles described above) of the adaptive visbreaker paradigm.

AVP — As an integrated simulator/optimiser model

In a neurodynamic environment, the quality of the system response needs to be economically quantified (Ozden, 1994). A systematic approach is to optimise the fuel oil blending module whenever the visbreaker paradigm produces data that are substantially different from the existing ones. The accuracy of these values depends on the computational hardware employed.

The operation's profit itself is a function of a multi-variable system, described below:

- The profit associated with selling the visbreaker's product.
- The profit associated with selling the marine fuel oil.
- The cost associated with purchasing the visbreaker's feed and fuel oil blending components.

The task is to evaluate the economics of the visbreaking operation by changing the decision parameters of the model. In essence, this concerns changing the unit's operating condition or feed quality. In this particular case, we intend to investigate the effect of changing the unit's severity of operation.

The problem solving approach is shown below:

Goal: Evaluate the economics of the visbreaking operation.

Decision Parameter to change: Visbreaker's severity as represented by the average soaker temperature.

Stage-1: Obtain the product pricing from OilNet (Oil&Gas information network) and other sources such as the Petroleum Economist journal or New York Mercantile Exchange.

Stage-2: Calculate the streams' value and volume balances using the global refinery linear program.

Stage-3: Data Management (PI, Excel, Visual Basic)

Stage-4: Neural Network Fabrication-Topology formation

Stage-5: Learning, Network Reciprocation, Calibration & Training

Stage-6: Neural Network Production

Stage-7: Fuel Oil Recipe- Optimisation

Stage-8: Computational results

Stage-9: Iteration to calculate the economics as a function of unit severity

Using the blending matrix presented in the Table 4-9, we have produced economic data related to the operation of the adaptive visbreaker paradigm. These are presented in the following tables. The refinery stream prices are in fact the shadow prices generated by the global refinery linear program (GLP). In this respect, we have produced a mathematical model of a complex refinery running 100,000 barrel per day of Arab crude. The selling price of petroleum products was obtained from the Petroleum Economist (PE) journal (average - first half 1996). For the sake of consistency, the selling price of all products is assumed to remain constant throughout this study. The estimated price of the various refinery products is given below:

Table 5-2 Product pricing

Product	Usage	Price $/ton	Source
Crude Oil	Crude Tower	94	PE
Gasoline	Final Product	183	PE
Jet Fuel	Final Product	180	PE
Diesel	Final Product	171	PE
Marine Fuel	Final Product	90	PE
Refinery Fuel	Furnace Fuel	40	GLP
FCC Diesel	Marine Fuel Oil Cutterstock	169	GLP
FCC Residue	Marine Fuel Oil Cutterstock	59	GLP

It can be seen from the above table that the selling price of the white products (Gasoline, Jet, and Diesel) is much higher than that of the marine fuel oil. The objective is to blend the visbreaker's bottom residue to a final marine oil specification, minimising the usage of the white products (cutterstock) and thus maximising the total operating profit.

The above prices are used in the integrated simulator/optimiser for the blend optimisation. At this stage, the model is ready to provide the product yield, properties and economic data related to the visbreaking operations. The investigation will evaluate the effect of increasing the unit's severity on the residue make and properties. In other words, by changing the unit's operating condition, we will measure the effect of increasing the temperature T, while the feed rate per day of operation TRP, feed quality f_q, and soaker average pressure P remain constant. This is shown below:

System Input $I = \begin{bmatrix} fq \\ U_c \end{bmatrix}$ **(5.2)**

where;

f_q = feedstock quality

u_c = unit's operating conditions

$$\text{Operating condition} = \boldsymbol{u_c} = \begin{bmatrix} T \\ TRP \\ P \end{bmatrix} \qquad \textbf{(5.3)}$$

TRP = Transit period in $s.m^{-3}$

T = Temperature in °C

P = pressure in PSIG

In this respect, we have used the reciprocated paradigm to predict the visbreaking yields and properties of the bottom residue, when the temperature is the only stimulus to the neural network system. A total of 10 cases were used. The results generated by the reciprocated visbreaker paradigm were subject to evaluation by the GRG2 optimisation package on a personal computer. The times taken to process these ten cases are shown in the Table 5-3.

Table 5-3 Time used by the Computer to Process The Model

Stage	**Time - Minutes**
Neural Network Fabrication & Preparation	
Data Preparation, Data pre-processing	45
Topology Formation, Initial Training	129
Network Reciprocation	57
Neural Network Production/Response	
Recipe generation & Optimisation per case	11
Reporting & recording	14

It can be seen from the above table that once a neural network is formed, trained, and calibrated, several cases can be run in a relatively short period of time.

The adaptive visbreaker's response is in the form of a matrix as presented in Table 5-4, below.

Table 5-4 Experimental results from the Adaptive Visbreaker Model (variable = reaction temperature)

Case	Temperature in Degrees F (C)	Conversion Volume %	CCR wet %	Residue Make VOL%	Operating Profit (Sales-Purchases-Operating expenses) in 1000 $ per day
1	780(415)	15.35	31.6	82.2	29.865
2	785(418)	15.88	31.19	83.4	30.087
3	791(421)	16.38	33.01	78.76	30.93
4	795(424)	16.80	33.7	77.15	31.340
5	801(427)	17.40	35.59	73.05	31.729
6	807(431)	18.21	37.33	69.64	32.965
7	811(433)	18.83	37.58	69.18	34.870
8	815(435)	19.37	39.11	66.47	35.110
9	817(436)	21.89	39.76	65.39	35.01
10	819(437)	22.09	41.08	63.29	34.167

It is known from thermodynamic theory as well as empirical studies, that increasing the furnace (or soaker) temperature results in an increase in the severity of the reaction, which intensifies the process of hydrocarbon decomposition. The results presented in the above table are in line with the empirical studies and the theory of thermal cracking. Furthermore, it indicates that increasing the temperature results in an increase in the volume conversion. The growth in the overall operations profit is also attributable to the increase in the conversion of black oil to white products.

In summary, the computational results presented above indicate that the operations profit increases with an increase in the operating severity and white oil production. However, increasing the reaction temperature beyond a certain temperature may result in polymerisation of the cracked molecules and thus asphaltenes formation. The increase in the asphaltenes affects the Conradson Carbon level and the storage stability of the fuel oil. As a result, the dispersion of the asphaltenes and dilution of the Conradson Carbon require additional amount of white oils. Consequently, this results in the quality imbalances. To obviate this difficulty, and to meet the stringent quality limits, the system optimiser needs to use increased volume of white oils which in turn results in a decline in the operating profit. Graphically, this is shown using Figure 5-9 to illustrate the effect of increasing the unit's severity (temperature) on volume conversion and CCR (weight %) of the residue.

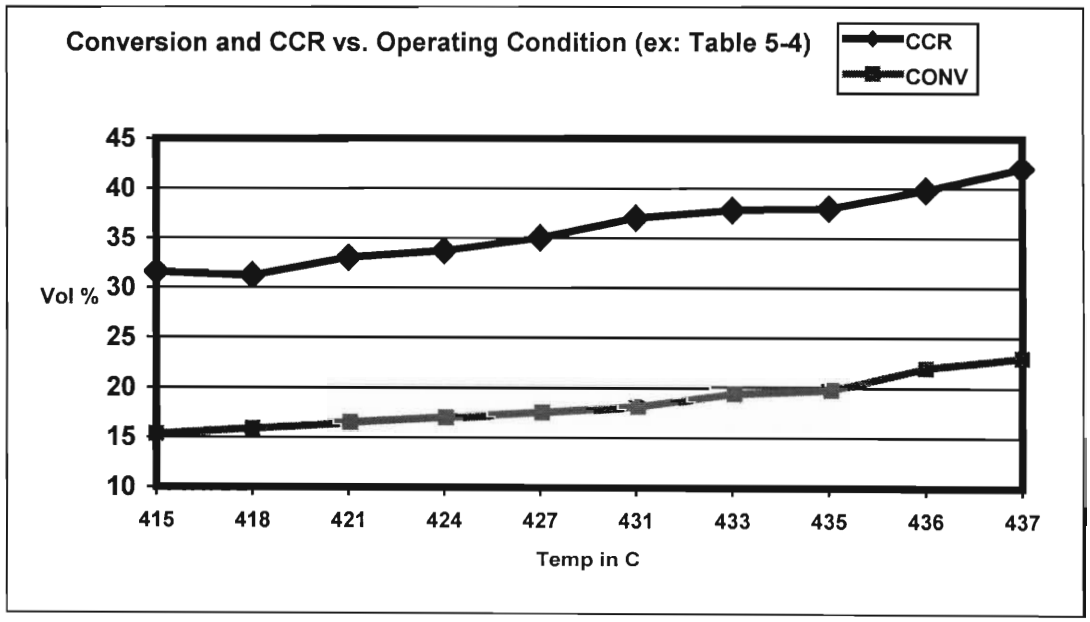


Figure 5-9 The effect of changing the paradigm's decision parameter – increasing the severity (Temperature) increases conversion and residue CCR.

Figure 5-10 is to illustrate the effect of increasing the unit's severity (temperature) on operating profit (visbreaking process + fuel oil blending).

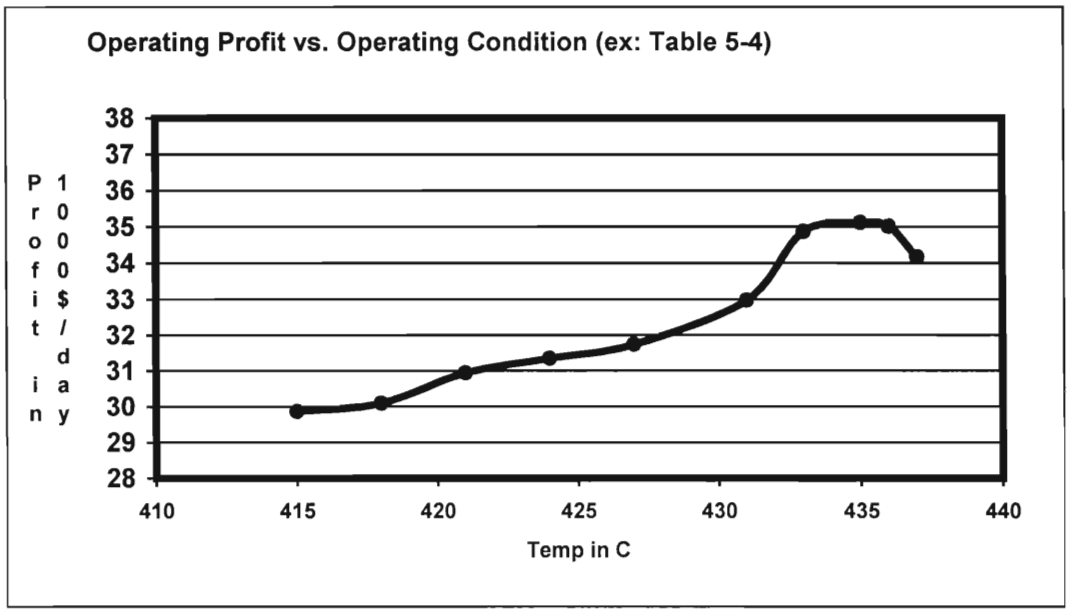


Figure 5-10 The effect of changing the paradigm's decision parameter – increasing the severity (Temperature) affects the operating profit.

The information given above is an excellent example of how an integrated knowledge-based system can assist scientists and engineers to evaluate the technical as well as the monetary value of their decision. Additionally, an integrated simulator/optimiser system is a valuable planning and scheduling tool that can be used to estimate the operating targets such as feed rate, severity, cutter type, inventory,……, and other important scheduling parameters.

The neural network's response to the variation in the soaker pressure was found to be negligible, the reason for which was found to be in the input data used in the training of the adaptive visbreaker paradigm. An examination of the data sets obtained from the first 141 days of visbreaker's operation shows little change in the pressure pattern.

Lastly, due to the variation in the residue content, hydrocarbon composition, metallo-organic compounds such as, nickel, vanadium, sodium, and potassium of crude petroleum, the visbreaking yields of various crude oils were found to be vastly different. This of course affects the white oil production and ultimately the refinery's profit. Consequently, refinery's crude mix and purchasing policy needs to be revised.

AVP — As a vehicle to improve the accuracy of the global refinery LP

As mentioned earlier, the major goal of this study is aimed at improving the efficiency and accuracy of the refinery's planning systems and tools and in particular, the global refinery LP model that is used to evaluate the refinery's feedstock, and to optimise refinery operations. Accordingly, it is expected that the visbreaker's sub-model of the global refinery LP uses the same yield pattern that is generated by the proposed reciprocated visbreaker paradigm. This is to provide a crude-dependent visbreaking yield thus enabling the GLP to account for the visbreaking yield of various crudes and other heavy residues used as the visbreaker's feed. Since these models are run independently, some computational method needs to be developed.

The method developed for this thesis is to produce a crude dependent correction vector that can change the visbreaking base yield of the GLP. This correction vector should be inserted into the GLP's matrix as a column vector X for $X = (X_1, X_2, \quad , X_n)$, where the elements in bracket are the corrective coefficients of visbreaking yields. Using a crude's physicochemical property such as CCR, the dependency of the vector X with the associated crude oil can be established. The importance of the CCR and its relationship with the residue's asphaltenes are to be discussed in the next section, but for the purpose of clarification, some description of this term is given below.

One of the most important characteristics of the visbreaker's feedstock is the Conradson Carbon Residue (CCR). CCR is measured by a test used to determine the amount of carbon residue left after the evaporation and pyrolysis of an oil under specified conditions, expressed as weight percent (American Society for Testing Materials ASTM D-189). Additionally, the bunker fuel oil produced from the visbreakate should meet (among other requirements) the CCR specification stipulated by the international standards. Against this background, and for the purpose of creating a dependency, this thesis employs CCR as the dominant variable affecting the visbreakability of a crude.

Accordingly, a procedure to update the visbreaking yields (visbreaker sub-model) of a GLP has been developed. This is highlighted below (for the sake of clarity, some real-world examples are used to demonstrate the viability of the proposed method):

Step 1 - Laboratory testing of crude petroleum to determine its physicochemical properties including the CCR of various residue cuts.
(This is normally done at the refinery's laboratory. Alternatively, crude assay data can be purchased from a consulting firm or another oil company. Depending on the details and distillation cut point, an assay data bank may cost between 300 to 1000 US $ per individual crude. The number of crude assay data in the refinery's LP model depends on the availability of crude, process configuration, etc. Recently, the author had an opportunity to inspect a crude evaluation LP model of an International oil company with 250 crude assays. In this case, the crude assay formed a matrix of 250 columns by 198 rows).
The crude data bank should be accessible by both the AVP and the GLP.

Step 2 - To train the Adaptive Visbreaker Paradigm to produce a yields pattern for various feedstocks with different CCR quality.
This is done by using the reciprocated AVP to simulate the visbreaking unit as explained in chapter 5 of this thesis. For the purpose of this study, we have selected 8 crudes from middle east (Dubai, Arab Light, Iran Light, Basrah Light, Kuwait, Iran Heavy, Arab Medium, and Arab Heavy) having an API range of 28 – 34 degrees. These crudes are available to South African refiners.
The AVP was used to produce a yield pattern for each individual crude (8 runs). The input data covered all the available laboratory assay data on the vacuum residue of these crudes. For consistency, the operating conditions (temperature, pressure) were assumed to be constant. This of course, may not be the case in real world applications, as the severity of the operation is often changed to optimise the white oil production.

Step 3 - To prepare a matrix of visbreaking yield for each individual crude (obtained in step 2 of this procedure), using CCR as the dependent variable as shown in the following Table:

Table 5-5 Experimental results from the Adaptive Visbreaker Model (variable = Feed Quality, CCR).

Note: The visbreaking yield of vacuum residue (VR in weight percent) of various middle-eastern crude have been normalised to 100% . The abbreviation for the given crudes are:

DUR = Dubai ALR = Arab Light ILR = Iran Light

BLR = Basrah Light IHR = Iran Heavy KWR = Kuwait

AMR = Arab Medium AHR = Arab Heavy

Crude Type vs. VR's CCR

Crude	DUR	ALR	ILR	BLR	IHR	KWR	AMR	AHR
CCR	19	19	21	22	25	26	27	31

% Product Yields per Crude Type

Gas	3	3	2	2	2	2	2	2
Gasol	7	6	5	5	5	5	4	4
Kero	9	10	10	9	8	8	7	5
LGO	9	9	9	9	8	8	8	6
MGO	4	4	4	4	4	3	3	3
HGO	9	9	10	11	9	10	9	8
BOT	59	59	60	60	63	64	67	72

It can be seen that the visbreaking of the vacuum residue of the above crudes produces 7 products. Additionally, the visbreaker bottoms make (visbreakate) increases with an increase in the CCR of the feedstock (assumed to be vacuum residue of above crudes).

Step - 4 Using the data from the above Table, develop the corrective coefficients of the vector X (defined as the CCR of visbreaker feed). This is achieved by the following methodology:

Calculate the slope b of the linear regression line through data points in an array Y (product yield), and X (CCR) for the number of data points n, using the following equation:

$$b = \frac{n\sum XY - \left(\sum X\right)\left(\sum Y\right)}{n\sum X^2 - \left(\sum X\right)^2} \qquad \textbf{(5.4)}$$

Here, the slope is the vertical distance divided by the horizontal distance between any two points on the line, which is the rate of change along the regression line.

Using the above equation, the slope of 7 lines representing 7 visbreaker products from 8 crudes can be calculated.

Next, the base yields are assumed to be from the crude with the lowest CCR, in this case, using Dubai crude with the VR's CCR of 19% (first column of Table 5.5). We recall that the basic idea is to insert the base yield into the GLP's visbreaker sub-model and to change these yields with a change in the CCR of crude's VR, using the correction vector X. Accordingly, a change in the CCR of the visbreaker feed affects the visbreaking yield of the global refinery LP.

The method applied in generating the correction coefficients (elements of vector X) is to use the slope b to linearise the yield pattern produced by the adaptive visbreaker paradigm. The difference between the highest and lowest linearised yield is the correction coefficient for that particular product. The following example illustrates how the correction coefficient for the visbreaker bottom (visbreakate) has been generated:

The yield pattern produced by the adaptive visbreaker paradigm is shown in Table 5.5. The required data arrays are:

Crude	DUR	ALR	ILR	BLR	IHR	KWR	AMR	AHR
CCR%	19	19	21	22	25	26	27	31

BOT%	59	59	60	60	63	64	67	72

Using equation 5.4 calculate the slope of the linear regression line through data point CCR and BOT (visbreaker bottom or visbreakate). In this case b = 1.0518. The linearised yields are calculated as follows:

Linearised Yield of a crude = (CCR of crude – Base CCR) * b + Base Yield

Using the above expression, the linearised yield of the visbreakate can be calculated. This is shown below:

Crude	DUR	ALR	ILR	BLR	IHR	KWR	AMR	AHR
CCR%	19	19	21	22	25	26	27	31

BOT%	59.0	59.0	61.1	62.1	65.3	66.4	67.4	71.6

Clearly, it can be seen that the yield penalty by moving from a crude with the VR's CCR of 19 to a crude with the VR's CCR of 31 is equal to (71.6 – 59 = 12.6 % or simply, 12.6 / (31–19) = 1.0518. Expressed in percent (incremental) visbreakate make for an increase of 1 CCR.

This value is in fact the correction coefficient used in the correction vector X.

By repeating the same procedure, we can now generate the correction coefficient(s) for every product produced from the visbreaking of vacuum residue of various crude as listed above (Table 5-4). This is illustrated as follows:

Table 5-6 Correction Coefficient for Vector X (Yield Change Vector for a Change in feed's CCR)

Visbreaking Product	Correction Vector X , for 1 CCR Change (expressed in percent)
Gas	– 0.0047
Gasol	– 0.1972
Kero	– 0.3039
LGO	– 0.3547
MGO	– 0.1016
HGO	– 0.0896
BOT	+1.0518

Step - 5 Modify the visbreaker sub-model of the global refinery LP to include the correction vector X next to the column representing the base visbreaking yield. This is a simple task and it can be done by inserting a column labelled CCR (to represent the correction vector X) into this sub-model. Additionally, the modified sub-model should include an equality row to declare the CCR of the base yields. The basic idea is to adjust the base yield by the CCR differentiation, adding the elements of vector X to the base yields of their respective products. This is further explained by the following example:

Lets assume that a refinery is running a 100 % Dubai crude and wishes to examine the visbreakate make if Dubai crude is replaced with the crude from Kuwait. To achieve this, it is necessary to calculate the delta CCR between Dubai and Kuwait crude. Using the correction vector and the delta CCR, the new yields can be formed. This shown in Table 5-7:

Table 5-7 An example of using the Correction Coefficients to account for the visbreaking yields of the Kuwait crude.

	DUR Base Yield	Correction Vector X	New Yields For Kuwait Crude Having a VR's CCR of 26
CCR	19	Delta CCR = 26 – 19 = 7	%

New Yield % = Delta CCR * Correction Coefficient + Base Yield

Gas	3	– 0.0047	2.97
Gasol	7	– 0.1972	5.62
Kero	9	– 0.3039	6.87
LGO	9	– 0.3547	6.52
MGO	4	– 0.1016	3.29
HGO	9	– 0.0896	8.37
BOT	59	+1.0518	66.36

It can be seen that using the proposed mechanism it is possible to evaluate a combination or blend of crude oils. Using the mixed integer capability (MIP) of the global refinery LP it is also possible to evaluate a "mixed bag" or a crude parcel (a cargo consisting of several crudes), where the whole parcel is either selected or rejected.

Further refinement of the above sub-model is the addition of a row to alter the unit's capacity with the type of crude processed. This is to account for the "coke forming" property of a crude's VR which reduces the visbreaker's cycle length (discussed in section 2.2 of this thesis). To include this feature, the correction

vector needs to be extended to include a new element representing the "coke forming" property.

A simplified example of the visbreaker sub-model is shown in the following Table. In this example, RRR is a row identifier, followed by a text showing the name of visbreaker's product. BAS is a column heading to include the base yields. The heading XXX is a column heading to represent the correction vector X. Two different feedstock under FEED1 (Vacuum residue) and FEED2 (De-asphalter tar) are classified as the feed to the visbreaker sub-model. As discussed the coke formation results in a decrease in the visbreaker's cycle length. This is calculated by the row 19 (R19) of the following Table.

Table 5-8 A sample of the visbreaker sub-model of the global refinery LP model that is used in crude evaluation.

RRR			XXX		
	**	BAS	CCR	FEED1	FEED2
**					
R01	VACUUM REIDUE			1.0000	
R02	DEASPHALTED TAR				1.0000
R03	LOSS	1.0250		-1.0000	-1.0000
R04	OFF GAS	-0.0091	0.0010		
R05	PROPANE	-0.0081	0.0008		
R06	PROPANE BALANCE	-0.0081			
R07	ISO BUTANE	-0.0044			
R08	IC4 BALANCE	-0.0044			
R09	N BUTANE	-0.0044			
R10	NC4 BALANCE	-0.0044			
R11	C5-330 NAPH	-0.0661	0.0003		
R12	VISBR GAS OIL	-0.0678	0.0005		
R13	VISBREAKER FLUX	-0.0900	0.0009		
R14	VISB LIGHT VAC GAS OIL	-0.0777	0.0012		
R15	VISB HEAVY VAC GAS OIL	-0.0980	0.0015		
R16	VISBREAKER BOTTOM	-0.6100	-0.0062		
R17	CHARGE BALANCE ROW	1.0000		-1.0000	-1.0000
R18	CCR OF BASE YIELDS	22.0000	1.0000	999.0000	999.0000
R19	VISB CAPACITY	1.0000	0.0100		
R20	CCR REPORT	1.0000			
R21	AVE FEED CCR	22.0000	1.0000		
R22	PLT FUEL MMBTU	0.1500			
R23	POWER KWH	1.0150			
R24	STEAM MLBS	-0.0890			
R25	COOL H2O MGAL	0.6910			
R26	SO2 CONTROL LIMIT	0.0001			

Other rows and columns represent customised features of the LP model. In the example above, row 20 and 21 are for reporting purposes. Row 22 to row 26 represent the plant's utility consumption and sulphur Di-oxide emission control.

It is clear that the yield pattern obtained from the adaptive visbreaker paradigm can be used to equip the global refinery LP with the capability of differentiating between the visbreakability of various crude. As a result, the GLP can be used to economically evaluate various feedstocks. This is shown below.

In the following example, the significance of using different crude with different visbreakability is demonstrated. In this case the yield pattern produced by the AVP has been copied to the refinery global LP model. Accordingly, using the refinery's global LP model the economics of processing 100,000 bbl per day of Arab Light (ALR) versus Iran heavy (IHR) at different visbreakate make can be calculated. This is shown in the following graph:

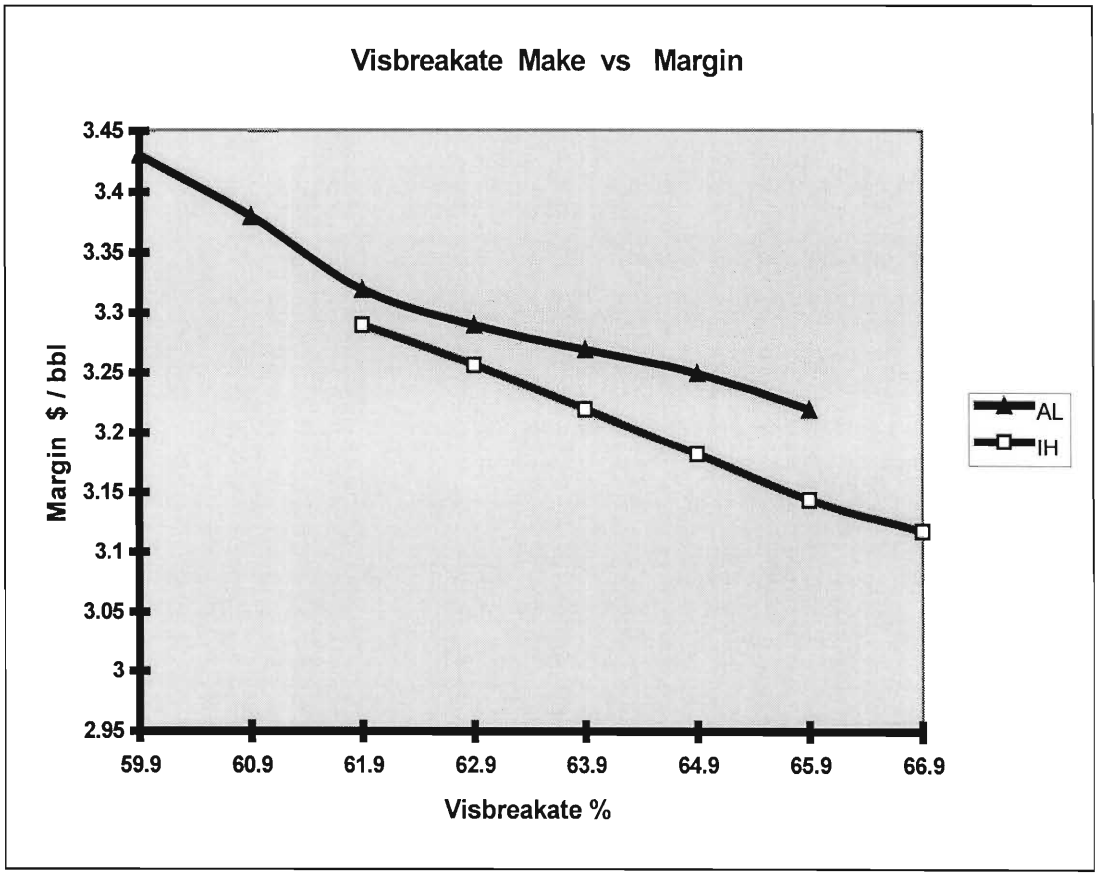


Figure 5-11 The effect of changing the Visbreakate make of different crude.

It can be seen from the above graph that the refinery margin is highly sensitive to the visbreakate produced by two different petroleum crudes. The deterioration in the visbreaking yield produces a ±0.19 $/bbl penalty for Arab Light and ±0.15 $/bbl for Iran Heavy. The overall penalty (by moving from Arab Light to process Iran Heavy with high visbreakate yield) is ± 0.28 $/bbl change in the daily margin. For a 100,0000 bbl/day refinery, this value translates into $28000 per day of operation. This amount is of course significant and can influence the decision making chain involved in the crude evaluation and selection process.

As seen in Table 5-4, the adaptive visbreaker paradigm can be employed to produce a detailed picture by predicting the residue make as well as the quality of the visbreaker bottoms. Accordingly, to maintain an accurate refinery LP model, a frequent update of the GLP's correction vector is necessary. This of course requires an input from the adaptive visbreaker paradigm.

The material presented in this section shows the feasibility of the application of the adaptive visbreaker paradigm to predict the cracking reaction yields. Additionally, the proposed integrated system allows dynamic monitoring of the residue properties as applicable to fuel oil blending optimisation. It was also demonstrated that through interaction the global refinery LP model can be equipped to differentiate between the visbreaking yield of various crude oils.

Besides the known parameters affecting the visbreaker's operations, there are other practical constraints, which are often difficult to define, quantify, or model. These are discussed in the forthcoming section.

5.4 Practical Considerations and Future Research Direction

In the last section of this chapter, we discuss another important characteristic of the visbreaking operation; namely fuel oil stability.

A stable fuel oil is a complex solution of asphaltenes and malthenes. According to the Institute of Petroleum IP375/IP390 test methods, the precipitation of asphaltenes from a residual fuel during storage and handling causes severe difficulties, which in extreme cases can render the fuel unfit for use. Once out of solution, it is extremely difficult to re-peptise the asphaltenes into their original state.

The precipitation of asphaltenes results in further polymerisation and sludge formation. Consequently, the use of such an unstable oil causes filter plugging and other mechanical problems.

From the practical standpoint, this is a disaster. Firstly, the instability phenomenon may occur up to several days from the date of manufacture. Thus a product that meets all the specification-related tests on the date of transfer to the customer may be unfit to use when needed. Such products must be returned to the refinery for correction. This can be constrained by storage tank limitations. Secondly, to re-peptise an unstable fuel oil, the severity of the visbreaking operations must be greatly reduced to ensure that the freshly-made products are able to re-establish and stabilise the colloidal suspension. Undoubtedly, the financial loss is enormous. In view of the above, the stability of visbroken fuel oil is generally accepted as the criterion limiting conversion of the visbreaking process.

The adaptive visbreaker paradigm is not equipped to predict the stability of the final fuel oil recipe, for the following reasons:

- There are no universally agreed upon criteria (or definitions) of stability.
- The stability of the fuel oil is often measured using different laboratory test methods.
- The thermal and chemical ageing of the fuel oil can not scientifically (or mathematically) be related to the feed's quality, operating conditions, or blending procedure (addition of aromatics followed by olefinics and lastly paraffinic materials).

To expand on the fuel oil storage stability problem and its possible causes, we provide the following explanations.

In the previous chapter, we commented that, beyond a certain point, an increase in the severity of the operation often results in, firstly, asphaltenes precipitation and secondly, an increase in asphaltenes formation. As discussed, asphaltenes are polycyclic and the most polar compounds found in crude oil, and in their natural form, these highly complex macromolecules are dispersed in the gas oils and other components of visbreaker feed. In general, the asphaltenes and high molecular weight aromatic malthenes form a stable colloidal system. This complex system can be visualised as the cross-linked or associated condensates of a multi-component system. This is made of individual molecules of aromatics, paraffins, naphthenics, macrocyclics and heterocyclics, in which the bridges or links can be cleaved under selective chemical or physical conditions. Transition metals such as nickel and vanadium are also present in the macrocyclic or heterocyclic systems in the form of porphyrin or non-porphyrin. Free radicals sites of asphaltenes are associated with the aromatic moieties of the asphaltic skeleton. The concentration of these organic radicals in asphaltenes is relatively high, of the order 10^7 to 10^8 radicals/g asphaltenes. The chemical activity of these radicals is of considerable importance with regard to the polymer, mesophase and coke-forming propensity of the asphaltenes (Khulbe *et al*, 1996). For simplicity, often the petroleum fraction which is

benzene soluble and normal pentane insoluble is generally referred to asphaltenes.

According to Hus (1981) "the micelle consists of core asphaltenes to which high-molecular weight aromatic hydrocarbons from the malthenes fractions are absorbed. To these high-molecular weight hydrocarbons, other hydrocarbons with somewhat higher hydrogen content are absorbed, until the micelles at their periphery contain hydrocarbons with a hydrogen content which is about equal to that of the continuous malthene phase".

In a stable fuel oil, the system of absorbed malthenes is such that all absorption forces are saturated. The micelle is then in physical equilibrium with the surrounding oil phase. In other words, the asphaltenes are peptised.

The absorption equilibrium can be disturbed in several ways, for instance, by adding hydrocarbons with a higher hydrogen content (aliphatic, or paraffinic hydrocarbons) and by increasing the temperature. Part of the absorbed compounds then dissolve in the continuous malthene phase, whereby the asphaltene cores precipitate.

During the visbreaking process, the continuous oily phase is cracked to small molecules. Also, new asphaltenes are formed from malthenes, and the malthene phase composition changes in character, so that eventually the equilibrium between asphaltenes and malthenes is disturbed to such an extent that part of the asphaltenes will flocculate. At this point, the cracked fuel oil becomes unstable.

In recent years, scientists have tried to introduce an early-warning system enabling refiners, firstly, to select an optimum visbreaker severity and secondly, to produce a stable fuel oil blend. The problem is, however, compounded by the fact that there is no universally accepted test method to approve or reject a batch of the fuel oil. In general, the stability of fuel oil is a function of:

- Feed-stock quality

- Operating condition
- Components used in blending the fuel oil

The experimental work by Castellanos *et al* (1991) with the Maya and Isthmus crude's at the Azcapotzalco refinery in Mexico city, suggests that the operating conditions (in term of the temperature and residence time) are key elements of the visbreaking operation. Their kinetically-derived model uses up to ten pseudo-components to characterise and categorise the various hydrocarbons according to their carbon number and hydrogen content. The model is, however, blind to the residue quality and its consequent effects on fuel oil blending.

According to C.J. Kuo (1984) from Singapore Petroleum, the stability of the fuel oil is also affected by the coke formation phenomena. He states that the petroleum coke formed during cracking apparently also affects the stability of visbroken fuel oils. When the coke is freshly formed, the particles are so fine that they can be easily suspended in the petroleum oil phase and partially, if not all, pass through the filter of the hot filtration test (IP370). Pilot plant tests also indicate that the resins present in the feedstocks act as the peptising agent and therefore their presence results in a higher visbreaker conversion and better fuel oil stability. Based on the colloidal solution theory of phase equilibrium, Kuo has defined a "stability factor" that is quality dependent. The experimental work with Chinese and Arab crudes indicates that the stability factor **SF** is closely related to the visbreaker's feed quality as shown below:-

$$\mathbf{SF = (A + R) / (S * CCR)} \qquad \mathbf{(5.4)}$$

where

A = Aromatics, in weight percent

R = Resins, in weight percent

S = Saturates, in weight percent

CCR = Conradson Carbon Residues, in weight percent

The CCR in the above equation is intended to reflect asphaltenes, as they can be correlated by the following empirical equations (suggested by Kuo):

For atmospheric residues, asphaltenes $\mathbf{ASP}_{AR}$, weight percent are estimated from:

$$\mathbf{ASP}_{AR} = \mathbf{0.2854\ CCR\ +\ 0.0049\ CCR^2} \qquad \mathbf{(5.5)}$$

For vacuum residues, asphaltenes $\mathbf{ASP}_{VR}$, weight percent are estimated from:

$$\mathbf{ASP}_{VR,,} = \mathbf{0.3373\ CCR\ +\ 0.0058\ CCR^2} \qquad \mathbf{(5.6)}$$

The process weight percent conversion at 662°F (350°C) **CONV**, is obtained from the following equation:

$$\mathbf{CONV = -\ 0.7922\ CCR\ +\ 41.804\ (SF)} \qquad \mathbf{(5.7)}$$

Where: SF = Stability Factors as defined in the equation (5.4)

The empirical equations presented above are of great value to a refiner, when the feedstocks quality, or unit operating condition is fairly constant. Unfortunately, this is not the case in the real world. Moreover, some scientists believe that various correlation's made of paraffin content, asphaltenes, and characterisation factor **K** of the feedstocks cannot fully describe the behaviour of certain feedstocks. Others believe that the metallo-organic compounds of the residue also improve the condensation and polymerisation process leading to asphaltenes formation (Holmes, 1993).

In order to illustrate the effect of asphaltenes' precipitation, two microscopic photographs of the stable and unstable fuel oil have been prepared. In this respect, the specimen of colloidal suspensions is photographed using a laboratory microscope. These photographs are presented as Exhibits-1 and 2 in Appendix-5 of this thesis.

From the theoretical arguments presented above, we conclude that the process of thermal decomposition of the heavy hydrocarbons is indeed of a

complex nature. Thus far, there exists no kinetically-based model that can satisfactorily predict the visbreaking yields or fuel oil stability.

It was demonstrated that an ANNs system based on neuroengineering technique can predict the yields of the visbreaking process unit. As stated earlier, an artificial neural network is a massive processing element that can learn from historical data in order to predict the future trend. If a refiner can categorise and monitor the relevant parameters (involving feedstocks, the visbreaking process and fuel oil blending) then the knowledge-based system presented in this thesis can be expanded to accommodate fuel oil stability.

In this respect, it is not necessary to change the structure or the topology of the adaptive visbreaker's paradigm. What we are proposing is in fact an addition of a neuro fuzzy element to the AVP. Fuzzy logic is an area of research based on the work of L.A. Zadeh (1973). It is a departure from classical two-valued sets and logic that uses "soft" linguistic system variables and a continuous range of truth values in the interval $[0,1]$, rather than strict binary (True or False) decision and assignments. Fuzzy logic is used where a system is difficult to model exactly (but an inexact model is available), is controlled by a human operator or expert, or where ambiguity or vagueness is common (Yager *et al*, 1994).

In this respect Zadeh wrote:

"More often than not, the classes of objects encountered in the real world do not have precisely defined criteria of membership. For example, the class of animals clearly includes dogs, horses, birds, etc, as its members, and clearly exclude such objects as rocks, fluids, plants, etc. However, such objects as starfish, bacteria, etc, have an ambiguous status with respect to class of animals".

A typical fuzzy system consists of a rule base, membership functions, and an inference procedure. Neuro fuzzy combines the fuzzy logic and neural

network approaches to predict the so-called the grey or dusky areas. The rationale behind combining fuzzy logic and neural networks is because the fuzzy systems have no memory by themselves. Moreover, the learning capability of a hybrid fuzzy-neural net is superior to that of fuzzy logic alone (Harris *et al*, 1996).

In general, fuzzy sets divide their universe of applications into three parts, the positive (or right), the negative (or left), and a borderline (or a centre, usually graduated). In our case, these parts can be assigned to different sediment levels, representing the fuel oil stability status.

The proposed neuro fuzzy complex is an enhancement to the existing knowledge-based system. In this respect additional learning enables the system to act as the "Early Warning System" that tracks the operating condition and the feed quality to predict the fuel oil stability. The input data required in building the neuro fuzzy complex is given below:

- Feed Composition (AR, VR, TAR, Hdon)
- Feed Quality (K factor, API, PNA, CCR, Asphaltenes, VBI)
- Operating Condition (TRP, Soaker Temperature)
- Fuel Oil Blending (Residue CCR, API, VBI, Vol %, Cutterstocks %, PNA and stability test pattern)

Using the Flame Ionisation technique, the average boiling point of heavy hydrocarbons can be measured. In this respect, the American Standard for Testing Materials, test method D 2887 can be utilised to determine the boiling range distribution of petroleum fractions. This is needed to calculate the K factor. As defined previously, K factor is an empirical value that provides an insight into the composition of feedstocks and products related to petroleum refining processes.

Gel Permeation Chromatography can also be used to determine the asphaltenic, paraffinic, and volatile aromatic content of heavy fuel oil. In addition, the fraction insoluble in n-pentane is an indication of the residue's asphaltenes content (Bakashi *et al*, 1987). The HDON stream (see below) is an aromatic-rich stream that can help to disperse the asphaltenes. The name HDON reflects the hydrogen donating capability of the cracked gas oil, which has a high aromatic content. Scientifically, the chemistry of hydrogen migration from materials such as the fluid catalytic cracker's cracked gas oil has not been proved. Nevertheless the addition of such rich aromatic materials should improve the asphaltenes' dispersion to form a more homogenous colloidal solution.

In this case, the fuel oil stability is defined as the total sediment in residual fuel as governed by the Institute of Petroleum IP 375/390 test methods. In this respect, the total sediment is the sum of the insoluble organic and inorganic material which is separated from the bulk of the sample by filtration through a Whatman GF/A type filter medium, and which is also insoluble in predominantly paraffinic solvent. Generally, a total sediment content of 0.1 weight percent is the maximum acceptable limit.

Often a problem can be split into sub-problems such that solving the sub-problems leads us to solving the problem. This method can be used to model the fuel oil stability problem. In this respect, let us assume that our aim is to model Y as a fuel oil stability. Mathematically, for a model of

$Y = f(\times_1 , \times_2)$, the relationships $\times_1$ and $\times_2$ belong to the universe U_1 and U_2 respectively. Each considered universe of discourse, U_i , can be covered by an arbitrary number of fuzzy subsets, and the *belongingness* of the independent variable, $\times_i$, to each particular fuzzy subset can then be described by the Membership Function (MF), which attains numerical values from 0 to 1. In Our case, three fuzzy linguistic variables (Right, Left, and Centre) are formed.
The relationships can be introduced using:

IF $< condition >$ **THEN** $< action >$

Or

IF $\times_1$ is MF_{1i} AND $\times_2$ is MF_{2i} THEN $y = w_i$

Where MF_{ij} (j =1,2; i=1,2,....*n*; n = number of fuzzy subsets) is the membership function describing the *belongingess* of $\times_j$ to the ith subset of the domain space. In this respect, the terms IF, THEN, OR, AND are often defined as the system's production rules (Shinghal, 1992).

In the light of the above description of the neuro fuzzy complex, the goal is to train and enhance the capability of the system to produce an appropriate action/reaction to a given condition (Walczak *et al*, 1994). Undoubtedly, the system needs to learn the pre-defined rules based on the historical pattern (plant data and laboratory test results).

According to Kosk *et al* (1992) fuzzy sets represent points in an n-dimensional hypercube. Each edge of the hypercube represents one element of the fuzzy set. The membership value of that element determines a point on the edge. When all the elements of the set are considered, these points on the edges define a point in n-space within the hypercube. If all the membership values are 0 or 1 then the points define the corners of the cube. This is consistent with Boolean logic. If all the memberships values are 1/2 then the point is the midpoint of the cube. This violates Aristotle's law of the excluded middle, A and not-A.

Further enhancement is an addition of the backward chaining programme (as an Excel add-in), where the system's rules can be run in a "goal driven" way. In backward chaining, if a piece of information is needed, the programme will automatically check all of the rules to see if there is a rule that could provide the needed information. The programme will then "chain" to this new rule before completing the first rule. The programme will then again automatically test this new rule. The logic of why the information is needed goes backward through the

chain of rules. This is a useful tool when some laboratory fuel oil stability data are either missing or lack the required accuracy.

Based on the three fuzzy categories of Right, Left, and Centre, we can now devise our fuzzy rules by introducing the following expression:

Fuzzy left = Comfort Zone: This is when the visbreaker feed is low in asphaltenes, visbreaker severity has been low, a cutterstock system with a low paraffin solvent has been selected.

Assume that fuel oil is definitely stable.

IF < Asphaltenes is Low AND Paraffin's is Low AND Severity is Low >

THEN < Sediment is close to zero AND Fuel Oil is Stable >

Fuzzy centre - Stable State: This is when the visbreaker has been processing a feed with low to medium asphaltenes at medium severity and the cutterstock system contains some considerable amount of paraffinic cutterstock. Assume that the fuel oil is almost stable (it may not be stable at all times and under all conditions).

IF < Asphaltenes is Medium AND Paraffins is Medium AND Severity is Medium >

THEN < Sediment is close to 0.06 AND Fuel oil is almost Stable >

Fuzzy right - Un-Stable Zone (Warning): This is when the visbreaker has been running a high asphaltene feedstock at high severity with a cutterstock system that contains large amount of paraffinic solvents.

Assume that fuel oil is definitely unstable.

IF < Asphaltenes is High AND Paraffin's is High AND Severity is High >

THEN < Sediment is over 0.09 AND Fuel Oil May Not be Stable >

The determination of the action variables is relatively straightforward, because there are basically only three conditions or things that can happen. Specific subsets can also be formed. Other linguistic terms (such as Very Low, Mild, and Very High) can also be used to describe the pertinent variables in the fuel oil stability system. In this respect, the visbreaker's severity is a multi-dimensional parameter whose 3 dimension(s) of High, Medium, and Low can occur in the Fuzzy-Right, Fuzzy-Left, and Fuzzy-centre parts of the proposed system. Membership functions (MF_1, MF_2, and MF_3) of the arbitrarily chosen three fuzzy (Low, Medium, and High) subsets of the universe of discourse can be shown in the following diagram:

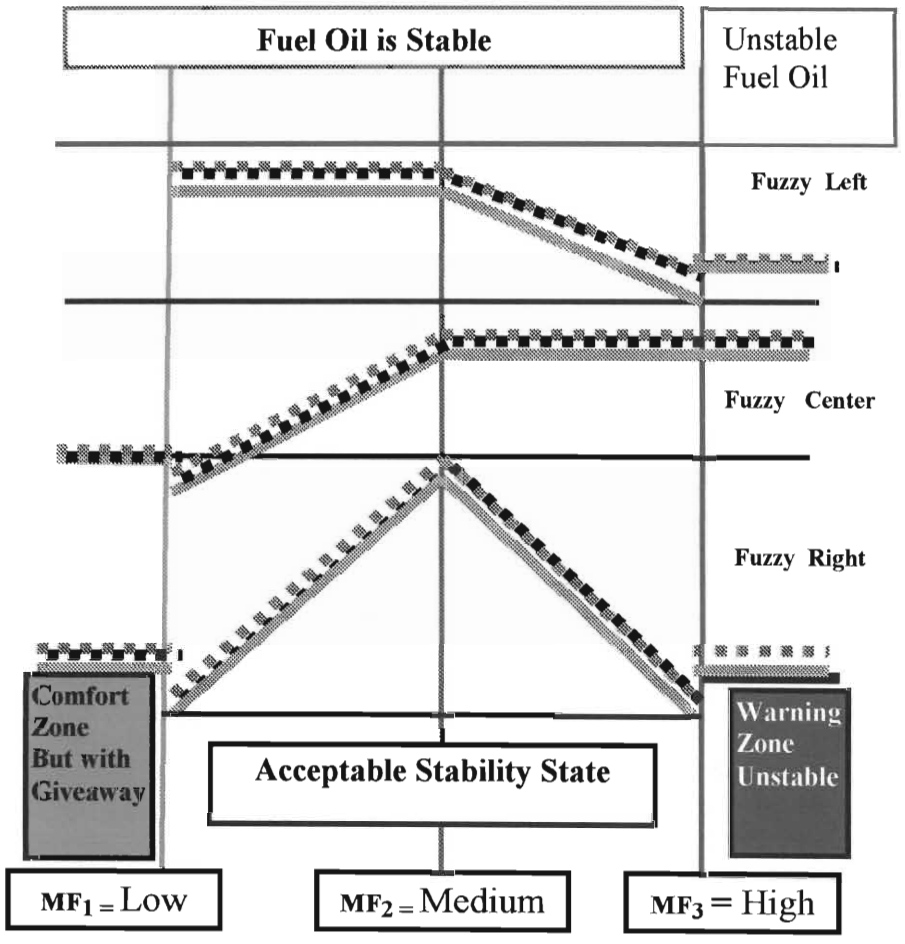


Figure 5-12 Schematic of The Proposed Neuro Fuzzy Complex to Foresee the Fuel Oil Stability Phenomena.

It was previously stated that there is no universally agreed upon test or method to measure the fuel oil's stability. As a result, the proposed neuro fuzzy complex should be used with caution. This is because, in the visbreaker unit, a number of reactions can take place, apart from cracking reactions. In particularly, condensation can occur when aromatic, polynuclear aromatics, and petroleum wax are present (Kok *et al*, 1996). These condensation reactions are largely responsible for asphaltenes formation which, at high conversion, can lead to the production of unstable fuel oil.

Accordingly, when dealing with fuel oil stability, a safe margin should always be kept to account for disturbances in the colloidal structure because of prolonged storage at elevated temperature, oxidation by air, etc.

Moreover, we should note that aromaticity is ***not*** the only parameter needed to be considered for the suitability of cutterstock (although aromatics are a better cutterstock than olefins, and olefins are better than paraffins). It is generally believed that metallo-organic compounds are also the cause of asphaltene formation and precipitation (Santarelli, 1992). Because of differences in the chemical and physical nature of petroleum residue, the stability may change after adding other products to a stable fuel oil.

Another problem is the availability of the meaningful data required to identify the cause and the nature of the unstable fuel oil. The following data sets are needed:

- Daily Plant Operating Data
- Daily Plant Yield Data
- Daily Laboratory Test Data on the visbreaker products and other potential blend components.
- Accurate records of the volume and property of each component of the blend
- Accurate records of the final blending volumes, procedure, and properties

In our case, the research into the second cycle of the visbreaking operation produced two instances of unstable fuel oil production. Unfortunately, due to the inconsistency in the plant and laboratory data, and the unavailability of a clear blending record, the real cause could not be established. Accordingly, the results obtained from the proposed neuro fuzzy complex could not be truly verified. In this respect, further experimental work is planned. This includes the use of a neuro fuzzy system as the early warning system to track the operating condition and the feed quality to predict the fuel oil stability.

As stated earlier, the work presented here is part of an ongoing research effort, to improve the refinery's planning systems and tools employed to increase the refinery's profitability. To achieve this objective, it is necessary to develop a computational method to model the visbreakability of various crude oils, simulate the visbreaking operations, fuel oil blending, and at the later stage the fuel oil storage stability problem. A neuro fuzzy addition to the adaptive visbreaker paradigm can act as an early warning system. However, due to overall system complexity, data inconsistency, and some unknown parameters, the prediction results should be treated with caution. The latter will be the subject of future research into the stability phenomenon and asphaltene precipitation. Recently, there have been some new and interesting research projects to study the nature of asphaltene and its effect on the stability of residual fuel oil (Tojima *et al*, 1997). The molecular structure and properties of asphaltene varies with factors such as the crude petroleum, processing severity, perception mode..etc. In order to model the asphaltene perception accurately, further research work in this field is required.

CHAPTER 6

DISCUSSION & CONCLUSION

Summary

As reported in section 1.3 of this thesis (Motivation of the research and objective of the thesis), since the refinery's profitability is highly sensitive to the visbreaking and fuel oil blending operations, a further initiative to develop an alternative method to simulate the visbreaking process, optimise the fuel oil blending, and equip the refinery LP with the visbreaking yields of various crude oils is well justified. Accordingly, the work done so far is summarised below:

- In the absence of complete scientific understanding of the visbreaking operation, using a neuroengineering procedure a mathematical model of the visbreaker model is developed (the adaptive visbreaker paradigm).

- Since the fuel oil blending can influence the visbreaking operation, firstly, a mathematical model of the fuel oil blending is constructed. Secondly, an integration of the AVP with the fuel oil blending model is proposed.

- To improve the predictability of the model, a network reciprocation mechanism is developed. Statistical methods were employed to measure the improvements claimed. Economic analysis proves that improvements resulting from the network reciprocation procedure are significant.

- The reciprocated visbreaker model is employed in 2 distinct roles. In the first role, the model is used to study the visbreaking operation and fuel oil blending, assisting the refinery planning and scheduling systems. A practical example of this application is given in section 5.3 of this thesis.

- In the second role, the adaptive visbreaker paradigm is used to simulate the visbreaking operation and to generate yield patterns. These data are used in the global refinery LP model, a planning tool used to evaluate a refinery's feedstock and to optimise a refinery's operation. To use the AVP's yield pattern, a correction vector is developed. This is to account for the visbreakability of individual crude oils available to a refiner. The analysis performed shows that the proposed procedure has improved the accuracy of the LP model. Furthermore, it can influence the decision-making chain involved in the crude evaluation and selection process.

- The use of a fuzzy complex system as the early warning system to track the operating condition and the feed quality to predict the fuel oil stability is also researched. Further experimental work in this field will be also the subject of future research into the stability phenomenon and asphaltene precipitation.

In view of the above, it can be concluded that, the work presented in this thesis demonstrates the practicality of the methods and models developed and comply with the objective of the research outlined in section 1.3 of this thesis.

Discussion and Conclusion

In today's competitive world, most organisations are feeling the pressure to change. This pressure stems from such factors as the drive for profit improvement, actions by competitors, regulatory activities, customer and employee needs, and the introduction of new technology. In the refining industry, profit improvement and regulatory actions clearly head the list of

change drivers. In the past decade, the economics of the industry have been hindered by requirements for large mandated capital expenditures, whilst experiencing volatile crude and refined product prices. Consequently, the constant evaluation of available resources and the optimisation of the decision-making process are a prerequisite to survivability. This of course requires access to various sophisticated planning tools and systems. Against this background, in recent years, mathematical programming and associated techniques have been widely used as decision-making tools.

The cost of purchasing petroleum crude is the highest single cost to a refiner. As the differential between heavy, light and sweet crude increases, the incentive to convert the bottom of barrel becomes more attractive. According to the Petroleum Economist (December 1995), the overall refinery conversion margin is expected to increase from $1.65 per barrel in 1996 to $3.00/ barrel by the year 2000. Although the forecast is based on the Salomon Brothers' recent European market research, the situation in other parts of the globe is not far from this forecast. Based on an analysis of refineries without conversion capacity, the study forecasts that there could be plant closures of up to 1 million barrels per day of refining capacity by the year 2000. Furthermore, Salomon sees the differential between light and heavy crude increasing from less than $1 per barrel now to $2–3/ barrel by the year 2000.

Moreover, with widening light-to-heavy differentials, refiners will probably choose to process heavier crude oils in the future. These indications coupled with heightened environmental awareness and continued increases in distillate demand are expected to increase interest in processing routes that improve white oil yield and reduce production of heavy fuel oil.

According to Sloan (1991) the bottom-of-barrel conversion encompasses two broad alternatives: carbon rejection and hydrogen addition. The selection of the best option depends on many factors: specific crude availability, market conditions and product distribution for existing refinery units. Previously, many refineries had sufficient markets for heavy or marine fuel oil, so that bottom-of-

barrel conversion was not needed. Due to the new environmental regulation this is no longer the case. As refiners have begun to see heavier crude feedstocks, the push to convert heavy fuel to higher value light products has become stronger. As reported in chapter 1, the market demand for increased volumes of lighter distillates and gasoline coincides with the lower demand for heavy fuel oil. Therefore, conversion of the bottom of a heavy crude barrel is essential for a refinery to remain viable. The economics of residue upgrading, based on the real-world data, was demonstrated in chapter 1.

Among the most popular carbon rejection conversion schemes is visbreaking; a mild thermal cracking process aimed at reducing the viscosity of vacuum residuum. This is done to minimise the amount of cutter-stock (light distillate products) needed to meet the viscosity specification of the finished product (marine fuel oil. As reported in chapter 2 of this thesis, the heavy gas oil produced may be used as a catalytic cracker feed. Since visbreaking is limited in severity by a number of factors, the reduction in refinery heavy residue yield is often less than for other bottom's conversion process. However, if the refinery is situated close to a major sea port, then the residue can be blended into bunker or marine fuel oil.

It is estimated that visbreaking accounts for about 22% of the world's residue upgrading units. The economics of converting the heavy residue into the lighter and more valuable streams, coupled with the installation of a modern visbreaker unit at the Engen Refinery in Durban, provided sufficient motive to build a model to simulate the unit's capability and estimate the economics of the visbreaking process and fuel oil operations. Furthermore, as discussed, the proposed model provides a crude-dependent visbreaking yield that is used in the refinery's global linear programme, a software employed to evaluate and select the crude needed and to optimise the refinery's operations.

The kinetic models of the visbreaker in particular have not been widely used by the petroleum industry. This is due to the complexity of the modern

visbreaking process, where the relationships between the various process parameters are often unknown or unattainable.

Due to the limitations of the kinetically-based model, an Adaptive Visbreaker Paradigm (AVP), based on the principles of an artificial neural network was constructed to study the visbreaking process. The neuroengineering technique has been employed to construct an empirically-based model to predict the yields of the visbreaking process. Since the visbreaking process is an essential precursor to fuel oil manufacture, the proposed model has been expanded to integrate the fuel oil blending and optimisation system. Accordingly, the adaptive visbreaker paradigm is designed to be used for two distinct applications. Firstly, as an integrated simulator/optimiser, to predict the visbreaking yields and to measure the economics of visbreaking operations. Secondly, as a vehicle to improve the accuracy of the global refinery LP. This is to help the refinery planners with the crude evaluation and selection process as well as the global optimisation of the refinery.

It was observed that due to fluctuations in the feedstock quality (due to variation in crude mix) and plant operating conditions, the prediction accuracy of the model needs to be improved. To improve the system's predictability, a network reciprocation procedure has been devised. Network reciprocation is a mechanism that controls and selects the input data used in the training of a neural network system. Using a genetic algorithm, the network reciprocation procedure minimises the system's prediction error by selecting the best available data sets. These selected data sets are eventually used to re-train the reciprocated network. Implementation of the proposed procedure results in a considerable improvement in the network's performance.

It should be emphasised that any data set originating from an unreliable or unstable unit operation should be detected and deleted during the data pre-processing stage of the neuroengineering procedure. The network reciprocation therefore is a procedure to continuously evaluate the valid data set and select those data whose contributions may result in improving the quality of the

paradigm's response. From this standpoint, network reciprocation differs from data pre-processing or other empirical methods used to detect the data outliers. Undoubtedly, some of outlier detection (Massart, 1995) models are useful diagnostic and identification tools, when single and multiple outliers already exist in the system. Unavoidably, the network reciprocation procedure becomes a complex method to use. However, it was discussed that the network reciprocation becomes a valuable tool when feedstocks quality is not consistent, for example, when a refinery is evaluating or using various mixes of crude oils, having different residue content and properties. It should be noted that this type of model delivers its best result when it has access to a large population of raw data. This is not a problem as the refinery operation is of a continuous nature, and therefore there is no limit to the number of process data available to the model. In reality however, the re-training of the model is not a simple task. This is not due to the data limitation, but rather the integrity of data received from the visbreaker plant, online analysers, and laboratory test results. A further difficulty is the scarcity of methods that determine the concentrations of different reactive species. Powerful analytical apparatus and chemical methods are expensive and not generally amenable to on-line operation. The information they provide is however, imperative to chose the correct operating parameters required by the adaptive visbreaker paradigm.

The preliminary results and associated graphs presented in chapter 4 of this thesis indicate that the implementation of the proposed network reciprocation procedure has indeed produced a complex neural network suitable for studying the visbreaking process. Economic analysis proves that the improvements resulting from the network reciprocation procedure are significant.

In order to explain the performance of the visbreaking process, one must look very closely at the fuel oil blending operation, where the blending optimisation program produces the system's optimal blend. Consequently, due to the complex interactions among the parameters determining the economics of the visbreaking process and fuel oil blending, the evolution of the proposed model to an integrated system becomes essential. This resulted in the formation

of an integrated knowledge-based system capable of representing the real world of the visbreaking operation. To select the optimum quantity of products, the fuel oil blending module of the proposed model uses sophisticated mathematical equations and an optimisation algorithm (fuel oil blending indices are presented in Appendix -1).

The computational results produced by the model prove that the economics of the visbreaking process is a multidimensional variable greatly influenced by the feed quality and the operating condition. The results presented show the feasibility of the application of an adaptive visbreaker paradigm in predicting the cracking reaction yields. Furthermore, the model allows dynamic monitoring of the residue properties to the point of fuel oil blending optimisation.

Besides the sensible results presented in the body of this thesis, there are some practical difficulties associated with neurally-based models in general, and the adaptive visbreaker paradigm in particular. Due to the variation in crude quality (frequent change of crude and other feedstock), precision of prediction was found to be low during the model cross validation and sensitivity analysis phase. Further research indicates that the major element of this problem is input data, sourced from the visbreaker plant. The wide variability in the input data coupled with data inconsistency can influence the models learning process. Using some pre-conditioned rule such as the proposed network reciprocation procedure can, somewhat, improve the predictability of the network. However, to improve the model's resolution, meaningful, consistent and coherent input data are also of importance. Moreover, the proposed system is difficult to operate and slow to converge. Consequently, more computational power is desirable.

In the second role, the AVP is used to simulate the visbreaking operation and to generate yields pattern that are used in the global refinery LP model. To reflect the variation in the visbreakability of individual crudes available to a refiner, a. procedure to generate a correction vector is developed. The analysis performed shows that the proposed procedure has improved the accuracy of the

LP model and can influence the decision-making chain involved in the crude evaluation and selection process. The refinery LP model is one the most important managerial decision tool used in the refinery-wide resource evaluation and optimisation. Accordingly, an accurate refinery LP model is the centre of an integrated decision support system.

Looking at some practical considerations in section 5.4, the fuel oil stability phenomena were discussed. In this respect, a fuzzy model was also proposed to act as the early warning system. In order to train, the fuzzy model, proper monitoring of the feed quality, plant operating condition, fuel oil blending, and tank batching records are required. These types of data are not freely and easily available. To provide such records, sophisticated, expensive control systems and equipment have to be purchased and installed.

In respect of the off-line modelling tools, it can be seen (Appendix -4) that extensive time and effort have been spent to evaluate and select a suitable mix of computational and modelling software. These include neural networks, genetic algorithm and other tools. Undoubtedly, the application of these software require comprehensive knowledge of refinery operations as well as mathematical modelling and computer proficiency.

It should be noted that the foundation of the adaptive visbreaker paradigm is based on the operation of a new visbreaker unit at the Engen Refinery in Durban. It is, however, possible to re-train the neural network paradigm and to learn other visbreaking process data for different working environments. In other words, the application of the neuroengineering technique, network reciprocation procedure, and LP correction vector mechanism is not limited to the visbreaking operation or to the existing Engen refinery configuration. In essence, the proposed models and procedures provide sufficient flexibility for further refinement or use at other locations.

As a concluding remark, we may add that the application of mathematical models such as the proposed integrated decision support system results in a

better understanding of the refinery process economics. In spite of their limitations, these models are useful planning tools that are used to measure the overall economics of the petroleum refining processes.

APPENDIX - 1

Terms Used in Blending the Petroleum Products

The petroleum refining industry, like other industry, uses terms which in most cases are specific to the nature of their business. The major terms applied to this project are described below:

API Gravity: Arbitrary scale for measuring the gravity or density of liquid petroleum products (expressed in degrees), adopted by the American Petroleum Institute (1983) . Its relation to specific gravity is shown below:

$$API = \frac{141.5}{SPG} - 131.4 \qquad \textbf{(A1.1)}$$

where the **SPG**. is the specific gravity of crude oil; a ratio of the density of the materials at 60^{o} Fahrenheit (15.5C) to the density of water at that same temperature meaning; the lower the API gravity, the more viscous or heavier the crude oil.

Conradson Carbon Residue (CCR) : A carbon residue test method for determining the amount of carbon (in percent weight) deposited after oil has burned. It indicates the relative carbon-forming tendency of an oil. Accordingly, materials with the high CCR content are classified as undesirable fuels.

Flash point : The lowest temperature at which, under specified test conditions, a petroleum product vaporises rapidly enough to form above its surface an air-

vapour mixture which gives a flash or slight explosion when ignited by a small flame. The flash point of an oil is an indication of the risk of fire or explosion associated with its use or storage. Flash point is an important specification for various petroleum products.

The Hu-Burns (1970) method is used to blend for the Flash point using the Flash Point Blending Index (based on conversion to the degrees Rankine) method calculated as follows :

$$\mathbf{FLI = 10^{(42.1093-14.286 * LOG10(FL+R))}} \qquad \textbf{(A1.2)}$$

where

FLI = Flash point blending index.

FL = Flash point in Degrees Fahrenheit F.

R = Degrees Rankine = 459.69.

To convert the FLI to Flash point (FL):

$$\mathbf{FL \text{ in degrees } F = (10^{((LOG10(FLI)-42.1093)/(-14.286))}) - R} \qquad \textbf{(A1.3)}$$

KFACTOR : Watson characterisation factor, or Kfactor is a calculated value which has been used widely as a parameter for correlating properties of petroleum products.

The defining equation is:

$$\text{Kfactor or } \mathbf{K} = \frac{\sqrt[3]{\mathbf{MeABP}}}{\mathbf{SPG}} \qquad \textbf{(A1.4)}$$

Where **MeABP** is the mean average boiling point of the fraction in degrees Rankine, and **SPG** is the specific gravity of the material; a ratio of the density of the materials at 60° Fahrenheit to the density of water at that same temperature. The Watson characterisation factor ranges from 9 for highly aromatic materials

to almost 16 for the highly paraffinic compounds. The use of characterisation factor takes into account the major differences in charge stocks (feed). However, the boiling range, degradation by previous cracking, entrained carbonaceous material, metallic containment's, high percentage of nitrogen, or extremely high percentages of sulphur are extra factors all of which influence the cracking yields,

Pour point : The lowest temperature at which an oil will pour when chilled without disturbance under specified conditions. It indicates the temperature below which it may not be possible to use an oil without some heating to maintain flow from storage.

The pour point index is calculated as follows (HPI, 1979) :

$$\mathbf{PPI = (10000(PP+R)^{(1/0.08)}) / ((140+R)^{(1/0.08)})} \qquad \mathbf{(A1.5)}$$

where

PPI = Pour point blending index.

PP = Pour point in degrees Fahrenheit F.

R = Degrees Rankine = 459.69.

To convert the PPI to Pour point (PP):

$$\mathbf{PP \text{ in degrees } F = ((PPI*(R+140)^{(1/0.08)}) / (10000^{(0.08)})) - R} \qquad \mathbf{(A1.6)}$$

Sulphur content : A measure of sulphur in the oil, expressed in percent weight of sulphur. Sulphur is an undesirable product. The sulphur content of most petroleum products is limited by environmental regulations.

Specific gravity : The ratio of the weight of given volume of material to the weight of an equal volume of some standard substance, in our case distilled water at 60 degrees Fahrenheit (F) .

Viscosity : The measure of the internal friction or resistance to flow of a fluid. The kinematic viscosity, which is measured in centiStoke (cSt) at 122 degrees Fahrenheit (F) equal to 50 ^{o}C, will be used .

The kinematic viscosity of petroleum products is converted into the viscosity blending index by the following equation (HPI, 1979) :

$$\mathbf{VBI = (41.10743 - 49.08758(LN(LN(cSt+0.8))))} \qquad \mathbf{(A1.7)}$$

where

VBI = Viscosity blending index.

cSt = Viscosity in centiStoke at 122 degrees Fahrenheit (50C).

To transform the **VBI** to Viscosity in cSt at 122 degrees Fahrenheit (50C):

$$\mathbf{Viscosity\ in\ cSt =}$$

$$\mathbf{= (EXP(EXP(VBI-41.10743)/(-49.08258))) - 0.8} \qquad \mathbf{(A1.8)}$$

APPENDIX - 2

Thermal Decomposition Theory

In addition to the quality and nature of the visbreaking feedstocks, the cracking process is time-temperature-pressure dependent. It was the great Swedish chemist Arrhenius, who first suggested that the temperature dependence of the specific reaction rate, k, could be correlated by an equation of the type:

$$\mathbf{Ln}\, k = \mathbf{Ln}\, \mathrm{A} - \frac{Ea}{RT} \qquad \textbf{(A2.1)}$$

That is, for many reactions it is found that a plot of $\mathbf{Ln}\, k$ against $\frac{1}{T}$ gives a straight line. The Arrhenius equation (Holland, 1989) is often written as

$$k = \mathrm{A}\, e^{-Ea/RT} \qquad \textbf{(A2.2)}$$

The factor A is called the pre-exponential factor or the frequency factor; Ea is called the activation energy, often expressed as kilo calorie per Mol. Collectively, the two quantities are called the Arrehenius parameters of the reaction as defined below:

A = pre-exponential factor or frequency factor.
Ea = activation energy, J/mol or calorie/mol
R = gas constant =8.314 J/mol.K=1.987 calorie/mol.K
T = absolute temperature, K

It should be noted that the temperature dependence of some reactions is not Arrhenius-like. It is, however, possible to express the strength of the dependence by defining an activation energy as:

$$Ea = RT^2 \left[\frac{dLnK}{dT} \right] \qquad \textbf{(A2.3)}$$

This definition reduces to the earlier one (as the slope of an Arrhenius plot) for a temperature-independent activation energy. Thus, by using $d(\frac{1}{T}) = -(\frac{dT}{T**2})$ the above equation can be re-written as:

$$Ea = -R \left[\frac{dLnK}{d(1/T)} \right] \qquad \textbf{(A2.4)}$$

which integrates to equation (A2.2) if Ea is independent of temperature. However, the definition in equation (A2.3) is more general than equation (A2.2), because it allows Ea to be obtained from the slope (at the temperature of interest) of a plot of **Ln** k against $\frac{1}{T}$ even if the Arrenius plot is not a straight line.

Equation (A2.3) shows that the higher the activation energy, the stronger the temperature dependence of the rate constant. That is, a high activation energy signifies that the rate constant changes rapidly with temperature.

The activation energy Ea has been equated with the minimum energy that must be possessed by the reacting molecules before the reaction will occur. From kinetic theory of gases, the factor $e^{-Ea/RT}$ gives the fraction of the collision between molecules that together have this minimum energy Ea. Although this might be an acceptable elementary explanation, some suggest that Ea is nothing more than an empirical parameter correlating the specific reaction rate to temperature (Truhlar, 1978). Nevertheless, postulation of the Arrhenius equation remains the greatest single step in chemical kinetics, and retains its usefulness today, nearly a century later.

The activation energy is determined experimentally by carrying out the reaction at several different temperatures. The equation (A2.4) is then used to plot the $\mathbf{Ln}\,k$ versus $\frac{1}{T}$ as shown below:

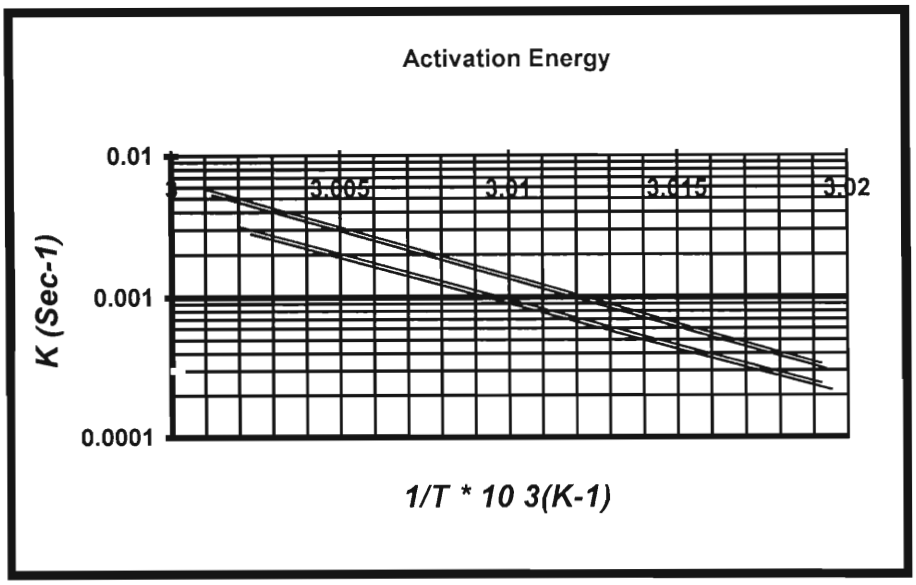


Figure A2-1 Diagram to calculate the activation energy for decomposition of hydrocarbons.

It can be seen from Figure A2.1 that the larger the activation energy the more temperature-sensitive is the rate of reaction. A number of correlation's can be used to estimate the activation energy; however, the determination of the change in rate of reaction with the temperature is valid only for a specific combination of activation energy and temperature.

The study of the thermodynamics of cracking leads to several interesting conclusions. Considering the thermal cleavage of the members of the paraffin series, two types of reaction can occur: dehydrogenation and true chain rupture (Kopsch, 1995).

Schultze (1937) has represented the variation of free energy *change* with temperature and composition for these types of reaction (under equilibrium conditions) by the following equations:

Free Energy Change of Reaction =

$$\Delta_f = -RT \operatorname{Ln} k \qquad \textbf{(A2.5)}$$

$$C_n H_{2n+2} \Rightarrow C_n H_{2n} + H_2 \qquad \textbf{(A2.6)}$$

$$C_{(m+n)} H_{2(m+n)+2} \Rightarrow C_m H_{2m+2} + C_n H_{2n} \qquad \textbf{(A2.7)}$$

In its simplest form, the dissociation of a compound into free radicals $|C_m H_{2m+2}\ ,\ C_n H_{2n}|$ is believed to be the most important reaction in the visbreaking process. These electrically-neutral but highly reactive particles are formed by scission of **C—C** or **C—H** bonds, with each fragment retaining one of the pair of shared electrons that made up the bonds. The free radicals are highly reactive, short-lived particles that, depending upon their size and environment, (1) react with other hydrocarbons, (2) decompose to olefins and smaller radicals, (3) combine with other radicals or (4) react with metallic compounds. The hydrogen, methyl and ethyl radicals are more stable than larger radicals, and they react with other hydrocarbons by capturing a hydrogen atom and forming a new radical. The larger radicals are unstable and decompose to form olefins and smaller radicals. The free-radical chain reaction is terminated when two radicals combine or when a radical reacts with a stable metallic compound. Alkyl chains on naphthenic or aromatic rings are presumed to react in the same way as paraffins.

The extent to which the thermal decomposition of heavy residue proceeds by the free radical mechanism is uncertain and cannot kinetically be proved. In the initial stages of cracking when paraffin molecules are large, rupture may occur at any carbon-carbon bond, and medium chain-length olefins and paraffins are obtained. When the cracking reaction has progressed further and it becomes more severe the smaller-chain paraffins begin to crack. The free radical theory does not account for the production of materials heavier than feed, such as those found in the visbreaker's bottom residue. This phenomenon is

presumed to result from the polymerisation of olefins and condensation of aromatics, although alkylation and other processes may also occur.

According to Fogler (1992), polymers are macromolecules made up of monomer units. Polymers and polymerisation can be classified by 1) composition/structure, 2) reaction mechanism, or, 3) process conditions. For example, based on the composition/structure of polymer product, polymerisation process are divided into *two* groups known as *condensation reactions* and *addition reactions*. In condensation reactions, often two monomers are reacted and a small molecule is formed in addition to the polymer. However, based on the reaction mechanism there are *three* types of polymerisation: chain-wise, stepwise and ring-opening. Chain-wise polymerisation itself can be either free-radical or ionic. Free-radical polymerisation is believed to be the major contributor towards the formation of the molecules larger than the ones found in the feed to the visbreaker unit. The basic steps in free radical polymerisation are initiation, propagation, chain transfer and termination. Depending upon some known and unknown factors the chain transfer process can be a free-radical transfer to a monomer of another species, or to the solvent. The termination itself can be a process of the addition, or disproportionation (Morrison *et al*, 1992).

Certainly, the empirical chemical kinetics provide sufficient theories (such as the Integrated Rate Law) to reveal some aspects of the complex reactions, for example, the dissociation of the heavy hydrocarbons. However these theories are often based on the process stoichiometries, the order of the process, and a set of dynamic variables, often difficult to isolate and impossible to control (Levenspiel, 1972).

According to Dente & Ranzi (1992), it is quite evident that termination reactions are in fact the reverse of chain initiation ones; moreover, radical-additions to double bonds can be related to radical-decomposition reactions. Most reactions involve radicals, but some purely molecular reactions also play a significant role. However, the key variable in the thermo-kinetic theory remains

the amount of heat required to initiate the process of visbreaking. It is noted that the thermal cracking of the crude's heavy residue results in multiple chemical reactions with unknown stoichiometry. Another complicating factor is the variation in the feedstocks quality, which varies with the petroleum crude type and the way that it is processed in other upstream refinery units such as:

- Crude distillation unit
- Vacuum distillation unit
- Propane De-asphalting unit

Research on the behaviour of various feedstocks (Brauch *et al.* 1996b) during the visbreaking indicates that sulphur as well as the asphaltenes contents, density and viscosity play a great role in the visbreaker's conversion. They have concluded that there is a good deal of "*individuality*" in the behaviour of various feedstocks used in the visbreaking process.

Beside the physical and chemical properties of the feedstocks, the visbreaking process is in fact a series of multiple and parallel reactions, which are temperature, pressure and time dependent. In its simplest form, in order for a single reaction such as the one presented in the equation (A2.6) to take place at about 752°F(400°C), that is to give negative value for the free energy change, the molecules must be the size of dodecane or ($\boldsymbol{n}$ = 12) or tridecane ($\boldsymbol{n}$ = 13). Similarly, dehydrogenation of the lighter molecules such as heptane can occur only at temperatures in excess of 1112F°(600°C). On the other hand the equation (A2.7) is thermodynamically possible for all paraffins above propane at the temperatures encountered in commercial visbreaking units. The typical carbon number(s) versus API gravity for the visbreaker's products is illustrated in the Table A2-1.

Table A2-1 Typical carbon number of the Visbreaker' products

Feedstocks	**[C10.....*n*]**	**API 6-13**
Gasoline(light naphtha)	[C5.....7]	API > 35
Distillate	[C8.....10]	API > 20
Residue (bottom)	[C10.....*n*]	API < 12

The theory of free energy can be extended to estimate the feasibility of a chemical reaction (Nelson, 1958). The common values of Δ_f (change in free energy as defined above) for hydrocarbon processing is tabulated below:

Table A2-2 Reaction Feasibility

$\Delta_f < 0$	**Reaction is well possible**
$\Delta_f = 0 \quad \Delta_f < 6$	**Reaction *May* be possible/ Doubtful**
$\Delta_f > 10$	**Reaction is in-feasible.**

In respect of the feedstocks's characteristics, the degree of viscosity and pour point reduction is a function of the composition of the residua fed to the visbreaker unit. Heavy feedstocks achieve pour point reduction from 15-35° F and the final viscosities from 25-75% of the feed, depending on the severity of the visbreaker. A high asphaltene content in the feed reduces the conversion ratio at which a stable fuel oil can be made (Gary, 1984), which results in smaller changes in the properties.

The properties of the cutter stocks used to blend with the visbreaker bottoms also have an affect on the severity of the visbreaker operation. The molecular structures of the compounds in petroleum which have boiling points above 1000°F (540^+ °C) are highly complex and historically have been

classified arbitrarily as oils, resins, and asphaltenes according to solubility in light paraffinic hydrocarbons.

It is generally believed that asphaltene formation from a predominately paraffinic feed is less severe when compared to that of aromatics and naphthenic feedstocks. This claim, however, does not always hold, especially when the feedstocks is subjected to high temperature and long residence time (Levenspiel, 1972). High pressure steam sometimes is used to control the residence time at a given level of pressure and at a given feedstocks flow rate. Generally, the steam injection helps to reduce the coking effect.

Many investigators (Rhoe *et al*, 1979) believe that the asphaltenes are not in solution in the oil and resins but are very small, perhaps molecular size solids, held in suspension by the resins. There is a definite critical ratio of resins to asphaltenes below which the asphaltenes will start to precipitate. During the cracking phase, some of the resins are cracked to lighter hydrocarbons and others are converted to asphaltenes. Both reactions affect the resin-asphaltenes ratio, the resultant stability of the visbreaker bottom product, and serve to limit the severity of operation.

APPENDIX - 3

Artificial Neural Networks – An Overview

It was stated earlier that artificial neural networks are essentially the pillars of the neuroengineering technique that is used to develop the adaptive visbreaker paradigm. Thus, it is necessary to provide an elementary view of the key elements, terminology, topology, and infrastructure of the neural networks system. Building an intelligent system that can model human behaviour has captured the attention of the world for years. Therefore, it is not surprising that a technology such as neural networks has generated great interest. In essence, neural networks are the quintessential complex adaptive system used in many real-world applications.

The perspective taken in this section and throughout this project is largely that of a scientist, emphasising the application potential of neural networks and drawing comparisons with other techniques that have similar motivations. As such, at any point, the focus will be on the application of neural networks' systems in a planning environment in the petroleum refining industry. In short, this thesis is not concerned with the physicochemical characteristics of the brain's neurons, neurology, biophysics, or bio-mathematical methods. It rather blends the principles of thermo-kinetics with those of artificial neural networks to address a chemical processing problem in the refining industry.

This section begins with a review of what neural networks are and why they are so appealing. Also referred to as connectionist architectures, parallel distributed processing, and neuromorphic systems, an artificial neural network (ANNs) is an information-processing paradigm inspired by the way the densely interconnected, parallel structure of the mammalian brain processes information. Artificial neural networks are collections of mathematical models that emulate some of the observed properties of biological nervous systems and draw on the

analogies of adaptive biological learning. The key element of the ANNs paradigm is the novel structure of the information processing system. It is composed of a large number of highly interconnected processing elements that are analogous to neurons and are tied together with weighted connections that are analogous to synapses.

Learning in biological systems involves adjustments to the synaptic connections that exist between the neurons. This is true of ANNs as well. Learning typically occurs by example through training, or exposure to a set of input/output data where the training algorithm iteratively adjusts the connection weights (synapses). These connection weights store the knowledge necessary to solve specific problems.

Although ANNs have been around since the late 1950's, it wasn't until the mid-1980's that algorithms became sophisticated enough for general applications. Today ANNs are being applied to an increasing number of real-world problems of considerable complexity. They are good pattern recognition engines and robust classifiers, with the ability to generalise in making decisions about imprecise input data. They offer ideal solutions to a variety of classification problems such as speech, character and signal recognition, as well as functional prediction and system modelling where the physical processes are not understood or are highly complex. ANNs may also be applied to control problems, where the input variables are measurements used to drive an output actuator, and the network learns the control function. The advantage of ANNs lies in their resilience against distortions in the input data and their capability of learning. They are often good at solving problems that are too complex for conventional technologies (e.g., problems that do not have an algorithmic solution or for which an algorithmic solution is too complex to be found). They are often well suited to problems that people are good at solving, but for which traditional methods are not.

There are multitudes of different types of ANNs. Some of the more popular include the multilayer perception which is generally trained with the backpropagation of error algorithm, learning vector quantization, radial basis function, Hopfield, and Kohonen, to name a few. Some ANNs are classified as feedforward while others are recurrent (i.e., implement feedback) depending on how data is processed through the network. Another way of classifying ANN types is by their method of learning (or training), as some ANNs employ supervised training while others are referred to as unsupervised or self-organising. Supervised training is analogous to a student guided by an instructor. Unsupervised algorithms essentially perform clustering of the data into similar groups based on the measured attributes or features serving as inputs to the algorithms. This is analogous to a student who derives the lesson totally on his or her own. ANNs can be implemented in software or in specialised hardware. For scientific applications, neural networks can be thought of as an architectural solution to common planning problems such as forecasting and optimisation. Just as in building architectures, there are many tastes and styles. Broadly speaking, artificial neural networks can be divided into two classes: those that involve learning and those that do not. The neural networks that involve learning and adaptation are sometimes called recurrent networks, or backpropagation networks. The neural networks that do not involve learning are sometimes called feed-forward nets.

Here, we note that the foundation of the Adaptive Visbreaker Paradigm is based on the prediction capability of the neural network system, that in turn, requires *Training*; a process that in this research work is defined as follows:

> "Training is a process used by the neuroengineering technique to teach the adaptive visbreaker paradigm, to *learn*, and to *forget*".

It is equally important to point out that any system with the capability to learn, and to forget, should also have a capability to recall what it has learnt. This definition leads us to conceptualise artificial neural networks as an information processing system.

Today's research in neural computation is largely motivated by the possibility of making artificial computing networks. Yet, as the term "neural network" implies, it was originally aimed more towards modelling networks of real neurons in the brain.

Although the biology is and has been the inspiration, much of the technology is trying to mimic nature's approach in order to acquire some of nature's capabilities (Holland, 1975). Assumptions that are not biologically accurate are used in building artificial, as opposed to biological, neural systems. The real motivation for studying neural computation is its robustness, flexibility, and simplicity. Its potential applications lie of course mainly in computer science and other applications such a chemical processing.

The neural networks field is also known as neurocomputing, associative networks, collective computation, connectionism, and probably many other things. For the purpose of clarity, the term artificial neural networks system (ANNs), or neural nets are freely used throughout this research work.

Next, we will briefly discuss the anthropomorphism, or the structure of the *neurons* themselves. The brain is composed of about 10^{11} neurons (nerve cells) of many different types. Figure A3-1 is a schematic drawing of a single neuron.

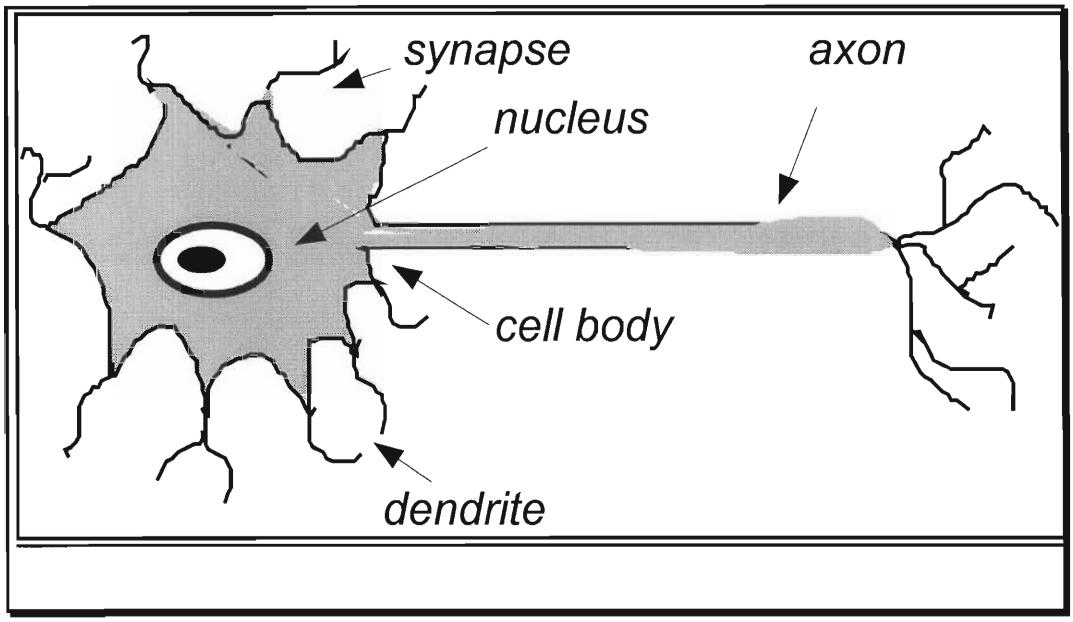


Figure A3-1 Schematic drawing of a typical genetic biological neuron.

It can be seen from the above diagram that, tree-like networks of nerve fibre called dendrites are connected to the cell body or soma, where the cell nucleus is located. Extending from the cell body is a single long fibre called the axon, which eventually branches or arbourises into strands and sub-strands. At the ends of these are the transmitting ends of the synaptic junctions, or synapses connected to another neuron. The axon is the nerve cell process that conducts impulses away from the cell body. The axon of a typical neuron makes a thousand synapses with other neurons. Although we could look at many other types of neurons, this one gives us the functionality and vocabulary required to present the analogies. In fact, there is a close analogy between the structure of a biological neuron and the artificial neuron presented in Figure A3-2 of this Appendix..

Generally, a neural network is characterised by :

Architecture: Pattern connections between the neurons.
Algorithm: Method of determining the weights on the connections.
Activation function.

Since that which distinguishes artificial neural networks from other approaches to information processing provides an introduction to both how and when to use neural networks, let us consider the defining characteristics of neural networks further.

A neural network consists of a large number of simple processing elements called neurons, units, or nodes. Each neuron is connected to other neurons by means of directed communication links, each with associated weight. The weights represent information being used by the network to solve a problem. Neural network can be applied to a wide variety of problems, such as storing and recalling data or patterns, classifying, grouping, performing general mapping from input pattern to output pattern, or finding solutions to constrained optimisation problems.

Each neuron has an internal state, called its activation or activity level, which is a function of the inputs it has received. Typically, a neuron sends its activation as a signal to several other neurons.

Figure A3-2 illustrates a typical neural network. In this diagram, neuron $\boldsymbol{Y}$ receives inputs from neurons $\boldsymbol{X_1}$, $\boldsymbol{X_2}$, and $\boldsymbol{X_3}$. The activation's (output signals) of these neurons are $\boldsymbol{x_1}$, $\boldsymbol{x_2}$, and $\boldsymbol{x_3}$, respectively. The weights on the connections from $\boldsymbol{X_1}$, $\boldsymbol{X_2}$, and $\boldsymbol{X_3}$ to neuron $\boldsymbol{Y}$ are $\boldsymbol{w_1}$, $\boldsymbol{w_2}$, $\boldsymbol{w_3}$, respectively. The ANNs input, $\boldsymbol{y\text{-}in}$, to neuron $\boldsymbol{Y}$ is the sum of the weighted signals from neurons $\boldsymbol{X_1}$, $\boldsymbol{X_2}$, and $\boldsymbol{X_3}$, i.e. ,

$$y\text{-}in = w_1 x_1 + w_2 x_2 + w_3 x_3 \qquad \textbf{(A3.1)}$$

The activation y of neuron ***Y*** is given by some function of its network input, ***Y*** $= f$ (***y-in***), e.g., the logistic sigmoid function (an ***S***-shaped curve) or any of a number of other activation functions.

$$f(x) = \frac{1}{1+exp(-x)} \qquad \textbf{(A3.2)}$$

It is important to note that a neuron can send only one signal at a time, although that signal is broadcast to several other neurons. It was mentioned earlier that neural networks consist of processing elements and weighted connections.

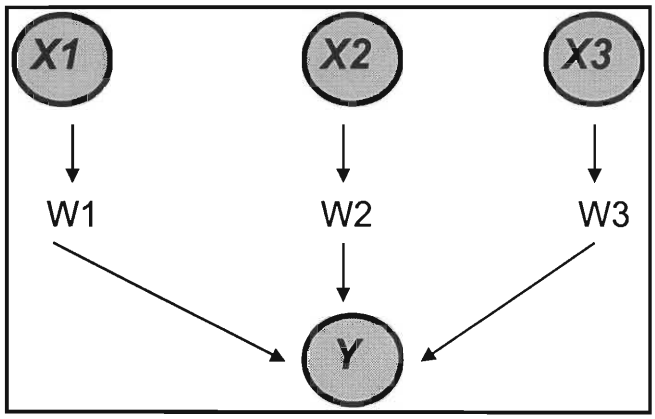


Figure A3-2 A simple artificial neuron

Warren McCulloch and Walter Pitts (1943) designed what is generally regarded as the first neural networks. These researchers recognised that combining many simple neurons into neural systems was a source of increased computational power.

In line with the aforementioned statement, let us suppose that neuron **y** is connected to neuron Z_1 and Z_2, with weights v_1 and v_2, respectively, as shown in the Figure A3-2. Neuron Y sends its signal **y** to each of these units. However, in general, the values received by neurons Z_1 and Z_2 will be different, because each signal is scaled by the appropriate weight, v_1 and v_2. In a typical neural network, the activation z_1 and z_2 of neurons Z_1 and Z_2 would depend on inputs from several neurons, not just one, as shown in the Figure A3-3. Although the neural network shown here is very simple, the presence of a hidden unit, together with a non-linear activation function, gives it the ability to solve many more problems than can be solved by a network with only input and output units (Sanchez *et al*, 1992). On the other hand, it is more difficult to train (i.e., find optimal values for the weights) than a network with hidden units.

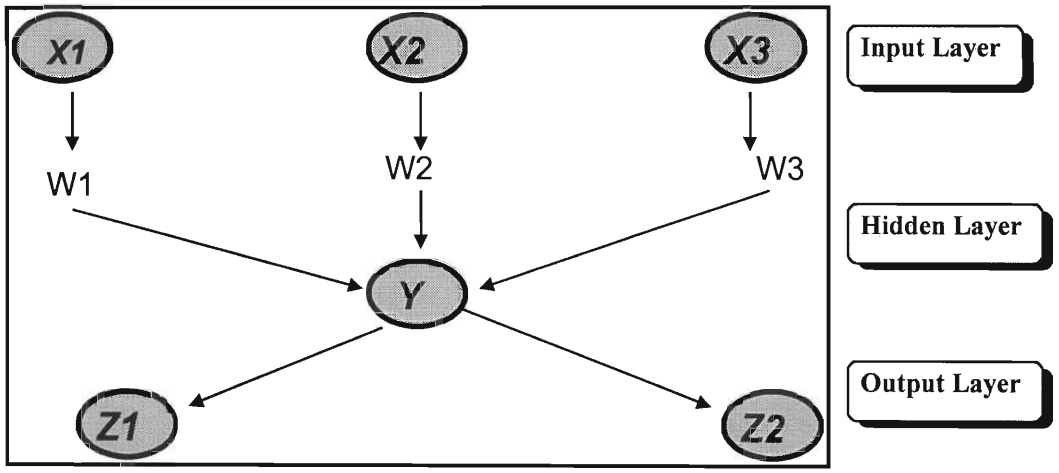


Figure A3-3 A Multi-layer artificial neuron

A multi-layer neural network can also solve more complicated problems than a single layer network and thus is the most likely candidate to be used in the initial design of the adaptive visbreaker paradigm. The three principle elements to be included in the design phase of the AVP are:

Topology – how the ANNs is organised into layers and how these layers are connected.

Learning – how information is stored in the AVP.

Recall – how the stored information is retrieved from the network.

After a description of the terminology used to describe neural networks systems, each of above mentioned elements will be examined in turn.

Terminology

Neural network's terminology remains varied, with a standard yet to be adopted. For clarity in further discussion, this thesis adopts the terminology proposed by Simpson (1991), described below.

Each neural network system has at least two physical components/connections and processing elements. The combination of these two components creates a neural network. In addition to the connections and processing elements, threshold functions and input/output patterns are also basic elements in the design, implementation, and use of artificial neural network systems.

Input and output vectors (patterns) are often denoted by subscripted capital letters from the beginning of the alphabet. For input patterns, this is shown as:

$$A_k = (a_{k1}, a_{k2}, \ldots\ldots a_{kn}); \qquad k = 1, 2, \ldots\ldots, m \qquad \textbf{(A3.3)}$$

and for the output patterns as follows:

$$B_k = (b_{k1}, b_{k2}, \ldots\ldots b_{kp}); \qquad k = 1, 2, \ldots\ldots, m \qquad \textbf{(A3.4)}$$

The processing elements in a layer will be treated in the same manner, where the collection of processing elements in a layer form a vector, and these vectors will be denoted by the capital letters from the end of alphabet. The input layer of processing elements is denoted by:

$$F_x = (x_1, x_2, \ldots\ldots x_n); \qquad \textbf{(A3.5)}$$

where each x_i receives input from the corresponding input pattern component a_{ki} The next layer of processing elements will be F_y then F_z (if this layer is necessary). This is illustrated in the Figure 2.10

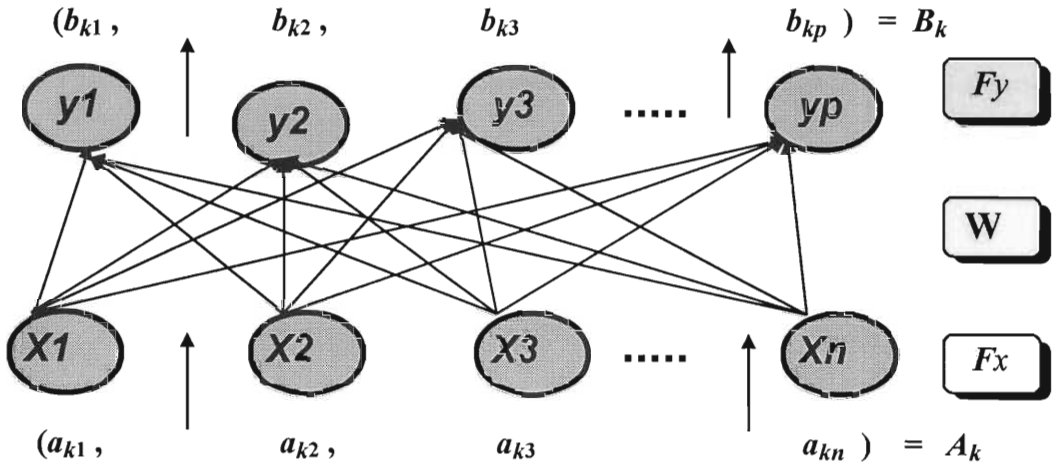


Figure A3-4 Illustration of the Artificial Neural Networks Terminology.

The second layer of the network (in this case the output) can be represented as follows:

$$F_y = (y_1, y_2, \ldots . y_p); \qquad \textbf{(A3.6)}$$

Weight connections are stored in weight matrices. The weight matrix **W** for the above network is presented in the Figure A3.5.

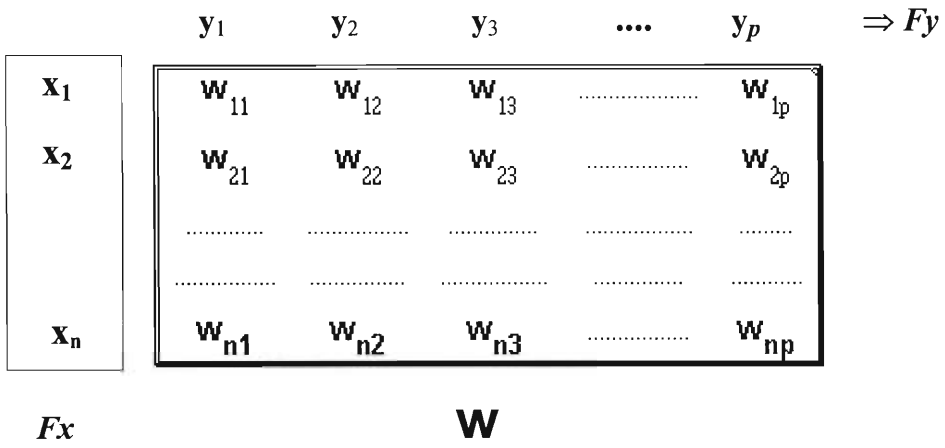


Figure A3-5 Illustration of the Weight Matrix.

Topology

It was mentioned earlier that a neural network consists of one or more layers of processing elements interconnected by weighted connections. The arrangement of the processing elements, connections, and patterns into a neural network is referred to as topology. Among the most common topologies are; Instars, Outstars, (Grossbeg, 1989), ADALINE (Adaptive Linear Neuron), and MADLINE (Multiple ADALINE),.....etc.

In addition to the common topology, both ADALINE and MADLINE use the least mean square (LMS) algorithm.

Learning

The most appealing quality of the artificial neural networks system is their ability to learn. Learning, in this context, is defined as change in connection weight values that results in the capture of information that can later be recalled. The methods used to adjust these connection weights are often referred to as the neural network algorithms. There are two distinct types of learning:

- Supervised.
- Unsupervised.

In *supervised* learning, the neural network system has access to the correct information, in other words, the answers are already provided. The system then tries to learn how to solve the given problem in order to produce the right answer. Learning is the most important part of the system training. The process of supervised learning is sometimes referred to as teaching the network, which thus acts as a machine learning device conditioned to provide the desired response to the stimulus provided by the training data. The goal of supervised method is to find a model – a general procedure - that will correctly associate the inputs with targets. In essence, learning requires historical data that describes sets of corresponding process input and outputs during a certain period of time (Joubert *et al*, 1996).

In *unsupervised* learning on the other hand, there is no information that could lead to the correct answer. The system has to guess and produce a pattern based on what it knows. The learning equations (often referred to as the learning rules) are in fact rules of algorithms applied to the networks. Inherent in any unsupervised learning system is an optimisation (or decision) criterion that is used for the evaluation of the result at the end of each cycle. This, however, is a very general one, such as minimisation of energy or distance, maximisation of profit, etc.

Among the most common learning rules (Zahedi, 1993) are:

- Hebb rule
- Delta rule
- Generalised delta rule
- Kohonen rule

Recall

Recall is a procedure to retrieve the information already stored in the neural network. The quality of the retrieved information is directly related to the method used in training the neural network. An alternative term is "system production" or production, often used to describe the neural networks response to the system's stimuli.

So far, we have defined artificial neural networks as information processing models and have characterised their nature. In the remainder of this section, we explain:

- The major application of neural networks
- How to build a neural network model
- How a neural network model works

We begin by listing the major applications of the neural network model. According to Werbos (1994), artificial neural networks have dual use as mathematical tools used for tasks ranging from reducing pollution through to political forecasting, and as models of intelligence. Among many of the problems which have already been successfully addressed by using neural computing are:

— Stock Portfolio Adviser

— Market Timing

— Credit Risk

— Word Recognition

— Object Recognition

— Jet Engine Diagnostics

— Paint Formulation

— Predicting Business Failure

. .....

It is this *predicting* capability of artificial neural networks systems that enticed us to use neural networks in this research work. According to Illingworth *et al* (1990), neural computing builds models based on historical data. Artificial neural networks systems can be used in any situation where there is an unknown relationship between a set of input factors and an outcome, and for which a representative set of historical examples of this unknown mapping is available. The objective of building a model is to find a formula or program that facilitates predicting the outcome from the input factors. This is particularly useful when modelling non-linear chemical process systems (Bhat *et al*, 1990).

The models that are expected to produce a prefect match are often referred to as the physical, as oppose to the behavioural applications, where the outcome is often an approximation (Berger *et al*, 1996). Some problems are physical in nature, meaning that although there are some underlying physical relationship between input and output, the exact correlation between predicted and real outputs can not be quantified. The adaptive visbreaker paradigm is an example of such a neural networks model.

Neural network model building requires careful planning at every stage. The required stages to model an ANNs are summarised as follows:

Required stages in paradigm building

Defining the system objectives

Collecting data

Domain dependent processing of raw data

Selecting, training, testing, and validation sets

Analysing and transforming data

Variable selection

Network construction, topology, and training

Model verification.

Defining the system objectives

It is necessary to clearly define the system's objectives, influencing parameters, perspective, and solution methodology. Computer software and other analytical tools are required both in the data pre-processing and model building stages. These need to be identified and evaluated.

Collecting data

The process of learning requires historical examples, and is based on the set of data used to prepare these historical examples. The data collection and pre-processing therefore plays a great role in the quality of the response or system performance. The process of collecting data also involves verifying it. Generally, there are several key points in this process. Three in particular are:

- Data formats: essential and recent data
- Field Usage: relevant, and related data
- Data Availability: consistent, and economically viable to acquire

Domain-dependent processing of raw data

Data pre-processing is another important step in the design and construction of neural network models. This process evaluates the raw data and provides a reduced but more tractable representation of the real world samples. There are two levels of data pre-processing required when trying to build a neural network model. The first level is domain-dependent pre-processing in which relevant features are derived from the raw collected data. The second level is generic in nature and is used to transform and shape the data into a useful form for interfacing with the neural network system.

Selecting; training, testing, and validation sets

The purpose of developing a neural network model is to produce a formula that captures essential relationships in a data set. Once developed, this formula is used to interpolate from a new set of inputs to corresponding outputs. In neural nets, this is called generalisation. The training set is the set of points that are used to fit the parameters of the model. The test set measures how well the model interpolates. It is used as part of the model building process to prevent over-fitting. The validation set is used to estimate model performance in a deployed system.

Analysing and transforming data

Converting data into a form suitable for building effective models is an iterative process that interacts with the model development process. At this stage, the critical issues are: Structuring or formulating the problem, and transforming enumerated data.

Variable selection

Picking the right input variable is critical to effective model development. A good subset of variables can substantially improve the performance of a model. The challenge is finding ways to pick good subsets of variables. A variety of techniques have been suggested for variable selection. Most of them fail to produce the best possible results. One of the most common approaches to variable selection is step-wise linear regression widely used in neural computing.

Network construction, topology, and training

Neural network models are referred to as "paradigms". There are many types of neural network models, but the majority of applications to date use some form of Multi-Layer Perceptions (MLP) due to its wide applicability and the compactness of its representation. According to Gelenbe (1992) the multi-layer ANNs is widely used in generalisation problems, where a network is expected to correctly predict outputs for inputs previously unseen during learning. Learning algorithms need to avoid over-fitting to successfully generalise. Over-fitting (or over-training) can be explained as a consequence of parameter redundancy; that is, the system has more parameters than needed for the solution of the problem. In curve-fitting, we might see this in a polynomial with too many terms: it can make a "better" fit to a set of data by adapting to, rather than smoothing out, the "wiggles" caused by noise. Backpropagation, stochastic backpropagation, and cascade learning, among the many, are examples of the learning algorithms used in generalisation problems.

Paradigm verification

Perhaps one of the biggest problems with neural net paradigms is how to quantify their respective performance. Statistical models often use the T-test to establish confidence intervals at the 90% or 95% certainty level (Willemse, 1994). Similar approaches can be taken with linear paradigms. In this case, the

residual errors are approximately normally distributed. If the residuals meet this requirement, the T-test can often be applied to either neural or linear models. When performing this test, it is essential that the data selected for validation has the same distribution as the main population. This is one of many ways to report on the model's performance and improving acceptance of the neural network paradigm.

A neural network is a massive system of parallel distributed processing elements connected in a graphical topology. By defining proper processing functions for each node and defining associated weights for each interconnect, it is possible to solve an optimisation problem relatively rapidly. System operators can consider a neural network as a large-dimensional non-linear dynamic system, which is defined by a set of first-order non-linear differential equations. In its simplest form, however, the output $\mathbf{S}_t$ of a linear neural network system is a linear combination of its inputs. Using this analogy, let us define a neural network system that at temperature t, receives an input vector $\mathbf{X}_t$ and predicts a desired response $\mathbf{d}_t$ using a weight vector $\mathbf{W}_t$ as shown in the following diagram:

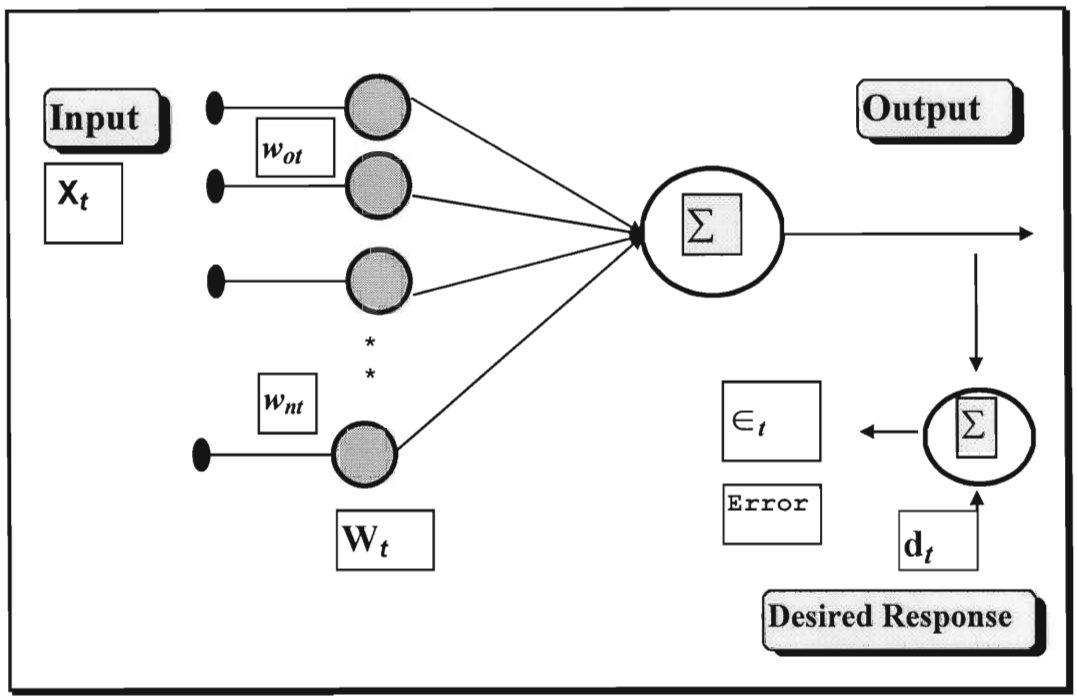


Figure A3-6 Illustration of the Actual Output vs. Predicted Output.

During the training process, input patterns and the corresponding desired responses are presented to the linear combiner. In this example, an adaptation algorithm automatically adjusts the weights so that the output responses to the input patterns will be as close as possible to their respective desired responses. There are many ways to generate approximations to the system's characteristic surface. One of the most popular method for adapting the weights is the simple least mean square (LMS) algorithm, often called the Widrow-Hoff delta rule (Fausett, 1994). This algorithm minimises the sum of squares of the linear errors over the training set. The linear error $\in_t$ is defined to be the difference between the desired response $\mathbf{d_t}$ and the output $\mathbf{S_t}$. In essence, the minimisation of the $\in_t$ over the regions $\mathbf{X_t}$ and $\mathbf{S_t}$ should provide optimality for the desired output $\mathbf{d_t}$. This is a simple example of how the learning algorithm can be used to train a network. Even though learning algorithms have successfully been used for many recognition problems, it is not clear if they can generalise well to previously unseen examples. As explained above, these algorithms tend to

minimise error of fit to learning samples. This may result in memorising the learning sample including any noise present. Such memorisation leads to poor prediction performance on unseen inputs, a phenomenon known as over-fitting.

Secondly, some of these learning algorithms do not provide robust stopping criteria to terminate the learning process. The typical stopping rules are based on a given number of learning iterations and a target value for the total error fit, which are to be supplied by the end user. An inexperienced end user has no guidance in selecting these values, leading to the selection of very small or very large values for the parameters. A large value for the target error of fit or small value for the number of learning iterations leads to under-fitting of the learning sample.

Finally, generalised learning algorithms are expected to filter out the noise present in learning samples. This implies that learning should terminate before the error of fit becomes less than the noise present in the learning sample. If the level of noise is known *a priori*, the end user can set the target value of the error of fit for terminating the learning algorithm. However, in the absence of any information about the noise level, learning becomes more difficult.

Due to the difficulties in learning for generalised problems, there is a need to evaluate the learning algorithms. An experimental framework to evaluate the algorithms can be defined around a set of generalisation metrics, and the framework should include the ability to measure the generalisation ability of different algorithms. Generalisation metrics are quantitative performance properties that characterise the ability of an algorithm to generalise previously unseen input vectors. A sample metric is the per-pattern error produced by a trained network over a set of testing samples. The trained network is the result of discovering the weights generated when using a given learning sample for a learning algorithm. Obviously, the testing samples are a set of previously unseen input-output vectors.

Other examples of metrics for generalisation performance include accuracy of prediction, shape of the learned function and ability to avoid over-fitting.

Accuracy in prediction of a test sample measures the number of correctly classified individual patterns within a sample, relative to the size of this testing sample. Accuracy of prediction is more appropriate than pattern per square error in classifications where the output takes discrete values. The shape of the learned function provides global information about the result of learning over the input domain.

The generalisation ability of learning algorithms depends on a number of parameters, called performance parameters. Some performance parameters are common to backpropagation and stochastic backpropagation. These include the number of learning iterations (also termed as nepoch), network size, and generalisation problem class (Gail *et al,* 1992).

Other parameters are specific to the algorithms. These include learning rate, momentum (for backpropagation), delta, stability count, starting temperature, and cooling factor (for stochastic backpropagation).

The algorithm-specific parameters are specified with the description of the algorithms. The number of learning iterations determines the quality of the learned weights. A low number of learning iterations can lead to under-fitting, since each iteration changes the weights by a small amount. For example, a network with no hidden nodes in the layers enables learning algorithms to generalise to non-linear functions. However, a large number of the hidden nodes also makes it easier to learn the noise and other peculiarities in the learning sample.

There are many ways to evaluate the effectiveness of a learning algorithm. When information over a wide range of target data is in hand, then the measure of the fitness is probably an attractive proposition (Gerald *et al*, 1983). At this

stage, we introduce the system's error or miss-match as the measure of the effectiveness of the learning algorithm.

$$\textbf{Error} = \frac{Yop - Top}{Yop} * 100 \qquad \textbf{(A3.7)}$$

where

where Y_{op} is the observed value of output o from training pattern p, and T_{op} is the desired or target output.

Another method often used to measure the pattern recognition ability of the neural network is to calculate the R-squared value. The R-squared values are often used to evaluate the estimates obtained from different prediction models. Creese & Li (1995) have compared the output of a neural network model with that of a linear regression model. They have shown that in linear regression analysis, R-squared, the coefficient of determination, is a measure of the effect of independent variable X in reducing the variation in Y, and is defined by the following equation:

$$R^2 = \frac{\mathbf{Ss} - \mathbf{Se}}{\mathbf{Ss}} \qquad \textbf{(A3.8)}$$

where

Ss = measurement of the variation in the observation Y_i (i = 1,2, ...n) when no independent variable X, as input is considered.

Se = measure of the variation in Y_i when the use of independent input variable X is considered. In this respect, the equation (2.32) can be written as;

$$\mathbf{Ss} = \sum_{i} (\mathbf{Y}_i - \overline{\mathrm{Y}})^2 \qquad \textbf{(A3.9)}$$

in this case the $\overline{\mathrm{Y}}$ can be shown as

$$\overline{Y} = \frac{\sum \mathbf{Yi}}{n} \qquad \textbf{(A3.10)}$$

and when X is in use:

$$\mathbf{Se} = \sum_{i} (\mathbf{Y}_i - \mathbf{Y}_k)^2 \qquad \textbf{(A3.11)}$$

where

$\mathbf{Y}_k$ = the estimated value using the model

$\mathbf{Y}_i$ = the actual value

$\overline{Y}$ = the mean value

for $\mathbf{0} \leq \mathbf{Se} \leq \mathbf{Ss}$

then $\mathbf{0} \leq \mathbf{R}^2 \leq \mathbf{1}$ **(A3.12)**

As **R**-squared increases, the total variation of **Y** is reduced. They have concluded that, in their line of work, the output of the neural network model agrees with the results obtained from the linear regression method .

In summary, it may be said that an artificial neural network is a modelling tool that can process information and carry out solutions almost simultaneously. In most cases, it learns by being trained. The technology is showing a great deal of promise in areas that have posed problems for conventional systems.

APPENDIX - 4

Decision Support Tools (Software evaluation)

As described in the section 4.1 of this thesis, using PIVAX™ and other local area network facilities, the plant and laboratory data is routed into an Excel™ database hosted by a PC. An Intel™ based computer is employed to run various software applications pertinent to both neuroengineering and the optimisation phases of the project.

Broadly speaking, the applicable software can be classified into the following category:

- Data Management
- Neural Networks' application
- Optimisation

Data Management

Data management is an essential element of this research work. In this respect, Microsoft Excel version 5C™ proved to be an excellent vehicle to perform tasks such as data collection and data pre-processing. Along with its powerful spreadsheet computation and data manipulation capability, Excel offers a few exceptional features described below:

- The connectivity to other LAN-based computer software using Microsoft Windows as the graphical user interface.

- The availability of the "Add-ins" applications in almost any field including artificial neural networks, fuzzy logic, genetic algorithms, and other scientific principles.

- The addition of Visual Basic for Applications provides an invaluable programming tool to this package. Visual Basic is a powerful programming language that can be used as the mathematical programming tool in many applications. Additionally, Visual Basic provides various facilities to design a graphical user interface.

Neural Networks' application

An extensive search was carried out to find a suitable neural network software able to read and process the Excel data to form the neural network's topology. Our investigation indicated that although many products are capable of reading the spreadsheet data, most are unable to produce a result that can be converted into the Excel or another spreadsheet format. This is not a serious problem, if the software is intended to be used in a stand-alone application. However, in an integrated networking environment, data portability is required for further refinement or processing. Having this in mind, we evaluated three products as described below:

1- NeuroForecaster

NeuroForecaster from Midaz Technic Co. is an advanced Windows-based, neural network tool. It is packed with the latest technologies including fuzzy computing and non-linear dynamics. When combined with Genetica™, the system is capable of building an intelligent neural network system and uses genetic algorithms to perform optimisation. NeuroForecaster is designed primarily for stock market forecasting and analysis, therefore, the package is not widely applied to the chemical processing environment.

2- NeuroShell & NeuroWindows

NeuroShell 2 and NeuroWindows are neural network programs from the Ward Systems Group, Inc. NeuroWindows is a powerful programmer's tool kit for neural network functions that may be called from Visual Basic or C and Pascal

which run under Windows. It is a function library in a Dynamic Link Library for an advanced user wishing to build his own custom interfaces or networks.

NeuroShell 2 is a Windows-based neural network package designed for non-programmers. NeuroShell 2 has a beginner's system, an advanced system and facilities for creating runtime versions of trained nets. The beginner's system has a subset of the advanced system's menus and routines. The network fabrication involves; data input, pre-network data operations, network formation, network application, post-network processing, and a results-output module. The data input module imports files into the program. This module is capable of reading Papyrus Clarity, Excel, and financial data in Equis Metastock format. The network fabrication module supports various neural network-building routines. One may choose from twelve network architectures. NeuroShell 2 support six kinds of backpropagation and three kinds of recurrent backpropagation, along with Generalised Regression (GRNN), Probabilistic (PNN), and Kohonen. The TurboProp backpropagation training algorithm does not require the specification of any momentum or learning-rate parameters, and trains a network automatically. Although several hidden layers can be formed, Ward cautions against increasing the number of hidden layers because of the increased training time and loss of meaning that occurs when more than one layer is fabricated. In this respect the allocation of the output layer's errors to the middle layer according to the connection weight is, in a very real sense, only a guess of what the middle layer's error should be. That guess becomes even more problematic when passed back another layer. In a multi-layers network, this results in compounding the guesses and subsequently decreases the system's performance and effectiveness

In summary, our evaluation revealed that the NeuroShell 2 and NeuroWindows are excellent neural networks programs to be used in financial, business, and in some of the chemical processing applications. An interface with Excel needs to be developed.

3- NeuralWare Software

NeuralWorks Professional, Explorer, Designer Pack, and Predicts are various products of NeuralWare, Inc. (A member of Aspen Technology Group). NeuralWorks Predict is the program that we have employed to fabricate the adaptive visbreaker paradigm. The major features of this product are discussed below.

Predict™ is a neural network package that integrates all the components needed to apply neural computing to a wide variety of problems (Suleiman *et al* 1997). The primary end-user interface to Predict is through Microsoft Excel. This provides a familiar front end for supplying data to and receiving results from the Predict "engine". The Excel interface also provides ready access to all the parameters that control the various algorithms, and allows the user to examine the results of all the following components of the trained paradigm:

- Train/test set selection
- data analysis and transformation
- Selected variables
- Network architecture

Within Excel , one can also use charting capabilities to analyse the results of the model. Third-party modules and add-ins are available to domain-dependent processing.

A secondary interface is the command-line interface. This allows all the functionality of Excel through a command-line language. Access to the various parameters is more involved and less intuitive than with Excel itself, but the advantage of the command line version is that a file of commands can be created to run Predict in batch mode.

Both Excel and command-line versions allow conversion of trained models into C, FORTRAN, or Visual Basic Code. The complete Predict functionality is also available for embedded systems support via Dynamic Links Libraries under Visual Basic and C/C^{++}, and via object libraries for UNIX system. Three levels

of interface address the diverse needs of the end-users, application engineers, system integrators, and neural network engineers. The complete system has six components.

The Train/Test selection component picks out training and test sets for model building. It tries to do this in such a way that the test set, or pattern is statistically close to the training set.

The Data analysis and transformation component automatically analyses data and transforms it into forms suitable for neural network application. This component expands categorical data into numeric data, shapes numeric data to get rid of skewness and other undesirable characteristics, deals with outliers in the data, and screens out data that contain no information. The user may change the transformation function and save the model under a different name.

The Input Variable selection component uses a genetic algorithm to search for synergistic sets of input variables which are good predictors of the output. Because of the evolutionary nature of the Input Variable selection algorithm, different initialisations of the algorithm will yield different variable sets. This tool can be used by experience users to build several paradigms based on different variable sets and combine the outputs of those models. Each model can be thought of as an expert system which uses a different set of criteria (the selected variables) to make its decision.

The neural computation component of Predict supports two proprietary non-linear feed-forward constructive algorithms. One of the algorithms is based on a non-linear Kalman filter (Pierre, 1992) learning rule and it is designed for very noisy regression problems. In this research work we have used the other one, the adaptive gradient learning rule. This is a general purpose learning algorithm suitable for multi-response predictive networks such as the many-to-many visbreaker paradigm.

As stated earlier, cascade correlation is the architecture used in the adaptive visbreaker paradigm. In cascade training mode, the neural network is constructed incrementally by adding nodes one or two at a time. Each hidden node or pair of hidden nodes has its weights trained from several initialisations. Each initialisation is referred to as a candidate. The best candidate is established in the network, and then all the weights to the output node(s) of the network are re-trained.

Optimisation software

This section describes three computer packages:

- Genehunter genetic algorithm package used in the neuroengineering process.
- Premium Solver used in the fuel oil blending and optimisation.
- Refinery and Petrochemical Modelling System (RPMS) used in modelling the global refinery configuration and optimisation.

Genehunter genetic algorithm

As reported in the chapter 4 of this thesis, initially, the generalised reduced gradient solver was used to minimise the degree of error associated with accepting a data set for the learning process. This method however, was found to be problematic, since a GRG2 solver often converged to a local minima. The experimental result indicates that a solver based on the fundamentals of the genetic algorithm is more suitable for the given binary integer and sparse problem.

Genehunter genetic algorithm from the Ward Systems Group, Inc. is an optimisation package used in the network reciprocation procedure. We recall from section 4.4 that a genetic algorithm was used in the neuroengineering process. The reason is that gradient descent and almost all other optimisation techniques can become stuck in any local minima of an objective or cost function. Genetic algorithms perform a global search and are thus not easily fooled by a local minima, most notably in the network reciprocation process that involves the minimisation of the error function Z

$$\boldsymbol{Z} = \sqrt{\frac{\sum(L(Yop - Top)^2)}{Np}} \qquad \textbf{(A4.1)}$$

here, $\boldsymbol{L}$ is an integer with the value of L= 0, or L= 1, that removes (or introduces) a data set into the overall computation. Most conventional optimisation packages are either unable to solve such problems, or the solution time is unacceptably long. Genetic algorithms (GAs), on the other hand, seek to solve optimisation problems using the methods of evolution, specifically survival of the fittest. Genetic algorithms have been also used for training recurrent neural nets, particularly for real time applications. GAs were thought to be an appropriate tool because they are frequently good for high-dimensional search spaces with rough landscapes. They also provide a wide coverage of the search space which should be useful for avoiding problems associated with local minima.

In a typical optimisation problem, there are a number of variables which control the process, and a formula or algorithm which combines the variables to fully model the process. The problem is then to find the values of the variables which optimise the model in some way. If the model is a formulation, then we will usually be seeking the maximum or minimum value of the formulation. The traditional optimisation programs tend to break down in combinatorial models or when the variables are non-continuous. Genetic algorithms, on other hand, are search algorithms founded upon the principles of natural evolution and selection. Possible solutions to the problem are coded as binary strings or "genes." The search is initialised with a random population of possible solutions. Each solution is tested against some criteria and numbers of the population are ranked according to their "fitness." Fit solutions are allowed to live and breed while unfit solutions die. An iteration is performed until solutions converge.

According to Goldberg (1989) in order for genetic algorithms to surpass more traditional cousins in the quest for robustness, GAs must differ from more normal optimisation and search procedures in four ways:

1. GAs work with a coding of the parameter set, not the parameter themselves.
2. GAs search from a population of points, not a single point.
3. GAs use payoff (objective function or fitness function) information, not derivatives or other auxiliary knowledge.
4. GAs use probabilistic transition rules, not deterministic rules.

Genetic algorithms require the natural parameter set of the optimisation problem to be coded as a finite-length string over some finite alphabet.

Genetic algorithms mimic evolution theory. In this context, the theory is that a population of a certain species will, after many generations, adapt to live better in its environment. The members of this population are called individuals. Individuals carry strings or chromosomes that are the values of variables of the problem. Roughly speaking, the strings of artificial genetic systems are analogous to chromosomes in biological systems. The formulation for minimisation (or maximisation) is called the fitness function. A standard genetic algorithm deals with a set (a population) of possible solutions (individuals) to a problem. Each individual is a point in the search space, so we can think of the genetic algorithm as a multi-point optimisation technique for multi-dimensional spaces. Usually, the size of the population is in the range from 20 to 300. Traditional methods require a starting point to begin the optimisation. Often the quality of the final solution is very dependent upon the position of the starting point in a search space, particularly for problems with a large number of local optima. Genetic algorithms, which offer many solutions and can search multiple points simultaneously, do not suffer as much from this drawback.

It was previously mentioned that populations are composed of individuals, and individuals are composed of chromosomes, which are equivalent to variables. Chromosomes are composed of smaller units called genes. A continuous chromosome is composed of either 8, 16, or 32 genes, which are implemented in the computer as binary bits. The two distinct values of a gene, 0 and 1, are called alleles, as shown below:

1	0	1	1	1	1	0

Multiple chromosomes make up the individual. Each partition is one chromosome, each binary bit is a gene, and the value of each bit (expressed as (1,0,1,1,1,0)) is an allele.

The genes in a chromosome can take on a wide range of values between the minimum and maximum values of the associated variables. There are only a finite number of values that the chromosomes can take on, however, and the number depends upon the precision sought. For example, if the desired precision is 8 bits, then there are 2^8 or 256 possible values for the chromosome, which will be evenly spread out between the upper and lower bounds of the given variable (Menczer *et al*, 1992).

Another type is the integer chromosome, a continuous' chromosome that can only take integer values. Integer chromosomes use only 16 bit resolution and their values range from -32,768 to +32, 767.

In our case, using the genetic algorithms (within the Genehunter package), we produced a mathematical formula to minimise the value of the fitness function $\boldsymbol{Z}$, while endeavouring to search for the value of the load factor(s) $\boldsymbol{L}$, where $\boldsymbol{L}$ is in fact a non-continuous function or an allele with a value of 0 or 1. To determine the best point at which to stop the genetic algorithm, we should compare the best fitness since the start of evolution with the best one reached in the current generation. If the best fitness for the current generation does not exceed the previous best fitness for a number of generations (typically 20-200), then the best solution has probably been reached. The results of minimising the fitness function $\boldsymbol{Z}$ in the reciprocation of the adaptive visbreaker paradigm is given in the following table.

Table A4-1 Fitness function of the network reciprocation

Function	Value	# of Generation	Time to converge- seconds
Minimisation	0.9902	86	2160

Premium Solver

Under an Integrated system, the Ward's genetic algorithms package can also be applied to other optimisation problems including the allocation of the necessary components to optimise the fuel oil blending operations. In practice, this is unfortunately found to be problematic. The major drawback in using a genetic algorithm in a non-linear blending problem is the time that it takes to produce a recipe that meets the required technical specification. In a dynamic environment, any change in the neural network's response(s) results in a change in the volume or the quality of the visbreaker's product. This of course, necessitates re-optimisation of the marine fuel oil blend.

The latest trend in petroleum product blending indicates that non-linear optimisation programs are gaining popularity. An interesting example of using non-linear programming in product blending is the Industry-University Collaboration Project (Waren *et al*, 1995), designed to update Texaco's blending system. Accordingly, to optimise the fuel oil blending pool, we have selected a fast optimisation package operating on a Generalised Reduced Gradient algorithm.

Generalised Reduced Gradient (GRG) algorithms, introduced by Abadie and Carpentier (1969) are widely used to solve small- to medium-size nonlinearly constrained problems. Premium Solver from Frontline systems is computer software that uses enhanced GRG code originally developed by Lasdon *et al.* (1992) to solve nonlinear problems. The GRG codes have successfully been used in various optimisations and pooling problems within the petroleum industry. It is known that the GRG method is subject to the intrinsic limitations of its ability to find the globally optimal solution. However, limited

guarantees can be made about the GRG method's ability to find a "local optimum", in particular where the objective function and all the constraints are twice continuously differentiable. When these are combined with prior knowledge of the problem structure in a specific case, the result will often be a definitive "optimal solution".

Depending on the computer's memory, Premium Solver is capable of solving non-linear problems with a maxim of 800 variables and 400 constraints.

Global Refinery LP

In many ways the refining industry was the investor and leader in the early development of linear programming in the industrial sector (Coxhead, 1992). Bonner & Moore Management Associates (B&M) are one of first pioneers in the field of LP and MIP applications in the refining and petrochemical industry. The Global refinery LP model was constructed, using the RPMS and GAMMA from Bonner & Moore (1990) as described below:

RPMS-PROGRAM **:** RPMS (Refinery and Petrochemical Modelling Systems) is a comprehensive system supporting the development and analysis of mathematical models of refining and petrochemical facilities. It is a system for the creation of models and reports for those models' solutions. RPMS accepts technology-oriented input, logical requests, and data tabulations and converts them into an LP matrix and associated reports. The user may supply all information explicitly, or may allow the system to retrieve information from any one of several system data bases or libraries to augment user-prepared input. Its function is to generate a model (matrix) for linear programming optimisation and to generate report s for publishing salient information from the optimal solution once one has been obtained. RPMS requires the support of a mathematical programming system (MPS) such as IBM's MPS X/370 standard, or CLP- Professional linear programming module from Bonner & Moore to perform the optimisation process.

The various modules of RPMS are, themselves, written in the GAMMA (modified C) language which is a B&M-proprietary high-level language for matrix and report generation, employing a relational-database and list-driven concepts. All input to RPMS is, therefore, in the form of the GAMMA data and information structures called "Tables".

The organisation of GAMMA reflects the general organisation of a mathematical programming systems (MPS) problem, in which three distinct phases should be developed:

- Data Definition.
- Problem Definition.
- Report Definition.

GAMMA is primarily a language for the generation of mathematical programming matrices, beginning with tables of business and technical data and control. The system allows for the generation of dynamic programs which conform automatically to changes in data availability, and which make it possible to communicate results from the mathematical programming system to the GAMMA program itself.

The program performs the following functions:

The data editor provides a method for manipulating data, and automatically imposes the correct GAMMA syntax.

The pre-processor process GAMMA source input, performs syntax and logic checking, and prepares input to the generator phase.

The generator processes input from pre-processor, databases, and MPS communication files, and can produce output to the MPS, and to the extract and publisher phase.

The extract processor processes input from the generator, MPS solution, and matrix data, and also provides input to the publisher phase.

The publisher processes input from the generator and extract phases, and accesses the MPS solution matrix data. The publisher also creates reports.

RPMS Solution technique: The engine used to solve the model is CLP (an adoption from the Constraint Logic Programming technique). CLP is a general purpose linear programming code, well-suited for use in the solution of complex, medium-sized linear programming problems for industrial applications on personal computers and workstations. It is oriented toward the IBM MPSX/370 version 2 standard with respect to its procedures and data input/output formats for linear programming applications.

The standard CLP does not include pure or mixed integer programming (MIP) features. However, the new generation of the CLP processor is based on the IBM™ OSL optimisation package that provides mixed integer programming facilities. CLP comprises two major processors, firstly, the CLPCOMP, which compiles a control language program by defining the logical sequences of the CLP procedure execution, and secondly, the CLP executor which accepts a compiled control language program and executes the procedure sequences applying the Revised Simplex Method briefly discussed below:

The method often used for initiating linear programs is called the phase I - phase II procedure. Phase I determines a canonical (standard representation of the problem) form for the problem by solving a linear program related to the original problem formulation. Phase II starts with this canonical form to solve the original problem. The revised simplex method, or the simplex with multipliers, as it is often referred to, is a modification of the simplex method that significantly reduces the total number of calculations that must be performed at each iteration of the algorithm. Essentially, the revised simplex method, rather than updating the entire tableau at each iteration, computes *only* those coefficients that are needed to identify the pivot element. Clearly, the reduced costs must be determined so that the entering variable can be chosen. However, the variable that leaves is determined by the minimum ratio rule, so

that only the updated coefficients of the entering variable and the current right-hand-side values are needed for this purpose.

It is now evident that this project is largely implemented by applying three mathematical programming techniques, namely; artificial neural networks, genetic algorithms, and optimisation either by linear programming or with the generalised reduced-gradient method. With this focus, we have been able to form an integrated knowledge-based system of data management, simulation, and optimisation.

It should be noted that the application platform is currently Microsoft Windows NT4™ running on a Intel™ based Pentium 166 computer and the IBM™ Optimisation Sub-routine Language (OSL) has replaced the CLP Linear Programming module.

At this stage, in order to illustrate a simplified but macroscopic view of the interactions between the aforementioned computer applications, we provide the following diagram:

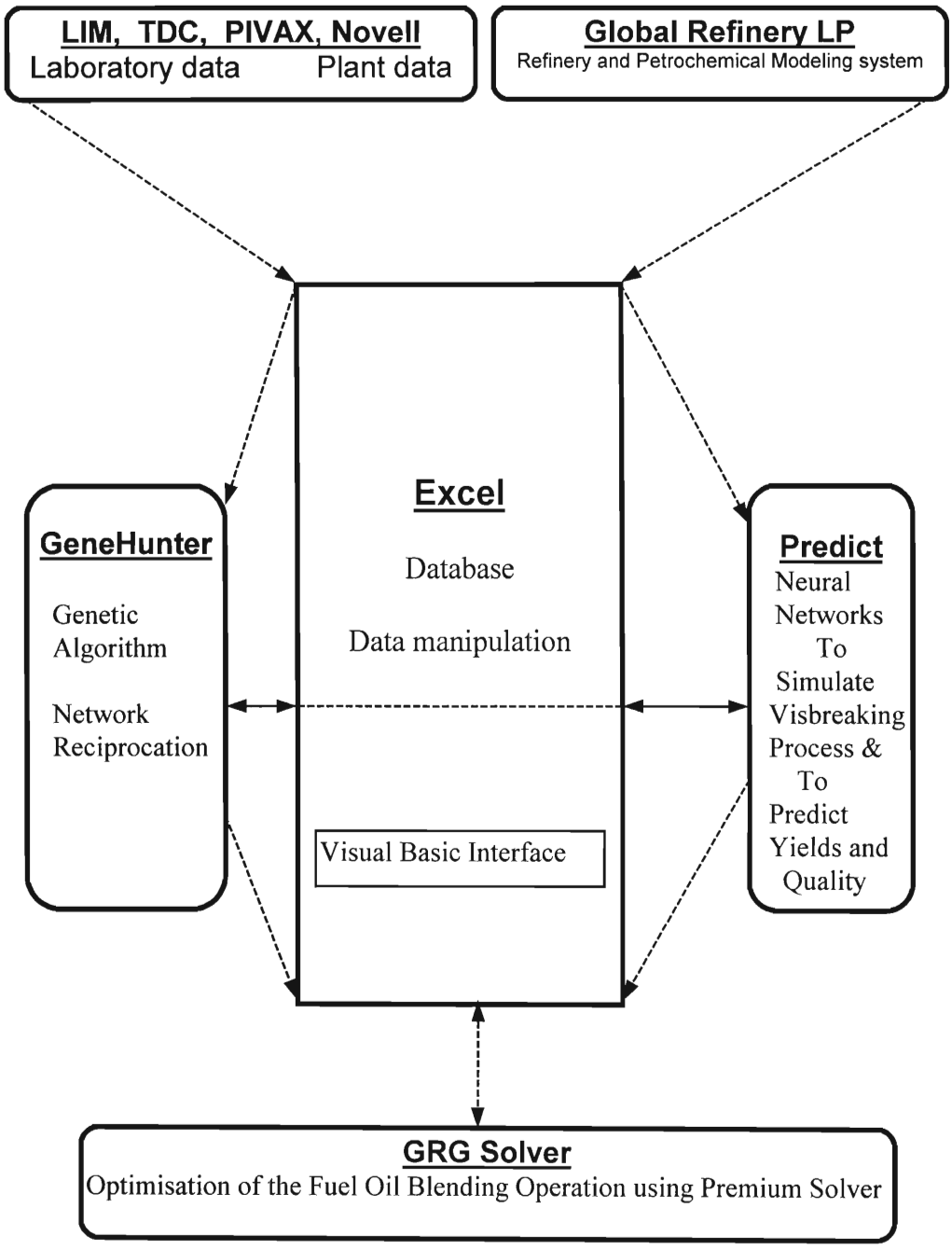


Figure A4-1 The interactions between various Decision Support Tools

APPENDIX - 5

EXHIBIT-1

Microscopic photography of the Asphaltenes:
Prepared by the Petroleum Section of the South African Bureau of Standards for this project.

Description:
Sample "A" contains 50 ml of Bunker Fuel Oil (BFO) with stability of 0.05% as measured by the Institute of Petroleum test method IP 375/390.

As explained in the section 5.4, fuel oils having IP 375 sediment contents of 0.06 (or less) are classified as the "Stable "fuels. In this respect, exhibit-1 is a microscopic photograph of a stable fuel oil, where both the large and small molecules of the asphaltenes are in solution with the peptising agent (gas oil).

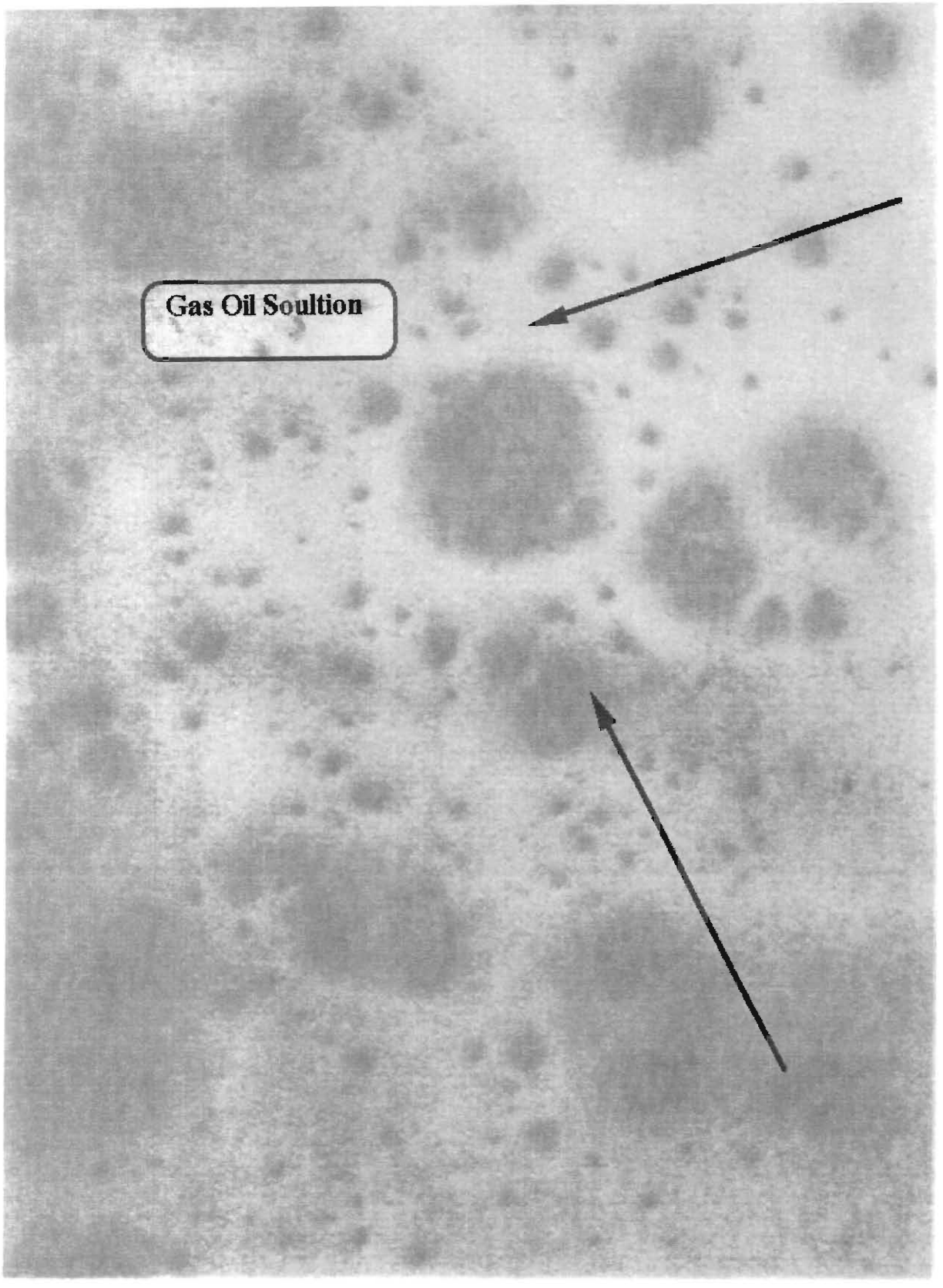


Exhibit - 1. Asphaltens are dispersed in oil solution.

EXHIBIT- 2

Microscopic photography of the Asphaltenes:

Prepared by the Petroleum Section of the South African Bureau of Standards for this project.

Description:

Sample "B" contains 50 ml of Bunker Fuel Oil (BFO) with stability of 6.1% as measured by the Institute of Petroleum test method IP 375/390.

As explained in the section 5.4, fuel oils having IP 375 sediment contents of 0.09 (or more) are classified as the "Unstable "fuels. In this respect, exhibit-2 is a microscopic photograph of an Unstable fuel oil, where the large molecules of the asphaltenes are not in solution with the peptising agent. Consequently, conglomeration and sedimentation of the asphaltenes produce unstable fuel oil.

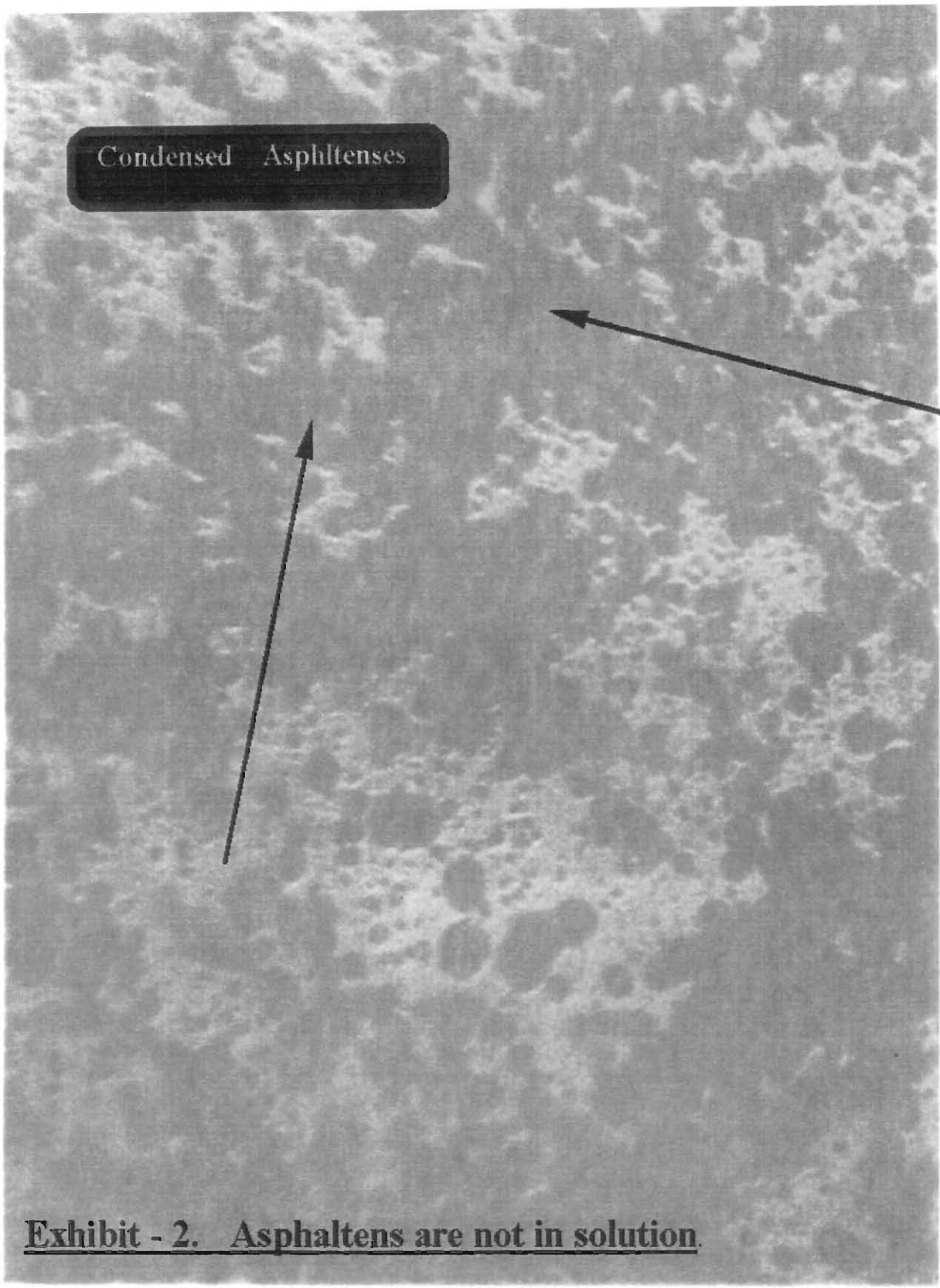


Exhibit - 2. Asphaltens are not in solution.

APPENDIX -6

List of symbols

Chapter-2 Fuel Oil Blending

P_b = property of total blend.

P_i = property of component ***i***.

W_i = weight fraction of component ***i***.

V_i = volume fraction of component ***i***.

X_i = mole fraction of component ***i***.

I_b = blending index for total blend.

I_i = blending index for component ***i***.

Chapter-2 Volume Conversion

X_i = Volume of white product ***i.*** produced by the visbreaker and n is the number of products.

V_f = Total volume of feed to the unit.

X_{max} is the maximum volume of cetane in millilitres that can be added to a gram of product without causing sedimentation.

Chapter-2 Soaking factors

F = soaking factor is defined as the equivalent coil volume in cubic feet per daily barrel of charge to unit.

V = coil volume in cu ft per bbl of daily throughput

D = feedstocks flow rate in bbl/day

P_t = pressure at a given point in the coil in PSIG.

K_t = reaction rate constant at a given temperature in Fahrenheit.

P_0, K_0 = standard reference values for P_t , K_t (relative cracking reaction velocity at temperature Fahrenheit)

Chapter-3 Feed & Quality Matrix

f_q = feedstock quality

u_c = unit's operating conditions

TRP = Transit period

VR = Vacuum Residue

AR = Atmospheric Residue

TAR = De-asphalter Residue

HDON = Hydrogen Donor, often high aromatic diesel stock

VBI = Viscosity Blending Index at 122 °F (50 °C)

CCR= Conradson Carbon Residue in weight percent

API = API degrees

KFC= K-factor (UOP K-factor or Watson K-factor, expressed as an index or a f actor defined in Appendix -1).

SUL = Sulphur content in weight percent

Chapter 3 – Cascade Correlation

Y_{op} i= Observed value of output o from training pattern p

T_{op} = Predicted value of output o from training pattern.

E = Sigmoid activation function used in cascade correlation

σ = The sign of the correlation.

o = Output for each candidate.

W = Weight

Chapter-4 System Profile - Error

ET = A percentage deviation from the original observed value.

Np = is the number of the test sets or samples.

RMS = Root Means Square of Error.

Z = Fitness or cost function

L = Defined as the load factor.

M_P = Mean of the predicted value in a given data set

M_A = Mean of the actual value in a given data set

C_d = The coefficient of the data variability

Chapter – 4 Fuel Oil Blending LP

Z = Profit in US $

W_f = Weight of fuel sold in ton

P_f= Price of the fuel sold in $/ton

d_i = Specific gravity of the component i at 60/60 °F (15/15 °C)

C_i = Cost of the component i in $/ton.

Q_i = Quality of the component i in the blend

Q_b = Quality of the final blend b

Q_s= Specified quality of the final blend b.

ϕ = Define as the fraction factor.

Chapter -5 Sensitivity Analysis

DUR = Dubai crude

LR = Arab Light crude

ILR = Iran Light crude

BLR = Basrah Light crude

IHR = Iran Heavy crude

KWR = Kuwait crude

AMR = Arab Medium crude

AHR = Arab Heavy crude

b = Slop of the linear regression.

Y = Data array (product yield),

X = (CCR) for the number of data points n

n = Number of observations

Chapter 5 – Fuel Oil Stability

SF = Stability factor.

A = Aromatics, in weight percent

R = Resins, in weight percent

S = Saturates, in weight percent

CCR = Conradson Carbon Residues, in weight percent

ASP_{AR} = Asphaltenes weight percent for atmospheric residues,

ASP_{VR}, = Asphaltenes weight percent vacuum residues.

CONV = The process weight percent conversion at 662°F (350°C)

MF_{ij} (j =1,2; i=1,2,....n; n = number of fuzzy subsets.

Appendix -1

FLI = Flash point blending index.

FL = Flash point in Degrees Fahrenheit F.

R = Degrees Rankine = 459.69.

PPI = Pour point blending index.

PP = Pour point in degrees Fahrenheit F.

R = Degrees Rankine = 459.69.

VBI = Viscosity blending index.

cSt = Viscosity in centiStoke at 122 degrees Fahrenheit (50C).

Appendix -2

A = Defined as pre-exponential factor or frequency factor.

Ea = Activation energy, J/mol or calorie/mol

R = Gas constant =8.314 J/mol.K=1.987 calorie/mol.K

T = Absolute temperature, K

Δ_f = Defined as the change in free energy.

Appendix -3

$\in_t$ = Defined as the linear erro.

$\mathbf{d_t}$ = Defined as desired output.

$\mathbf{S_t}$ = Defined as actual output

W = Weight

S*s* = Measurement of the variation in Y.

S*e* = Measure of the variation in X

$\mathbf{Y_k}$ = the estimated value of input

$\mathbf{Y_i}$ = the actual value of input

$\overline{Y}$ = the mean value of input

Appendix -4

Z = Objective function

L = Load factor having an integer with the value of L= 0, or L= 1,

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