THE SYSTEMS ANALYSIS OF AN ETHYLENE PLANT

A thesis submitted for the degree of

Doctor of Philosophy

by

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SUMMARY

This thesis is concerned with the systems analysis of an Ethylene Plant which is central to the operations of the BP Chemicals, Baglan Bay Factory. It describes how systems and techniques were developed in order to analyse the operation of the Plant.

The three main project activities described are:-

i) the development of a plant computer system

ii) the reconciliation of industrial flow data

iii) the modelling of the Cold End section of an Ethylene Plant.

The plant computer system developed for the Ethylene Plant complements and extends conventional information and control facilities. It is demonstrated how the computer system provided valuable assistance during the commissioning of the Ethylene Plant.

Data reconciliation is defined as the resolution of inconsistent raw data in a systematic and objective manner. From an analysis and modelling of the errors in industrial flow data a linear error criterion is shown to be suitable for reconciling such data. This enabled the versatile linear programming technique to be used for data reconciliation. The developed and implemented data reconciliation system for the Ethylene Plant, involving the acquisition, reconciliation, and reporting of flow data, is explained. This system provides management with high quality consistent data upon which to make decisions.

It is demonstrated, through the steady state modelling and simulation of the Cold End of the Ethylene Plant, how systems engineering concepts were applied to a large scale industrial process system. The Cold End is divided into its component sub-systems and those sub-systems which have greatest effect on system performance are modelled. A modular approach characterises the modelling work. This modelling study

is shown to provide an insight into the interactions and basic principles of operation of the Cold End sub-systems and to establish a foundation for future modelling work.

CONTENTS

PREFACE

BP Chemicals International Limited encourage collaboration between Industry and Universities. In 1971, BP Chemicals approached the Chemical Engineering Department of the University of Aston, in Birmingham, with the intention of setting up an industrially based Ph.D project. It was felt that by working together, it would be possible for both sides to capitalise on the rapidly growing expertise in the systems engineering and computer control field.

The No. 2 Ethylene Plant at Baglan Bay, South Wales, was selected as the general area of interest. BP Chemicals regarded the Ph.D project to be of direct benefit to the No. 2 Ethylene Plant and the Baglan Bay Factory as a whole, and also of potential use in the selection, design and operation of existing and future ethylene plants within the Company.

Throughout the Ph.D project, the author was a member of a project group within BP Chemicals, Technical Control Branch, which had responsibility for the development of a computer based information and control system for the Baglan Bay Factory. As the scope of the Ph.D work lay within the terms of reference of this project group, both the project group and the Ph.D project shared common interests. The Ph.D work program was, however, influenced by the priorities of the Factory, the Ethylene Plant and the computer project.

It was inevitable in a Ph.D project of this nature to draw on help and co-operation from individuals and groups associated with the project. Such assistance was recognised and acknowledged throughout the work.

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THE AUTHOR

The author was awarded, in 1965, a BP University Apprenticeship to study Chemical Engineering at the University College of Wales, Swansea. He graduated, in 1968, with a first class honours degree. Under the continued sponsorship of BP Oil he completed, in 1969, a Masters Degree in Systems Engineering at the University of Lancaster. Between 1965 and 1969 he spent periods totalling 18 months working at various BP establishments. In 1969, the author joined Technical Control Branch, BP Chemicals, at London, to work on the Computer Control and Information System for the Baglan Bay Factory. He transferred to Baglan Bay, South Wales, in 1971 and started work on the Ph.D project in September of that year.

INTRODUCTION

The Ph.D project set out to analyse an Ethylene Plant with a view to developing systems and techniques for improving its operation. The Plant, the No. 2 Ethylene Plant, is at the heart of the BP Chemicals Baglan Bay Factory and was commissioned during the Ph.D project. The project was tackled using systems engineering principles and advantage was taken of the availability of a process control computer.

The thesis has been divided into six chapters.

Chapter 1 introduces the project by describing generally the Factory, Plant and Computer Systems with which the project was concerned.

Chapter 2, the systems analysis, examines further these systems and establishes a set of activities for the Ph.D project. These activities are the setting up of a plant computer system, the reconciliation of data from a large scale industrial flow measuring system, and the modelling of a Section of an Ethylene Plant. The development of these activities is described in the subsequent three chapters.

Chapter 3, considers the development of the No. 2 Ethylene Plant Computer System, and its application during the commissioning of the No. 2 Ethylene Plant. The computer system was used to complement and extend existing information and control facilities. Applications of the powerful and flexible calculation, logging and alarming facilities provided by the computer are described, and the acceptance and use of the computer system are discussed.

The reconciliation of data derived from large scale industrial flow metering systems is examined in chapter 4. The chapter contains an analysis and estimation of the errors found in industrial flow data. Various mathematical techniques and criteria for reconciling data are assessed, and the development of a data reconciliation system for the No. 2

Ethylene Complex is described.

Chapter 5 describes how systems engineering was applied to the modelling and simulation of the Cold End of the No. 2 Ethylene Plant. The study was particularly concerned with the examination of the complex energy interaction between the process and refrigeration systems.

The conclusions drawn in Chapter 6 consolidate the major benefits and general points arising from the project.

CHAPTER 1

SYSTEMS DESCRIPTION

CHAPTER 1 - SYSTEMS DESCRIPTION

1.1 INTRODUCTION

Chapter 1 describes the systems within which the Ph.D work was carried out. A brief description is given of the historical development and current status of the Baglan Bay Factory. This Factory, which has an Ethylene Complex at its heart, has become one of the largest and most advanced petrochemical complexes in Europe. The computer control and information system that was designed to meet the requirements of the Factory is explained. The Chapter concludes with a description of the No. 2 Ethylene Complex, which was selected as the main area of interest for the Ph.D project.

1.2 THE BAGLAN BAY FACTORY

Throughout the 1950's petroleum chemicals and their derivatives had a growth rate that was about double the industrial average. This was a world-wide phenomenon which encouraged many major international chemical and oil companies into seeking a share of the market. In 1947, British Petroleum Ltd. and Distillers Ltd., pooled their experience and formed British Hydrocarbon Chemicals (BHC). The first BHC factory, which was built adjoining the BP Refinery at Grangemouth, Scotland, came into operation in 1951. In view of the continued rising demand for petroleum chemicals, BHC decided in 1961 to embark on a major new investment at Baglan Bay. The site offered good road, rail and seaport facilities, good supplies of electricity and water, and close proximity to the BP Refinery at Llandarcy. At Baglan Bay, the first Ethylene Plant of 50,000 tpa capacity came on stream in 1963.

At the beginning of 1967, BP acquired Distillers interests in

BHC and formed BP Chemicals. It was in 1967 that the new petrochemical complex at Baglan Bay was conceived. The expansion, which would make the Baglan Bay Factory one of the largest petroleum chemicals complexes in Europe, was completed in 1973. The new Baglan Bay Complex has been described by Routley (1) as possessing certain special features:-

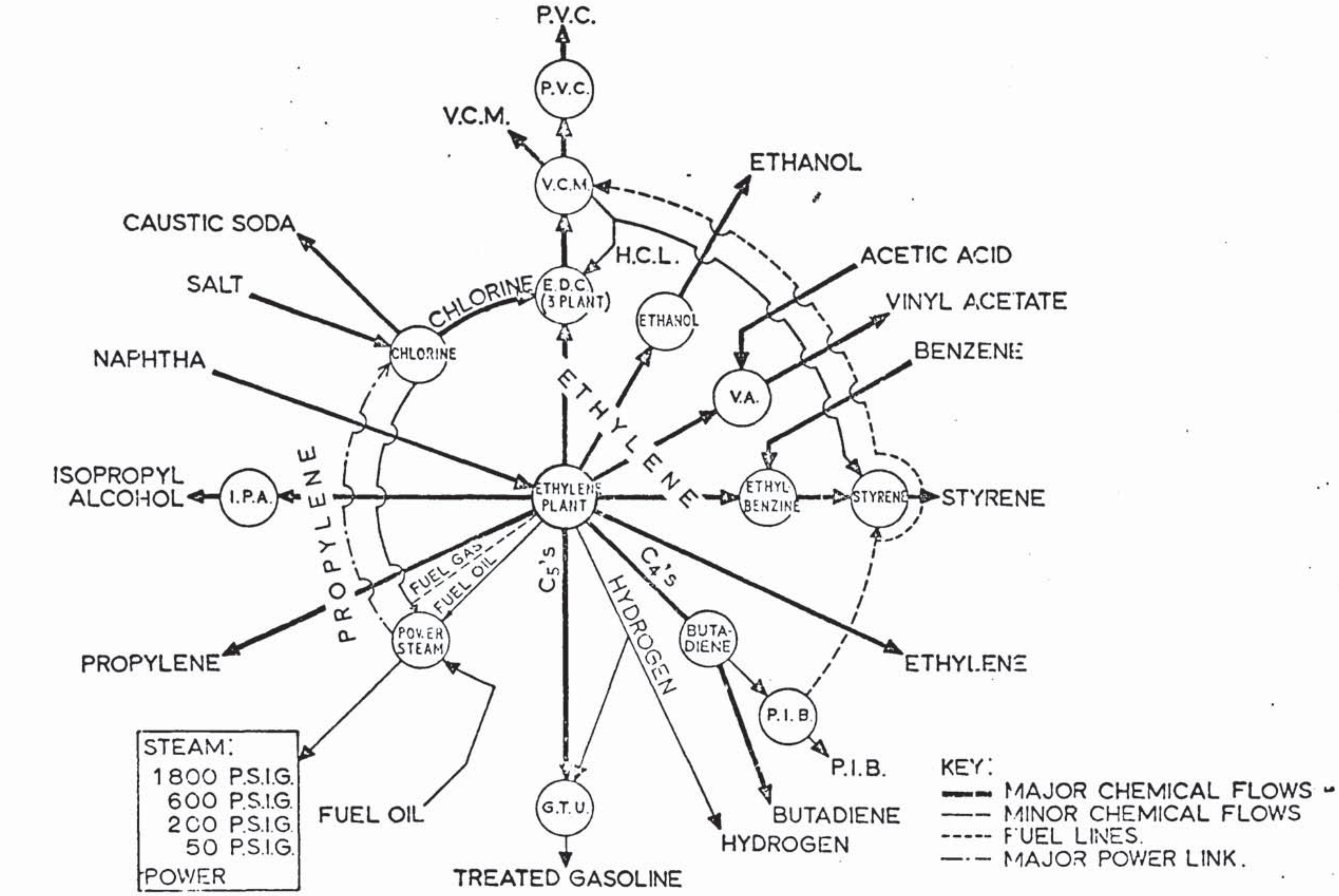
(i) the complex was built and commissioned almost as a single entity.

(ii) it is a highly integrated complex.

(iii) the complex contains a number of processes new to the Factory.

(iv) many of the plants use the most advanced technology.

The Baglan Bay Factory, incorporating the new Complex, is composed of 16 plants. The arrangement of the 16 plants, shown diagrammatically in Fig. 1.1, has been compared (1) with a 'spoked wheel'. At the 'hub of the wheel' is the 340,000 tpa Ethylene Plant backed up by the Power and Chlorine Plants. From the Ethylene Plant radiate nine 'spokes', corresponding to the Ethylene Plant products (e.g. ethylene, propylene, C4's, gasoline, fuel oil, fuel gas and steam), which are further processed to give the final site products. Although fuel gas and steam are not classified as chemical products, they are, as utilities, important Ethylene Plant exports essential to the operation of the downstream plants. The 'radial spokes' of the 'wheel' are further complicated by considerable crosslinking. Not only is there extensive interaction between process and fuel gas streams, as shown in Fig. 1.1, but also between the four different steam pressure levels used on site. The main raw material feedstock to the Factory is naphtha, which is primarily supplied from the nearby BP Llandarcy Refinery, and supplemented by naphtha imported through Swansea Docks. Other major raw materials are salt, benzene, fuel oil and acetic acid. The majority of the 13 final



SIMPLIFIED NETWORK DIAGRAM FOR THE BAGLAN BAY COMPLEX (1973) FIG. 1-1 site products are sold, or used in other BP factories to manufacture plastic and synthetic materials (e.g. P.V.C. is used to make cable sheathing and gramophone records). Gasoline produced by the Gasoline Treating Unit (GTU) is returned to the nearby Llandarcy Refinery. Hence, the Baglan Bay Factory is a complex and highly interactive system.

1.3 THE BAGLAN BAY FACTORY COMPUTER SYSTEM

The complex and highly interactive nature of the new Baglan Bay Factory pointed to the need for more sophisticated control techniques, than those provided by individual contractors, if the site was to be operated as an integrated factory.

A systems study was instigated by Technical Control Branch, BP Chemicals, to determine the preferred control strategy for the Factory. The results of the system study highlighted (1) the need for:-

(i) information from sensing devices which would be reliable, meaningful and readily accessible by all levels of management.

(ii) some form of mathematical aids/models to assist management in decision taking at the supervisory control and production scheduling levels.

The study recommended the installation of a computer control and information system for the Factory. The computer system was aimed at providing:-

(i) automatic data acquisition and processing.

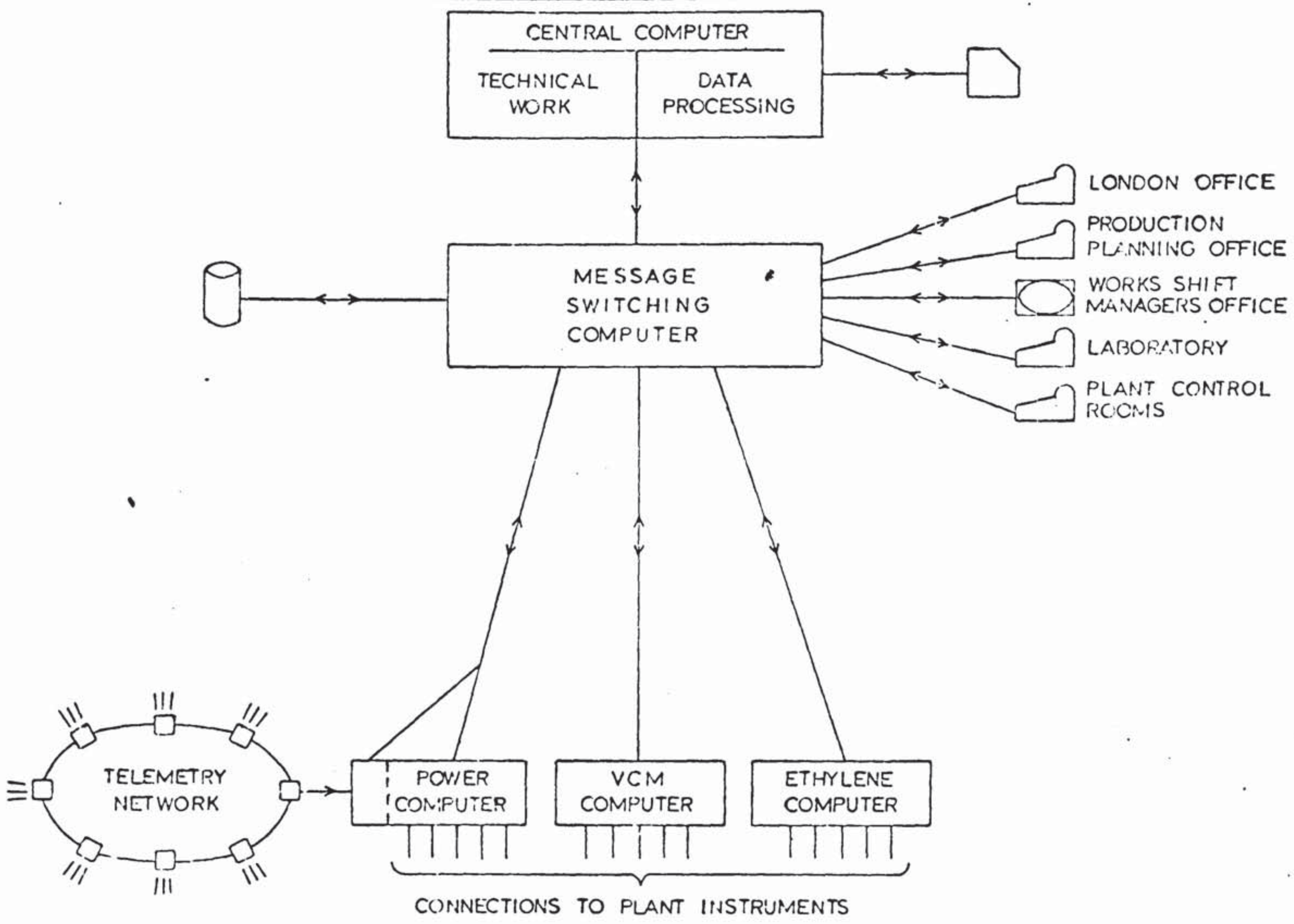
(ii) automatic data transmission and improved data presentation.

(iii) facilities to operate mathematical models to assist management in decision taking.

The design of the system to meet these aims was based on a hierarchical multi-digital computer configuration as shown in Fig. 1.2. It was structured in a modular fashion. The modular concept was deliberately employed to reduce the effect of system failure and to allow proven technology and equipment to be used. This approach was also better suited to meet the commissioning requirements of the Factory. Three Ferranti Argus 500 plant computer systems were installed on the Ethylene, VCM and Power Plants. Their initial role was logging and presentation of local plant data. Supervisory control was planned for a later stage but no DDC control was envisaged, except in special cases where highly non-linear or interactive control loops exist. Conventional analogue equipment is used at Baglan Bay for direct control on all plants.

The three plant computer systems are linked directly to a message switching computer, also a Ferranti Argus 500, which is housed in the main computer suite. Attached to the message switching computer are disc store units on which all relevant data for site control are held. On plants without process computers, automatic data collection is effected by a telemetry network. Information from this network is transmitted to the message switching computer via the Power Plant computer system. Site personnel have access to the information files on the message switching computer discs via teleprinter or visual display unit links located in all plant control rooms plus certain other offices.

Supporting the three plant computer systems and the message switching computer system is the central computer, an ICL 1904A, which is linked into the system via the message switching computer. The central computer, in addition to its commercial data processing commitment, is used for developing and running the models and other supporting technical work required by the plant computers. This hierarchical form of computer system design enables the data storage requirements of the plant



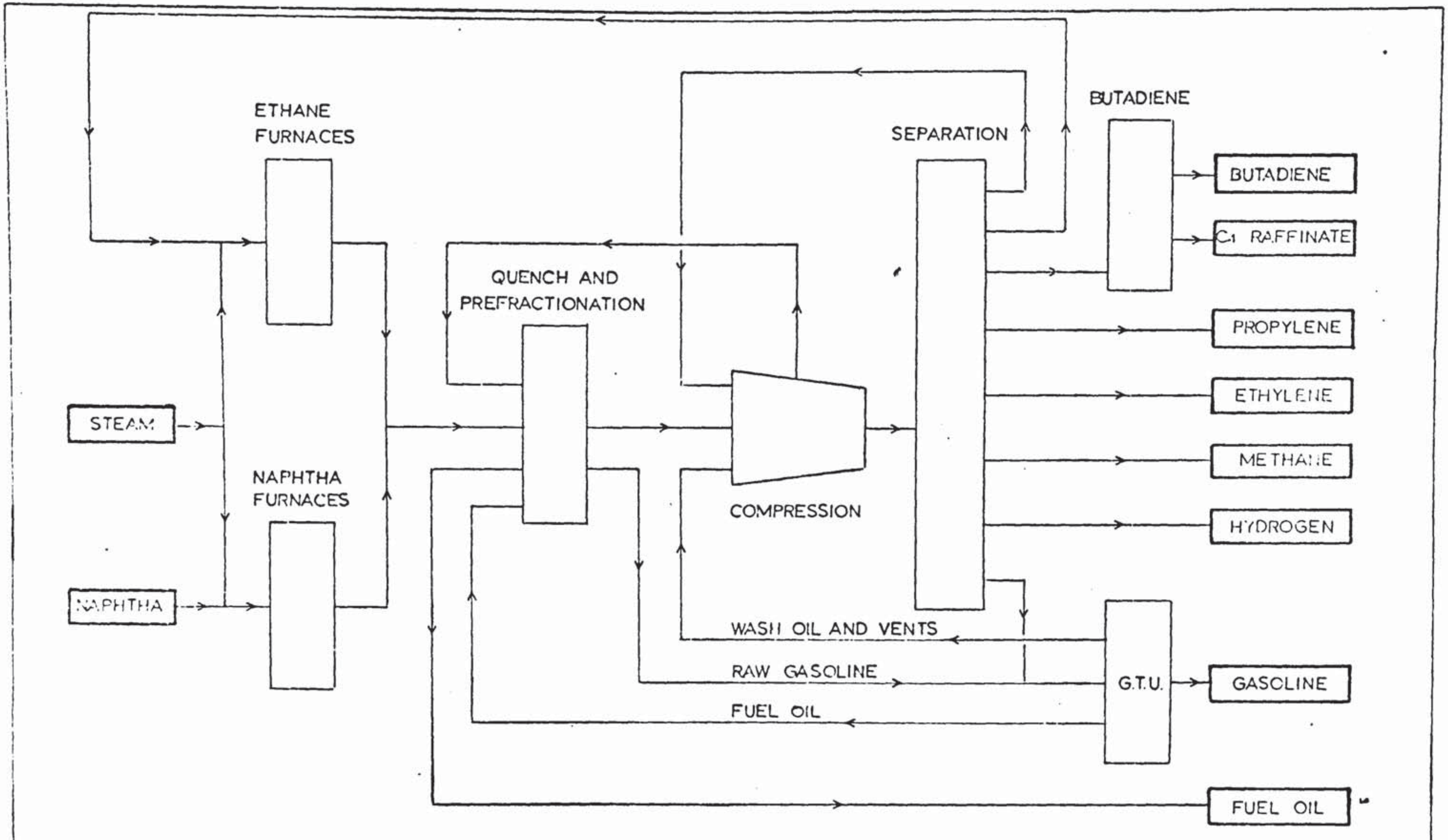
BAGLAN BAY ·FACTORY COMPUTER CONTROL & INFORMATION SYSTEM (FIG 1-2) computers to be kept to a minimum whilst still providing powerful facilities for data storage and modelling applications.

1.4 THE NO. 2 ETHYLENE COMPLEX

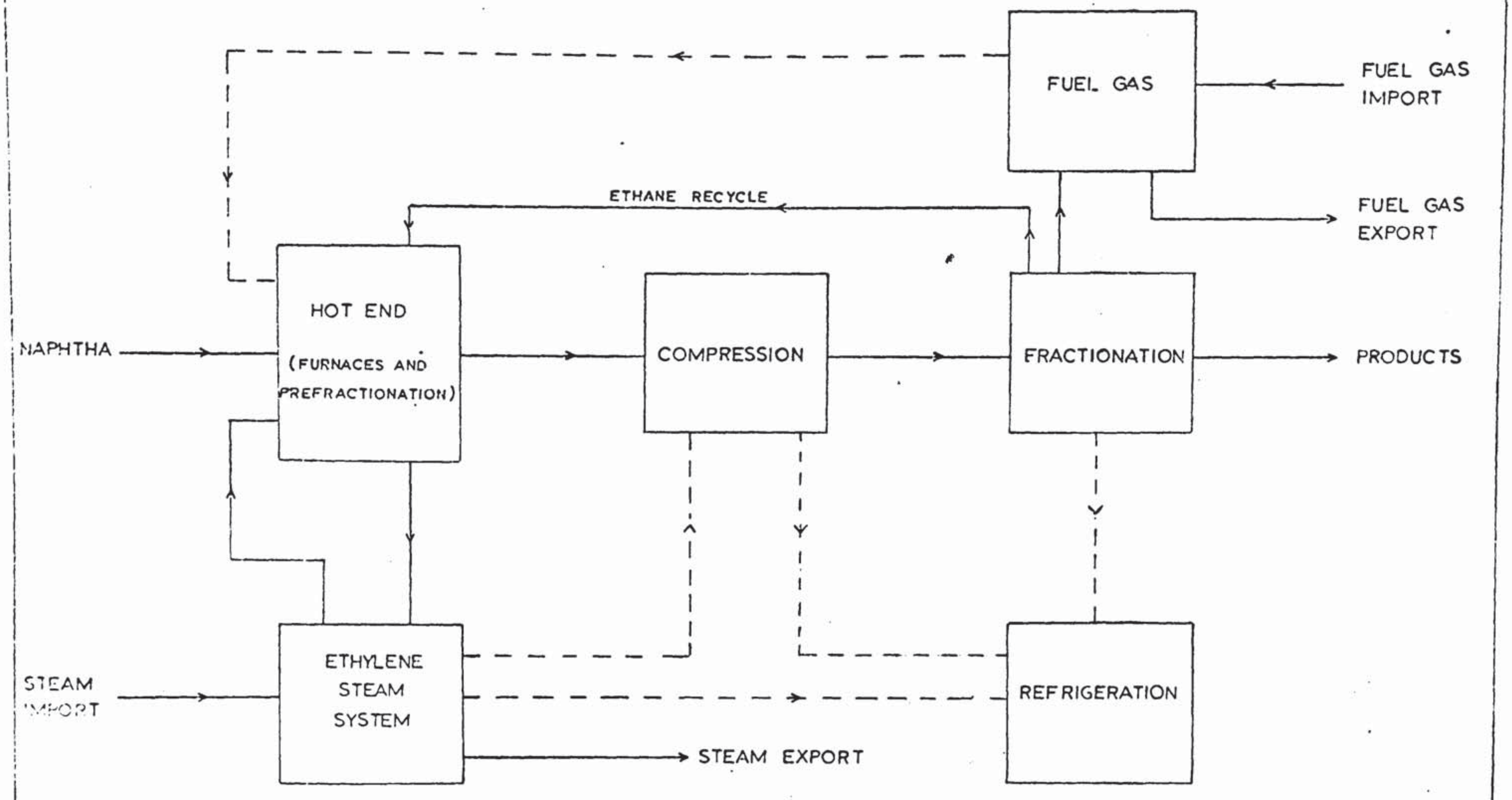
The No. 2 Ethylene Complex, consisting of the Ethylene, GTU and Butadiene Plants, is at the heart of the Baglan Bay Factory and its successful operation is the key to the profitability of the site. The No. 2 Ethylene Complex, which was designed and built by Stone & Webster, can be divided into the following sub-systems:

	SUB-SYSTEM			
i)	Furnace	HOT END	ETHYLENE PLANT	ETHYLENE COMPLEX
ii)	Prefractionation			
iii)	Compression	COLD END		
iv)	Fractionation			
v)	Refrigeration			
vi)	Fuel Gas			
vii)	Steam			
viii)	BUTADIENE EXTRACTION			
ix)	GASOLINE TREATING UNIT			

A simple schematic of the Complex is shown in Fig. 1.3. Fig. 1.4 is a block diagram showing the major material and energy links between the sub-systems of the Ethylene Plant. The furnace and pre-fractionation sub-systems are closely allied and form the 'Hot End' of the Plant. The three remaining sections, compression, fractionation and refrigeration, are inter-related and constitute the 'Cold End' of the Plant. This natural division of the Plant into two major sections is recognised in the management and operation of the Plant. The Fuel Gas



NO 2 ETHYLENE COMPLEX - SIMPLIFIED REPRESENTATION (FIG 1-3)



BLOCK DIAGRAM OF ETHYLENE PLANT SHOWING PRINCIPAL MATERIAL AND ENERGY FLOWS. (FIG 1-4)

KEY.
ENERGY FLOW
MATERIAL & ENERGY FLOW

and Steam sub-systems, although not classified as Ethylene Plant sub-systems, are closely interwoven into the operation of the Plant and the Hot End in particular. The main features of each of the Ethylene Complex sub-systems are summarised as follows:-

i) Furnace

Naphtha feedstock is cracked at high severity in 10 furnaces. High pressure steam is generated in heat exchangers immediately after the furnace exit. Ethane, produced by the naphtha cracking and recovered by the fractionation system, is cracked to produce ethylene, and high pressure steam is again generated.

ii) Prefractionation

The furnace effluent gases are quenched with oil and low pressure steam is generated. The prefractionation section recovers fuel oil and the majority of the raw gasoline from the furnace effluent streams.

iii) Compression

The cracked gas from the prefractionation system and minor recycle streams from the fractionation system are compressed in 4 stages and dried. The compression system is a major user of steam.

iv) Fractionation

The dried gas, cooled against various process streams and by refrigeration, is separated in the distillation train into the following major product streams:-

a) ethylene

b) propylene

c) raw C4's

d) raw gasoline

e) high and low purity hydrogen

C2 and C3 acetylenes are removed in hydrogenation units. Vent streams from the fractionation system are recycled back to the compressors for further recovery. The ethane is recycled to the ethane furnaces.

v) Refrigeration

The refrigeration system, employing ethylene and propylene as refrigerants with cascade cooling, is used to liquefy the cracked gas before fractionation, and provide reflux in the low temperature fractionation system. The refrigeration system, through energy exchange, is closely interlinked with the fractionation system. The refrigerant compressors are a major user of steam on the Plant.

vi) Fuel Gas

The fuel gas system is fed by methane from the fractionation system and supplemented, as required, by imported fuel gas. The fuel gas is used to fire the furnaces and any excess is exported to the Factory. Facilities are provided for the additional make-up of fuel gas from liquid C3's and C4's.

vii) Steam

Steam is used within the Ethylene Complex at 4 pressure levels. The Ethylene Plant generates steam at the highest and lowest pressures, and excess or deficiencies are balanced against the Factory steam systems.

viii) Butadiene Extraction

Butadiene is recovered from the raw C4 stream by extractive distillation using acetonitrile. Butadiene-free raffinate is produced as a co-product.

ix) Gasoline Treating Unit (G.T.U.)

Raw gasoline from the Ethylene Plant is selectively hydrogenated to give a single gasoline product. A side stream is recycled to the Ethylene Plant compressors for use as a wash oil, and refined gasoline is returned to Llandarcy Refinery.

Thus, having described the main features of each of the Ethylene Complex sub-systems, reference to Figs. 1.3 and 1.4 shows how these systems are highly interlinked through both material and energy exchange. The fractionation system provides fuel gas to fire the cracking furnaces of the Hot End, and the Hot End generates high pressure steam to drive the cracked gas compression and refrigeration compressors. The refrigeration system is closely integrated, through energy exchange, into the operation of the fractionation system. Flows are recycled from the GTU plant to the cracked gas compression system and ethane is a major recycle flow from the fractionation system to the Hot End.

1.5 CHAPTER REVIEW

It is evident from the Chapter that the Baglan Bay Factory and Ethylene Complex are highly complex and interactive systems involving advanced technology. A computer control and information system was provided to assist in the effective operation of the Factory. A systems analysis of the Ethylene Plant is described in the next chapter, and activities for the Ph.D project are defined.

CHAPTER 2

SYSTEMS ANALYSIS

CHAPTER 2 - SYSTEMS ANALYSIS

2.1 INTRODUCTION

The need to adopt the principles of systems engineering (2) in the analysis of large scale industrial systems, such as the systems under study, has emerged because of two basic reasons:-

i) Industrial plants have become increasingly complex.

ii) The automatic digital computer has provided the engineer with a tool of immense logical flexibility and computing power.

Systems engineering is not a new activity since its history is rooted in good industrial design practice. However, it emphasises the importance of examining overall system performance. Systems engineering is an orderly and well disciplined way of getting things done.

Characteristic features of the systems engineering approach are:-

i) A thorough investigation and statement of objectives.

ii) The formulation of performance criteria.

iii) The building of quantitative models to describe system performance.

iv) Simulation using the models to reproduce the actual behaviour of the real system to the accepted degree of accuracy.

v) Optimisation of the system.

vi) Implementation of systems study results.

vii) Retrospective appraisal and improved operation of the system.

In the application of systems engineering to specific problems, some of these features have greater or less significance than others. This project was concerned first with establishing the requirements of the systems under analysis. It then, through the application of the systems engineering tools of computers and computer techniques, designed and developed systems to meet these requirements. It was recognised that since the three year period of the project coincided with the construction, commissioning and post-commissioning periods of the No. 2 Ethylene Plant, the project had to respond to the changing demands of such an environment.

This chapter discusses the importance of No. 2 Ethylene Plant operations with respect to the Factory and highlights the key factors that affect such operations. The remainder of the chapter analyses the aims and development of systems that will contribute to the efficient operation of the No. 2 Ethylene Plant and the Factory. The effective use of the Ethylene Plant Computer System is defined. The problem and required solution to reconciling data from a large industrial flow measuring system are introduced. The need for a steady state computer model of the Cold End of the Ethylene Plant is discussed.

2.2 NO. 2 ETHYLENE PLANT OPERATIONS

The successful operation of the No. 2 Ethylene Plant is essential to the profitability of the Baglan Bay Factory. The No. 2 Ethylene Plant represents a large capital investment. There is a large increment between the values of feedstock and products, with ethylene, propylene and butadiene several times as valuable as naphtha feedstock.

Optimal operation of the No. 2 Ethylene Plant can be achieved by maximising:-

i) on-stream time of the plant

ii) plant throughput

iii) utilisation of ethylene and co-products as high value chemical feedstocks, as against low value fuel gas.

Whitehouse (3) identified the major factors affecting the operation of the Ethylene Plant as being:-

i) the scheduling and operation of the naphtha and ethane furnaces. Because of coke formation the furnaces have to be taken off stream periodically.

ii) the complex inter-relationships between sections of the plant. These include the effect of the refrigeration system on the fractionation and compression systems of the plant, and the effect of different cracking conditions on compressor capacity.

iii) planned and unplanned shutdowns on sections of the Plant which cause reduction of throughput and pose differing capacity constraints, e.g. partial loss of propylene refrigeration system capacity due to failure of a propylene refrigerant compressor.

iv) planned and unplanned disturbances on the Baglan Bay Factory leading to major short-term changes in the required product pattern. For instance, a plant such as the Ethanol Plant consuming ethylene might get into difficulties. If the Ethylene Plant is producing maximum ethylene, the short term loss in ethylene demand will affect the economic operation of the Ethylene Plant. It might become profitable to alter plant conditions to produce maximum propylene for the duration of the Ethanol Plant upset.

v) changes in naphtha feedstock quality which will lead to changed product patterns and demand changes to furnace conditions.

With these factors in mind, it can be appreciated that the efficient operation of the No. 2 Ethylene Plant depends on relating the operation of one part of the Plant to the Ethylene Complex and Factory as a whole, and then taking action in the context of the whole. To achieve such operation it is essential to be able to monitor and control plant performance accurately.

2.3 NO. 2 ETHYLENE PLANT COMPUTER SYSTEM

The acquisition and utilisation of reliable information for the monitoring and control of a plant of the size and complexity of the No. 2 Ethylene Plant are formidable problems. They can be solved by the effective use of an on-line plant computer system. The computer system can be used to:-

i) automatically display and log plant measurements.

ii) provide flexible and comprehensive alarm facilities.

iii) perform arithmetic and logical operations on plant measurements to enable key performance indices and summaries of plant performance to be produced as required.

iv) implement direct control or supervisory control of the plant.

On-line plant computer systems have been successfully used to effect improved control of large Ethylene Plants (4).

A recommendation (3) was made to install a process control computer on the No. 2 Ethylene Complex as part of the Baglan Bay computer control and information system.

The Ethylene computer system was to be installed in parallel with the conventional analogue recording and control equipment. This was to ensure that any unforseen problems with the computer system did not affect the commissioning of the No. 2 Ethylene Plant. The role of the computer system was to complement and extend the conventional control and information facilities. This arrangement was seen to have one major disadvantage. Since the initial operation and control of the plant were not dependent on the availability of the computer system, the acceptance and use of the system might prove more difficult to establish. The Ethylene computer system was to be developed in stages. Initially the computer system would be concerned with data logging and information reporting, but it was ultimately intended to extend its function to supervisory control of the plant.

As the commissioning of the No. 2 Ethylene Plant fell within the timescale of the Ph.D project, the objectives of the plant computer system over this period were defined as:-

i) the establishment of a reliable computer data acquisition system.

ii) the effective application of the computer system during plant commissioning.

To meet these objectives the following tasks were defined:-

i) to check rigorously the performance of the computer hardware and software as supplied by the computer manufacturer.

ii) to perform comprehensive checks on all plant signals to the computer.

iii) to prepare technical software to complement and extend conventional control and information facilities.

iv) to ensure that personnel were adequately trained in the use of the computer system.

v) to provide guidance and help to users of the plant computer system and generally promote the computer system facilities.

The development and application of the plant computer system are discussed in Chapter 3 of the thesis.

2.4 DATA RECONCILIATION

Accurate and reliable plant data are required to enable management to monitor the performance of plants. Such data are also needed for the maintenance of production records, and as input data to any mathematical models which will assist decision-taking,

At Baglan Bay there has been an attempt to ensure that high quality and reliable data are available from key points across the Factory. Instrumentation was installed of higher quality, than has hitherto been necessary, together with additional instrumentation to provide back up information for cross checking purposes. The acquisition of this information is accomplished by the Factory on-line computer system. On the No. 2 Ethylene Complex approximately 630 inputs are monitored by the computer system. These include some 120 flows which are required for plant section and battery limit accounting. Although particular care has been taken to ensure that the flow data from instruments are reliable and accurate, it is inevitable in a large scale industrial flow measurement system that data inconsistencies will occur. Such inconsistencies will arise due to a number of reasons, such as instrument faults and human errors. At Baglan Bay, where the volume and value of flow data have considerable significance, there is need for an automatic method for reconciling such data and being able to produce rational material balances across the Factory.

An example of the kind of situation that can arise due to inconsistent data is demonstrated by considering the situation shown in Fig. 2.1. Plant A produces material X which is either consumed by user plants B, C and D or sent to storage. On a typical day plant A claims to have produced 980 tonnes of X, whereas the user plants claim to have consumed 786 tonnes between them with 94 tonnes sent to storage. This leaves 100 tonnes of X unaccounted for.

The situation suggests a number of alternative explanations:-

a) One, or maybe more, of the user plants are receiving more X than they have monitored.

b) Plant A is producing less of X than it claims.

c) Material X is being lost from the system (i.e. through leakages, tank losses etc.).

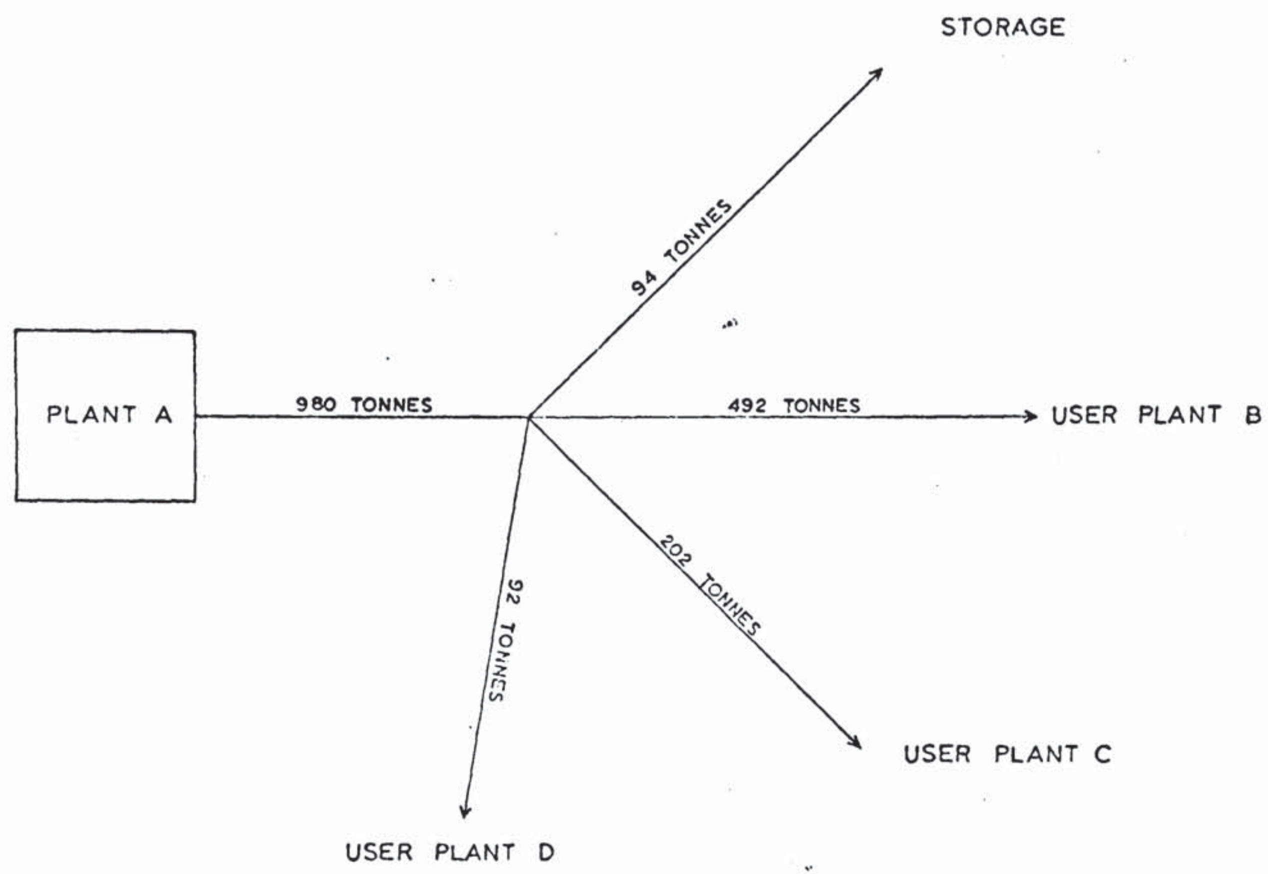
d) A combination of (a), (b) and (c).

A consistent and systematic procedure is required to solve this problem that will examine all the flow and level measurements taking into account the relative accuracies of the measuring devices.

The name 'data reconciliation' has been used to define a particular form of activity at Baglan Bay. To clarify the meaning and context of data reconciliation and associated terms used in the thesis, the following definitions are introduced:-

Data Reconciliation

Is the resolution of inconsistent raw data in a systematic and objective manner.



DATA RECONCILIATION EXAMPLE - UNRECONCILED FLOWS (FIG 2-1)

Data Reconciliation Technique

Is the mathematical technique used to reconcile the raw data.

Data Reconciliation Error Criterion

Is the criterion used by the data reconciliation technique to reconcile the raw data.

Automatic Data Reconciliation

Makes use of a computer in the application of the data reconciliation technique.

Data Reconciliation System

Involves the collection, checking, reconciliation and reporting of data.

In consideration of the selection of a data reconciliation technique for reconciling data obtained from a large scale industrial flow system, such as found at Baglan Bay, the following requirements were defined. The technique should:-

i) attempt to produce a reconciled set of data that is more correct (i.e. closer to the true data) than the unreconciled raw data.

ii) ensure that the material balances are satisfied and that the reconciled data are technically meaningful (e.g. material balances should not be satisfied by reversing the direction of uni-directional flows).

iii) take account of the accuracies of the various measurements when reconciling the raw data.

iv) attempt to identify which measuring instruments are in error.

v) attempt to locate sources of unmeasured material loss in the system and provide estimates of the magnitude of the losses.

vi) be computationally efficient and reliable.

vii) be capable of handling all relevant data.

Chapter 4 analyses the errors found in industrial flow data and establishes a data reconciliation technique and error criterion that satisfy the above requirements, and are thus suitable for reconciling data from large scale industrial flow measuring systems. The application of the technique to the reconciliation of data from the No. 2 Ethylene Complex is described. The No. 2 Ethylene Data Reconciliation System forms a major part of the Baglan Bay Factory Data Reconciliation System.

2.5 ETHYLENE PLANT MODELLING AND SIMULATION

2.5.1 General

The highly interactive nature of the Baglan Bay Factory makes it important to ensure that decisions taken in one part of the Factory are not taken without consideration of the remainder of the Factory. A need was recognised (1) for some form of mathematical aids/models to assist management in decision-taking at the supervisory control and production scheduling levels.

Five major reasons why the operation of the No. 2 Ethylene Plant would benefit from the building of quantitative models are:-

i) the large tonnage and cash throughput of the plant.

ii) the range of co-products.

iii) the necessity for the integration of the individual unit operations e.g. naphtha and ethane furnaces with compressor capacity.

iv) the necessity to match production levels and patterns with product demands.

Wider benefits from the application of such models would be in selection, design, and operation of existing and future Ethylene Plants.

A steady state computer model which simulates the operation of the Ethylene Plant was seen to be the vehicle by which supervisory control could be achieved. From this comprehensive steady state model, simple regression models could be developed which could be used to cater for the hour by hour control of the plant. Supervisory control would be implemented using the Factory and Plant Computer Systems.

In consideration of the scope of any modelling work, the confidential nature of the Ethylene Plant cracking furnace design and operation precluded any analysis of the furnace system from forming a part of the Ph.D project. This left six other potential areas of the Ethylene Plant available for detailed analysis:-

i)	Prefractionation	
ii)	Compression	)
iii)	Fractionation	) COLD END
iv)	Refrigeration	)
v)	Fuel Gas	
vi)	Steam	

The prefractionation, steam and fuel gas systems are closely linked to the furnace area. It was decided that any detailed analysis and modelling of the Ethylene Plant, for the purpose of the Ph.D project, would be devoted to the three systems (i.e. compression, fractionation and refrigeration) constituting the Cold End. The high degree of inter-linking between these three systems necessitates an examination of their combined performance. It is important to achieve optimal operation of the Cold End since the complexity of Cold End design makes any capacity up grading of the initially designed and installed system extremely difficult and costly. The development of a model of the Hot End of the

Ethylene Plant was the responsibility of another member of Technical Control Branch.

2.5.2 Cold End Modelling and Simulation

The Cold End of the Ethylene Plant achieves its separation of cracked gas products by first compressing the gas, and then subjecting it to a series of fractionations. The physical properties of the cracked gas products demand high pressures and low temperatures to achieve such separations. High pressures are produced by the cracked gas compression system and a cascade propylene/ethylene refrigeration system is employed to produce low temperatures.

2.5.2.1 Cracked Gas Compression System

The cracked gas compression system represents the main material link between the Hot End and the fractionation system of the Cold End (Fig. 1.4). It also has some energy exchange with the propylene refrigeration system. The modern trend on ethylene plants has been to install a large single compressor train, since centrifugal compressors have proved reliable. However, on the No. 2 Ethylene Plant, a decision was taken to install a parallel train of centrifugal compressors due to special circumstances of location and history - i.e. in event of failure of the No. 2 Ethylene Plant there exist no alternative sources of ethylene plant products near Baglan Bay; and, at the time that the process design of the plant was being finalised, the performance of certain large centrifugal compressor installations were open to question.

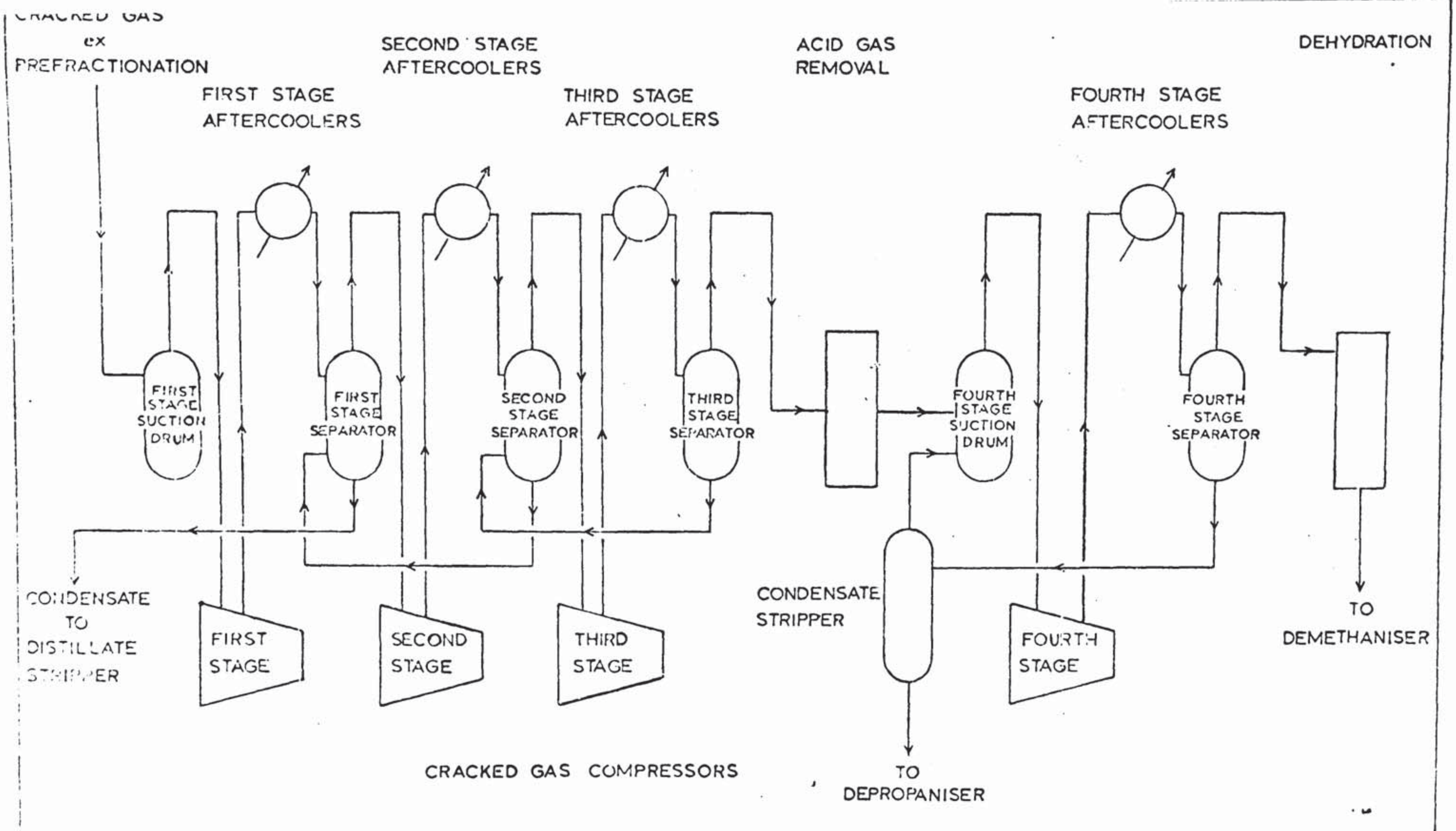
During the compression of the cracked gas, condensation of the heavier hydrocarbons and water occurs between the compression stages. The gas discharging from each compression stage is cooled in aftercooler heat exchangers and flows to a separator, where the condensed water and hydrocarbons are removed, and are flashed back into the lower pressure separators. (See Fig. 2.2). The uncondensed vapours are passed to the next compression stage. Too high an interstage temperature will result in insufficient of the heavier components being removed from the cracked gas. This will inefficiently load the next compression stage. Conversely, too low an interstage temperature will remove excess of the light components from the cracked gas and inefficiently load the previous compression stage. Therefore, judicious selection of cracked gas interstage temperatures is important in the efficient operation of the cracked gas compression system.

A steady state computer model of the compression system can be used to examine the effect of different interstage temperatures on compression system performance. A computer model is appropriate since the compression system is characterised by recycle streams making an iterative form of solution necessary.

2.5.2.2 Refrigeration and Fractionation Systems

The cascade propylene/ethylene refrigeration system employs different levels of refrigerant, analogous to conventional steam utility systems which have steam available at various pressures and temperatures. The Ethylene Plant has been designed such that the refrigeration system should respond to, and meet, the changing energy requirements demanded by the process systems. This position will prevail until refrigeration capacity becomes limiting. Under this situation, the refrigeration system will become the dominant system and will strongly influence plant performance.

Zdonik et al (5), in their review of Ethylene technology, regard the refrigeration system of an Ethylene Plant as very important, since it represents a large part of the plant investment, and its



CRACKED GAS COMPRESSION SYSTEM (FIG 2-2) continuous and efficient operation is essential to the best performance of the plant. They consider the principal design aspects[1] of the refrigeration system as:-

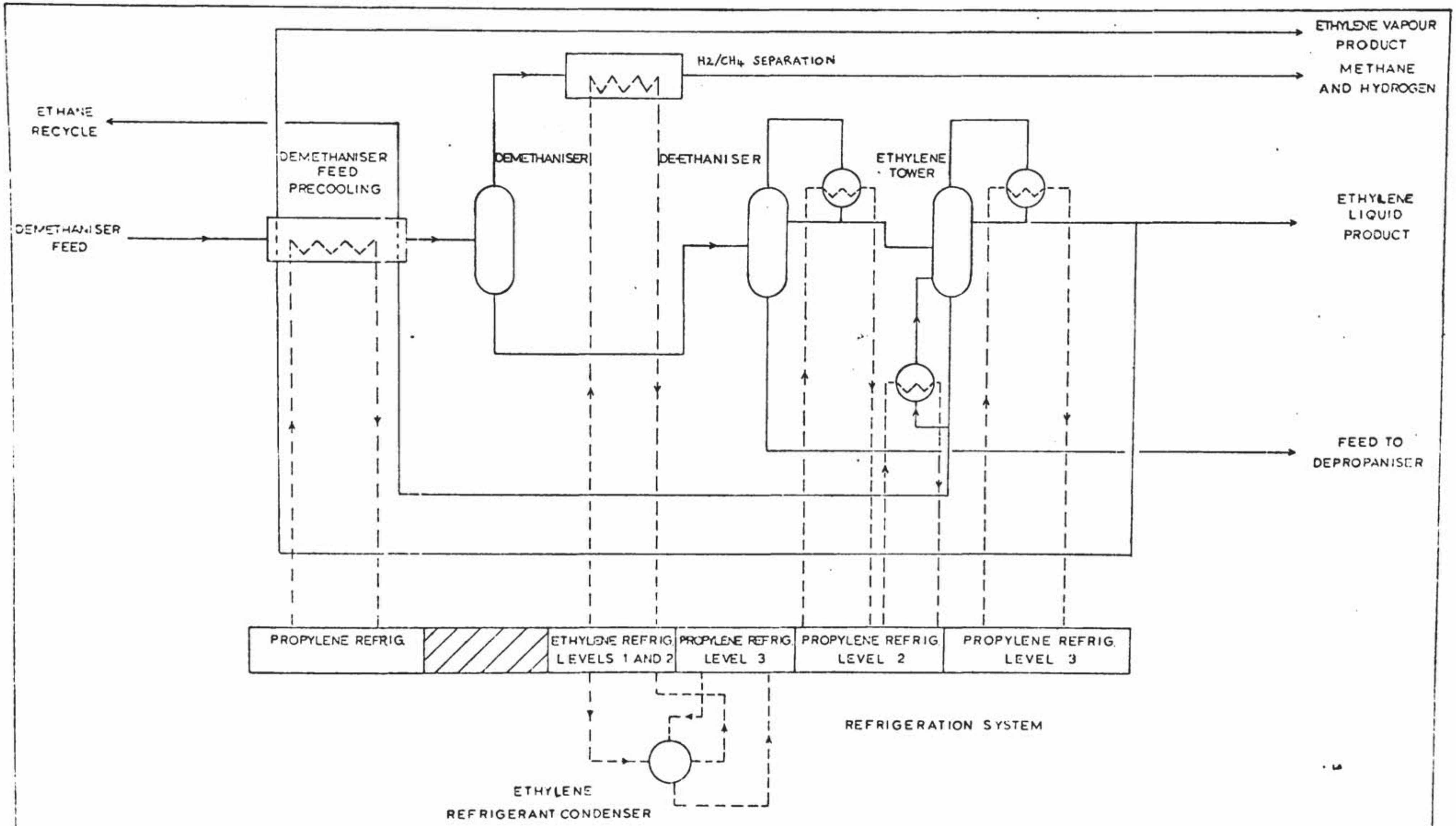
i) economy of operation.

ii) flexibility with respect to change in load resulting from variations in quantity and composition of the plant feedstock.

iii) automatic adjustment to normal changes in coolant demand.

Plant investment costs and operating costs are closely related to the installed compressor horsepower. Zdonik et al comment that it is not expedient to have the refrigeration system too closely integrated with the process system. Although such close integration may reduce the theoretical compressor horsepower, it will usually result in a sacrifice of plant flexibility. In such instances, an upset in one part of the fractionation recovery system is transmitted through the system, and due to the interlocking of too many process sections, the restoration of normal operating conditions will require considerable time and will cause loss of production.

A preliminary examination of the Cold End systems suggests that the key to the efficient operation of the Cold End lies in the understanding of the complex energy interactions between the refrigeration and process fractionation systems. An appreciation of the high degree of energy interaction between the process and refrigeration systems can be gained by reference to Fig. 2.3, which is a schematic showing the major process fractionation units that use refrigerant with the refrigerant flows interwoven amongst the process flows. The figure shows how different temperature levels of refrigerant are used at different stages in the process.



SCHEMATIC DIAGRAM SHOWING MAJOR INTERACTIONS BETWEEN FRACTIONATION AND REFRIGERATION SYSTEMS (FIG 2-3)

KEY
—— PROCESS FLOWS
– – – REFRIGERANT FLOWS

A steady state computer simulation model will enable one to assess and predict the effect of process changes on the refrigeration system and vice versa.

The fractionation system modelling should primarily be concerned with establishing the fractionation system energy demands on the refrigeration system.

The modelling and simulation of the Cold End is described in Chapter 5.

2.6 CHAPTER REVIEW

The Chapter, after discussing the important factors affecting Ethylene Plant operation, identified three major Ph.D project activities that would contribute to the efficient operation of the Ethylene Plant and Baglan Bay Factory. These activities were the development and application of the Ethylene Plant Computer System, the reconciliation of flow data, and the computer modelling and simulation of the Cold End of the Ethylene Plant. The objectives of the Plant Computer System and the tasks required to meet these objectives were stated. The need for reconciling data was discussed and the requirements of a technique to reconcile mass flow data at Baglan Bay were specified. Finally, reasons for modelling the Cold End were established and general features which characterised its performance were discussed.

The following chapters describe the development of each of these main project activities.

CHAPTER 3

NO. 2 ETHYLENE PLANT COMPUTER SYSTEM

CHAPTER 3 - NO. 2 ETHYLENE PLANT COMPUTER SYSTEM

3.1 INTRODUCTION

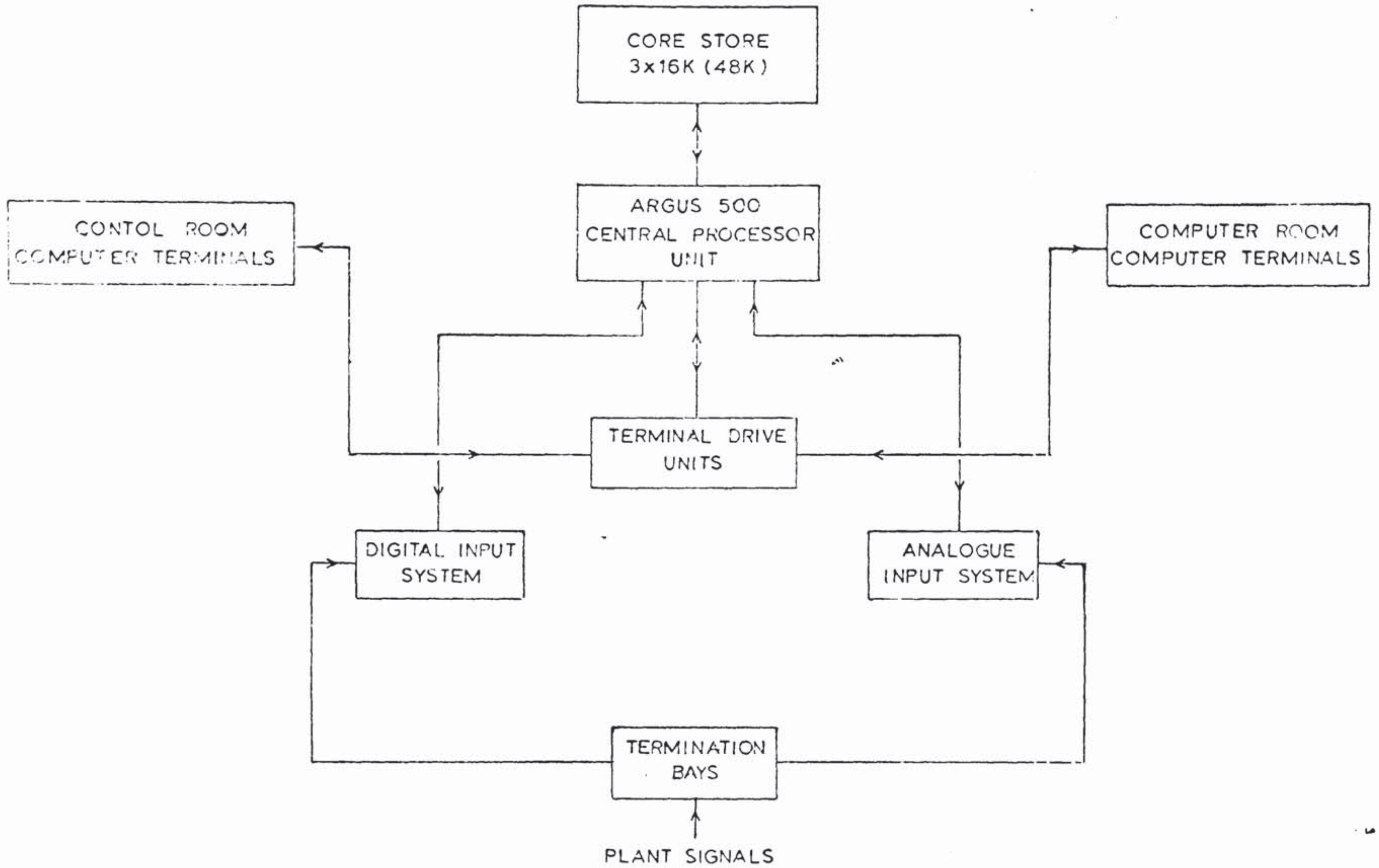
Chapter 3 describes the development and application of the No. 2 Ethylene Plant Computer System. The objectives of the computer system and the tasks defined to meet these objectives were defined in the previous chapter.

The chapter begins with a description of the principles and main features of the Ethylene Plant Computer System. Special purpose terminology defined by the computer manufacturer and used to describe computer system facilities, is introduced. This terminology is referred to in the subsequent sections of the chapter. The important activities of preparing and developing the computer system are discussed. It is upon these activities that the successful application of the computer is based. The role of the computer system during the pre-commissioning and commissioning of the Ethylene Plant is described and the chapter ends with an evaluation of the success of the computer system.

3.2 DESCRIPTION OF NO. 2 ETHYLENE PLANT COMPUTER SYSTEM

The No. 2 Ethylene Plant Computer System basically consists of a Ferranti Argus 500 computer with a Ferranti Consul R control software package. The computer system has 48K of core store and provides, in its present form, comprehensive data logging, alarming and calculation facilities. It has the potential to be used for direct digital or supervisory control of plant operations. Detailed descriptions of the Ethylene Plant Computer System are given in (6,7) and a simple schematic of the computer system is shown in Fig. 3.1.

The Ethylene Plant Computer System is concerned with the:-



ETHYLENE PLANT COMPUTER SYSTEM SCHEMATIC (FIG 3-1)

i) acquisition of basic plant data.

ii) processing of data.

iii) outputting of derived and basic data.

Before discussing the important features of each of these functions, the scope of the Ethylene Computer System will be described.

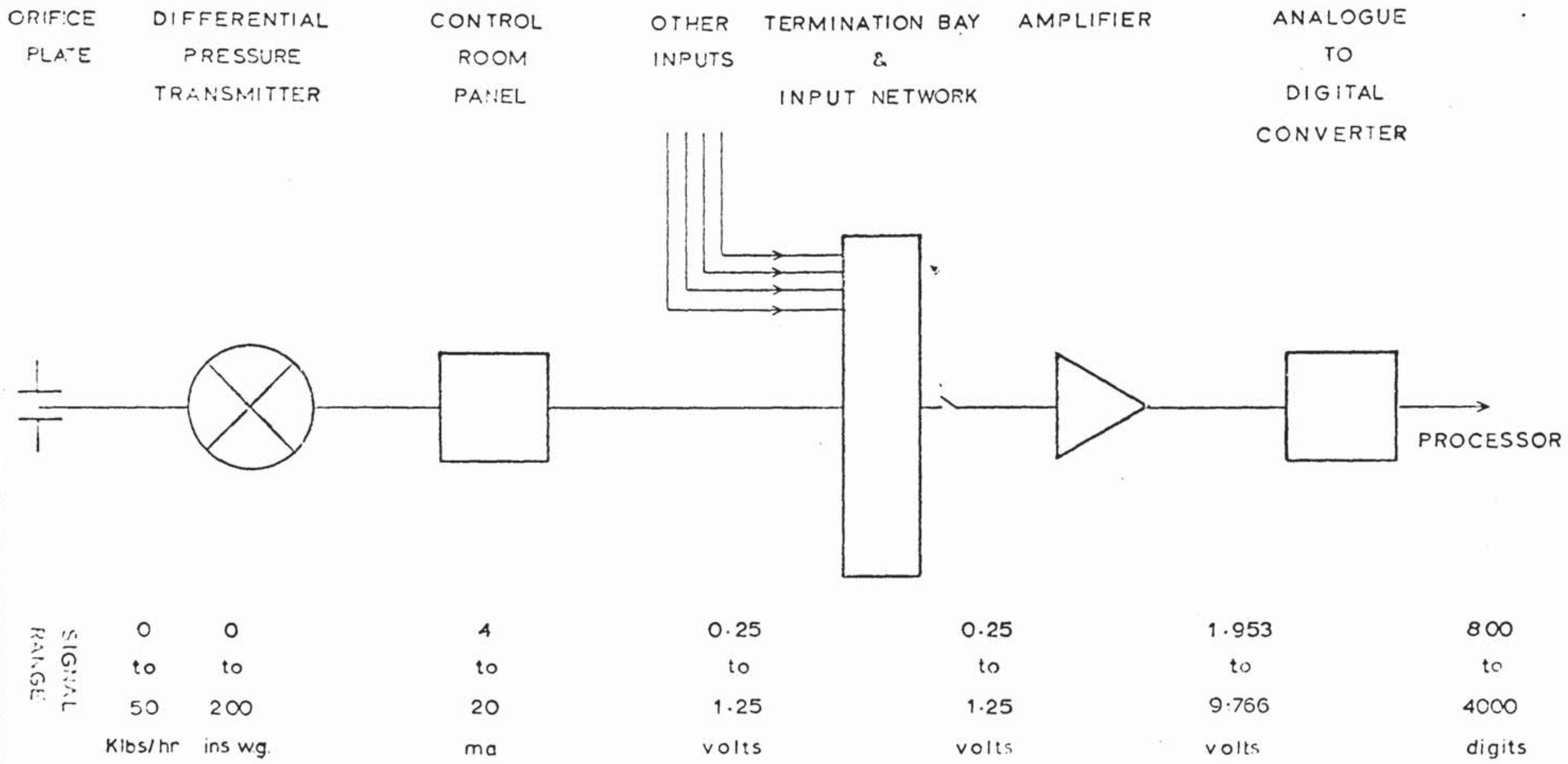
3.2.1 Scope of System

The No. 2 Ethylene Plant Computer System serves the Ethylene, Butadiene and GTU Plants. Computer inputs are taken from some 630 instruments, (Ethylene 540, Butadiene 70 and GTU 20) which include orifice plate flow meters, thermocouple and resistance thermometers, and on-line analysers. The choice of inputs was based on the requirements of the system for accounting, scheduling and control of certain key areas of plant. For the Ethylene Plant most plant sections were comprehensively covered, whereas on the GTU Plant only battery limits streams were selected. On the Butadiene Extraction Plant key flows, temperatures and all on-line analysers are input to the computer system.

3.2.2 Acquisition of Data

The acquisition of plant data is performed by the computer analogue and digital input systems. The computer analogue system is concerned with the transmission of primary signals from the plant instruments, their subsequent hardware filtering to remove signal noise, and their conversion into digital values. Fig. 3.2 traces the path of an analogue signal from an orifice plate flow meter to its conversion to a digital value in the computer.

Process signal inputs arrive at the computer directly from the plant instruments, or indirectly via the main control room instrument panel Fig. 3.3. The inputs direct from the plant are generally



DIAGRAMMATIC REPRESENTATION OF INSTRUMENT SIGNAL TRANSMISSION

(FIG 3-2)

'low level' signals (i.e. less than 100 mv) whereas the inputs via the control room instrument panel normally exist as 'high level' signals (0-1.25v). Whenever convenient, signals have been taken from the control room panel recorders and controllers to reduce cost. Most temperature inputs are direct from the plant. As resistance thermometers are fundamentally more accurate than thermocouples, resistance thermometers have been used below 750^{o}F and thermocouples above this temperature. This has meant that on the Ethylene Plant, thermocouples have been used on the Furnace Section and resistance thermometers elsewhere. Bridge circuits for the resistance thermometer sensors direct from the plant are located in the computer termination bays (Fig. 3.3). In designing the computer analogue input system particular attention was paid to signal noise rejection in the cabling.

Digital inputs to the computer digital input system are of two main types - pulse frequency inputs and digital logic inputs. Pulse frequency inputs originate from positive displacement and turbine flow meters, whereas digital logic inputs of the isolated contact type are used for detecting stream and component signals from on-line analysers.

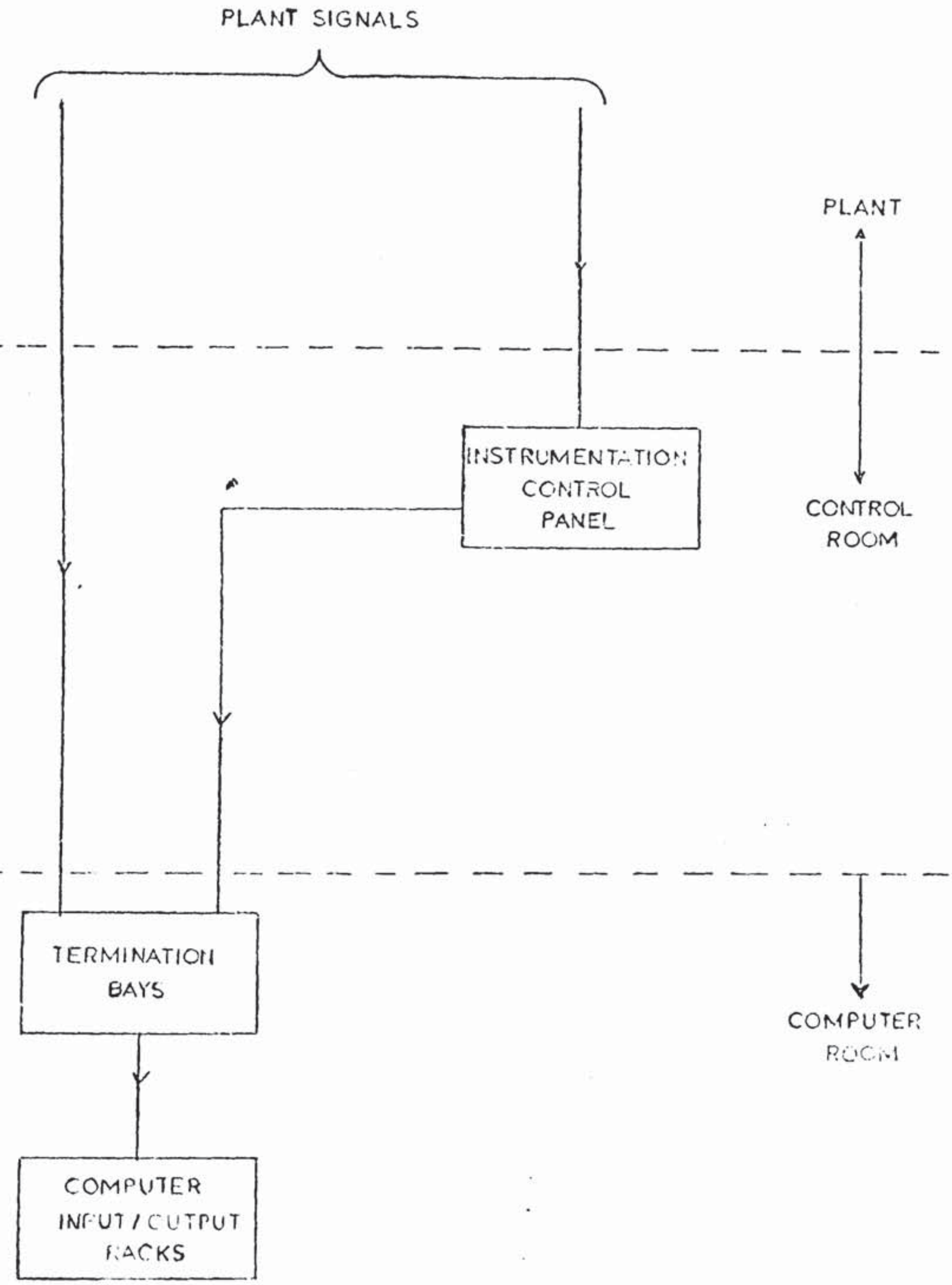
3.2.3 Processing of Data

The processing of plant data is accomplished in two stages:

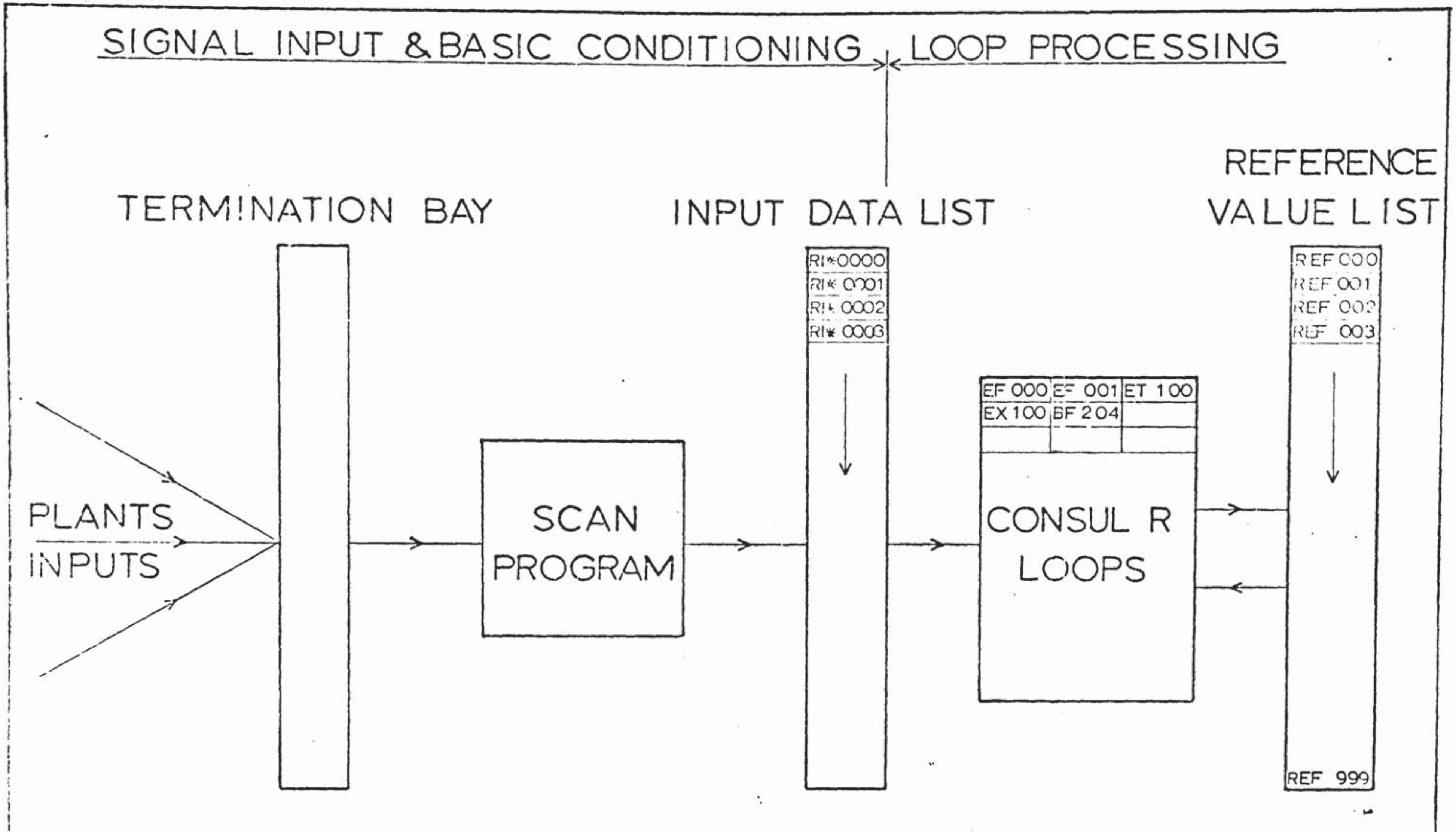
i) Basic Conditioning

ii) Consul R Processing

The first stage provides numerical values proportional to the plant measurements; the second stage converts these values into meaningful engineering quantities and further processes them as required. These stages are shown schematically in Fig. 3.4.



COMFUTER / PLANT INTERFACE (FIG 3-3)



DIAGRAMMATIC REPRESENTATION OF PROCESSING OF DATA (FIG 3-4)

i) Basic Conditioning

Basic conditioning is performed by analogue and digital scan software programs in conjunction with the analogue and digital input systems. The programs control the scanning and initial storage of the computer inputs in the input data list (Fig. 3.4), and carry out any basic signal conditioning that is required. Scan rates may vary from 0.5 to 64 seconds for each plant signal and are determined by the nature and use of the signals. Flows and pressures are normally scanned every 4 seconds and temperatures every 16 seconds. The analogue scan program contains subroutines that perform basic signal conditioning facilities. These facilities include a smoothing subroutine to remove signal noise; a linearisation subroutine which is used to scale thermocouple and resistance thermometer signals; and a square root subroutine which is used to square root the signals from differential pressure type flowmeters.

ii) Consul R Processing

The basic building blocks of the Consul R software are modular program subroutines called Loops. Consul R loops are identified by five character codes. The loop identification codes on the Ethylene Plant Computer System were designed to correspond to the measurement type and plant section with which the loops are associated. For instance, EF100 is flow loop 100 on the Ethylene Plant; BT123 is temperature loop 123 on the Butadiene Extraction Plant.

Loops can be sub-divided into recursive program macros called Algorithms. There exist 26 different algorithms in the Consul R software ranging from algorithms that perform simple arithmetical functions, such as adding the values of two computer inputs, to process control algorithms that simulate the control action of conventional three term controllers.

Loops are classified into 2 types:-

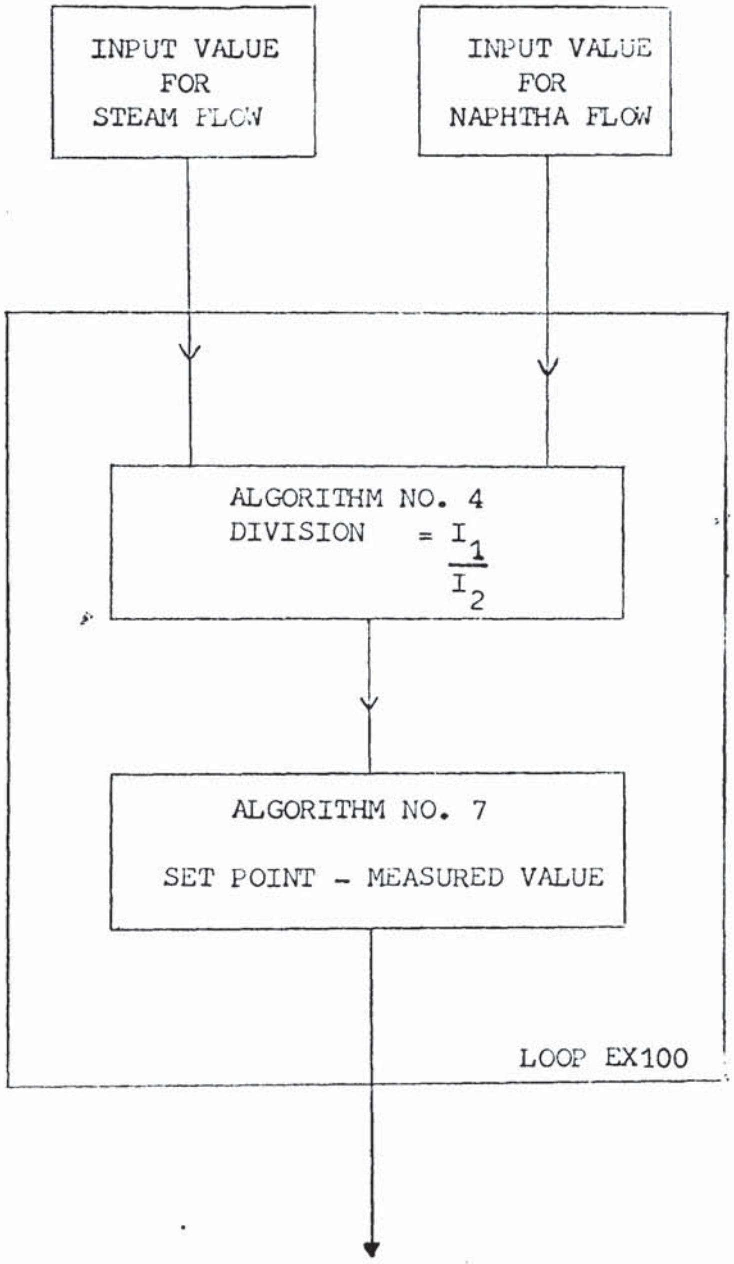
a) Read Only Loops which do no calculations but contain the equivalent of a display algorithm. All basic plant inputs are displayed through use of Read Only Loops.

b) Calculation Loops which perform arithmetical and logical operations on plant inputs stored in the computer. An example of how a calculation loop is constructed is shown in Fig. 3.5. This loop calculates the steam to naphtha flow ratio of a naphtha furnace. The loop identity is EX100. The loop contains the division algorithm (Alg. No. 4) and the set point/measured value algorithm (Alg. No. 7). This latter algorithm is necessary to display and put alarm limits on the output of the loop.

The frequency with which a loop calculation is executed can be specified to be in the range of 0.5 to 64 seconds.

3.2.4 Access and Output of Data

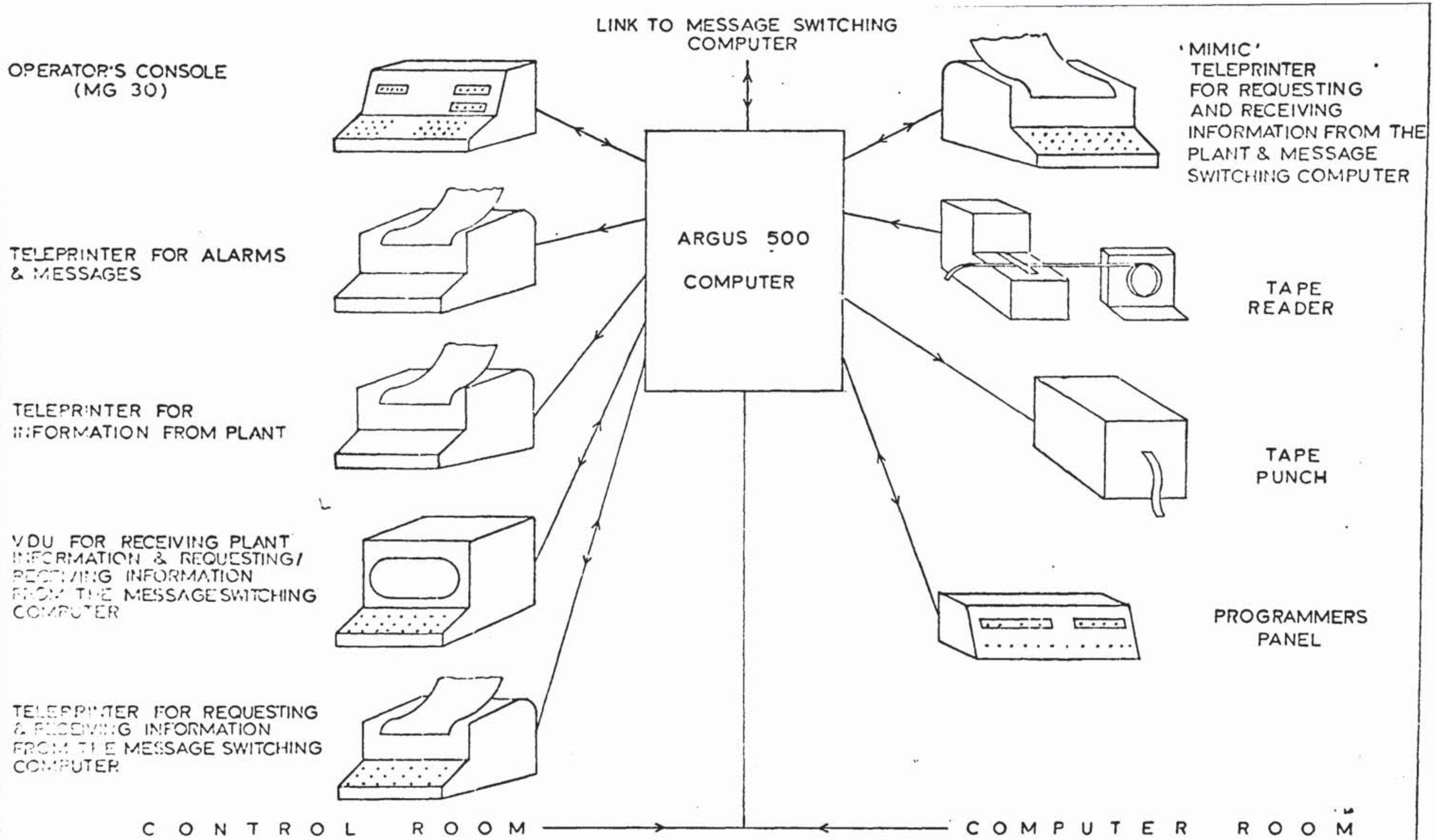
Users of the Ethylene Plant Computer System are able to access data using the terminal equipment shown in Fig. 3.6. Data can be accessed from two centres - the main control room and the adjacent computer room. This arrangement was designed to minimise interference between the technical and process operating requirements of the computer system. Process operating staff access data using the operator's console situated in the centre of the control room, while technical staff, who require data for technical investigations, use a 'mimic'-teleprinter located in the adjacent computer room. The 'mimic'-teleprinter is able to duplicate most facilities provided by the operator's console. These facilities include requests for



MEASURED VALUE = $\frac{\text{STEAM FLOW}}{\text{NAPHTHA FLOW}}$

STRUCTURE OF TYPICAL CALCULATION LOOP

EX 100 (FIG. 3.5)



PLANT COMPUTER TERMINAL EQUIPMENT LAYOUT (FIG 3-6) computer loops, logs and alarms. Changes to computer loops, logs or alarms, which can easily be implemented on-line using the operator's console or mimic teleprinter do not affect the operation of the rest of the computer system. A series of security levels operated by key switches prevent unauthorised personnel from making changes.

The programmers panel and paper tape punch shown in Fig. 3.6 are used in the loading of the computer system software from paper tape and in computer fault diagnosis. The computer terminal equipment are designed also to allow communication with the Baglan Bay Factory computer system.

Data can be output from the computer in a number of forms. Typed records can be produced on teleprinters found in the control room and computer room. Alternatively, the data can be displayed on a visual display unit situated in the control room, or punched on paper tape using the fast tape punch located in the computer room.

Computer logs are used to output groups of basic and derived data. The computer system provides comprehensive logging facilities in the form of trend logs, alarm logs, and specially formatted logs which contain selected loops specified by users of the computer system.

Powerful and flexible process alarm facilities are provided by the computer that enable basic and derived data, contained in Consul R loops, to be checked against upper and lower alarm settings. The computer indicates the presence of an alarm condition by producing a bleeping noise and flashing light from the operator's console, and printing an alarm message on the control room alarm teleprinter. Alarm indications can only be acknowledged from the operator's console.

Thus, having described the main features of the computer system, the development of the system to meet the objectives defined in Chapter 2, is discussed in the next section.

3.3 DEVELOPMENT OF PLANT COMPUTER SYSTEM

3.3.1 Plant Computer Acceptance Tests

Acceptance tests were performed on the Ethylene computer hardware and software as supplied by the manufacturer, Ferranti Limited. Such tests were carried out at both the Ferranti Works, Wythenshawe and at the Baglan Bay Factory. All tests were witnessed and approved by the author. The purpose of the tests was to ensure that the computer hardware and software met BP Chemicals standards as defined in (7), and to establish a basic reliable computer system upon which future development work could confidently be built.

Comments and details of the results of the acceptance tests are contained in (8). Of particular value were the elevated temperature tests on the computer hardware at the Ferranti Works. The object of the tests was to highlight any latent faults in the hardware. The tests enabled the performance of the equipment at elevated temperatures to be assessed (important when computer room air conditioning units fail) and provided a useful check on the reliability of the computer hardware before delivery to the Baglan Bay Factory. The significant amount of non-standard special-to-project software definitely warranted testing.

It was concluded that the nature and number of the faults discovered during the computer acceptance tests fully substantiated the rigour of the testing.

3.3.2 Checking of Computer Inputs

The checking of inputs from the plant instruments to the computer system extended over a six month period, prior to plant commissioning, and required the full time services of two instrument mechanics. The testing was divided into two parts - continuity checking to ensure that the wiring connections between the instruments and the computer were correct, and functional checking to ensure that the accuracy of signal transmission was within specification. To facilitate the functional checking of signals, the computer was used as a digital voltmeter and numerical values proportional to the signals were printed on a teleprinter in the computer room. A summary of the number and type of computer inputs checked is given in Fig. 3.7.

The checking of on-line analyser signals to the computer involved close collaboration with the on-line analyser commissioning team. Modifications to the analyser computer software proved necessary as a result of the testing. Problems caused by the length of time analyser digital input contact closures remained set had to be circumvented by increasing the scanning frequency of the computer digital scan program.

3.3.3 Development of Technical Software

3.3.3.1 Processing of Basic Plant Data

Basic plant data consist of data that are directly measured by plant instruments. Computer software, in the form of Consul R read only loops, was developed to enable the current values of basic plant computer input data (i.e. flows, temperatures, pressure etc.) to be displayed digitally in engineering units. Details of Ethylene computer inputs are given in (9).

The accurate monitoring of battery limit and certain internal flows was recognised as being important for enabling local plant management to maintain close control of plant performance. Consequently, particular attention was paid to the calculation and checking of flow factors that were used in the computer flow loops. A computer program (10) was

FIG.3.7 SUMMARY OF COMPUTER INPUTS

TYPE OF COMPUTER INPUT	SIGNAL RANGE	NO. OF COMPUTER INPUTS	COMMENTS
'High' level	0.25 - 1.25 v	393	All signals from control room panel recorders & controllers.
Thermocouple	0 - 50 mv	89	Essentially naphtha and ethane furnace temperatures.
Resistance Bulb	0 - 50 mv	78	Signals from duplex RT bulbs.
'Shared' Resistance Bulb.	0 - 20 mv	33	Signals shared with Control Room temperature indicator. Necessary when duplex RT bulbs were unavailable.
Analyser	0 - 12.5 mv	6	Single stream/one component analysers.
Analyser	0.25 - 1.25 v + digital logic signals	23	Multi-stream/multi-component analysers
Turbine meter	0 to 5 v pulsed signal	8	
TOTAL:		630	

developed on the Honeywell Computer Time Sharing Link to calculate computer flow factors for differential pressure type flow meters. Orifice plates and nozzles were used predominantly to measure flows on the No. 2 Ethylene Complex. During the period when flow meters were being checked, all No. 2 Ethylene Complex flow meter data were held on a computer data file. This enabled data to be easily amended and the computer calculations conveniently repeated.

The accuracy of mass flow measurements of certain key flows was improved by programming the plant computer to use temperature and pressure measurements to correct for variations in fluid density at line conditions. The software was designed to check each calculated line density and ensure that it lay between realistic limits. In the event of a calculated density lying outside limits, due perhaps to malfunction of either the temperature or pressure sensors, a constant density would automatically be substituted. The flows selected for this treatment included most gaseous battery limit product flows and certain liquid streams, such as naphtha import and gasoline product. Other computer flow loops used constant meter factors incorporating fixed densities.

3.3.3.2 Processing of Derived Data

The plant computer system enables arithmetic and logical operations to be carried out on the basic plant data inputs and the resulting derived data displayed. Discussions with Ethylene Plant management established the derived data that were required to enable more efficient operation of the Ethylene Plant to be achieved. Such derived data included:-

i) Steam/naphtha ratios on the furnaces.

ii) Reflux ratios of the fractionating towers.

iii) Hydrogen/acetylene ratios in the C2 and C3 hydrogenation units.

A series of computer calculation loops were defined using flow and on-line analyser inputs to enable process operating staff to effect improved control of the C2 and C3 hydrogenation units of the plant. A description of the computer facilities provided for the C2 hydrogenation unit is given in Appendix 1.

Computer software was prepared that averaged battery limit flows and certain internal plant flows over periods of 1 hour, 8 hours and 24 hours. The averaged flows were used to evaluate the production performance of the plant.

3.3.3.3 Alarming of Data

It was decided with Ethylene Plant management that the computer alarm facilities should complement and not duplicate existing control room panel alarms. Routine alarming of computer inputs would be the exception rather than the rule. Computer alarms were placed on plant measurements which did not have control room panel alarms but which were considered by Ethylene Plant management important enough to warrant alarm facilities. Computer high temperature alarm limits were set on the temperatues of the cracked gas leaving the transfer line exchangers of the naphtha and ethane furnaces. Computer alarm facilities were also used to ensure that stream component concentrations, as measured by the on-line analysers, remained within specification. Of particular concern was the concentration of acetylenes in the MAP tower base stream, since high concentrations of acetylenes are an explosion hazard.

It was decided also to use the computer as a pre-alarm on certain important plant measurements, to give process operating staff warning that a control room panel alarm condition possibly was imminent.

It was felt that the corrective action prompted by the computer pre-alarm would result in the control room panel alarm state being averted. Pre-alarm settings on the compressor flows would indicate an approach to a compressor surge condition before the surge control alarm and control system came into operation.

The ability of the computer to alarm derived data was used on the C2 and C3 hydrogenation units of the Ethylene Plant. The way in which this alarm facility was applied is described in Appendix 1.

3.3.3.4 Logging of Data

Comprehensive sets of computer logs were specified to record basic and derived data. The logs fell into two main categories:-

(i) operational logs which were directed towards process operating staff as aids in the minute-by-minute operation of the plant.

(ii) summary logs which were directed towards plant management as aids in assessing the short term performance of the plant.

Operational logs were defined for each of the main plant sections. The contents of the logs were essentially computer loops which displayed the instantaneous values of plant measurements. The format of the propylene refrigeration system log is shown in Fig. 3.8. The data are presented in two columns, one column for each refrigerant compressor.

Summary logs contain derived data such as average flows over an 8 hour shift and selected basic plant data which are indicative of the state of plant performance.

An alarm log was prepared which gave the alarm settings and instantaneous values of all computer inputs that had been given computer alarm facilities. The 12 available computer trend logs were allocated to

13.28 HRS 30/09/74 LOG 48

	H-C-3A		(PROPYLENE REFRIG.)		H-C-3B		
E	P603	MV	PSIG	E	T614	MV	DEG.F
E	P602	MV	PSIG	E	T615	MV	DEG.F
E	P601	MV	PSIG				
E	F600	MV	KLBS/HR				
E	P600	MV					
E	S610	MV	K.RPM	E	S620	MV	K.RPM
E	F832	MV	KLBS/HR	E	F833	MV	KLBS/HR
E	T800	MV	DEG.F				
E	F610	MV	KLBS/HR	E	F620	MV	KLBS/HR
E	P610	MV		E	P610	MV	
E	T610	MV	DEG.F	E	T610	MV	DEG.F
E	P611	MV	PSIG	E	P611	MV	PSIG
E	T611	MV	DEG.F	E	T611	MV	DEG.F
E	F612	MV	KLBS/HR	E	F622	MV	KLBS/HR
E	P612	MV	PSIG	E	P622	MV	PSIG
E	T612	MV	DEG.F	E	T622	MV	DEG.F
E	F613	MV	KLBS/HR	E	F623	MV	KLBS/HR
E	P613	MV	PSIG	E	P623	MV	PSIG
E	T613	MV	DEG.F	E	T623	MV	DEG.F
E	F614	MV	KLBS/HR	E	F624	MV	KLBS/HR
E	F615	MV	KLBS/HR	E	F625	MV	KLBS/HR

FIG. 3.8 Format of Propylene Refrigeration System Computer Log

various groups of users e.g. the Ethylene Plant technical section were allocated 2 logs and the instrument section 1 log. Each trend log enabled up to 6 computer loops to be logged at frequencies between 10 seconds and 10 hours. Computer loops could easily be inserted or removed from the trend logs either from the operator's console of mimic teleprinter.

3.4 APPLICATION OF PLANT COMPUTER SYSTEM

3.4.1 Training

It was appreciated that the success of the plant computer system was strongly dependent on its acceptance and use. Hence, the effective training of personnel in the use of the computer system was regarded as an important activity and considerable effort was spent in preparing a training programme. A series of training courses were given which were scheduled to allow personnel to familiarise themselves with the computer system before the start of plant commissioning. Plant management from foreman level upwards attended the courses. It was the responsibility of the process foremen to train process operators to use the plant computer.

Each training course took the form of a lecture supplemented by practical sessions using the computer system. The lecture provided a general appreciation of how the computer system operated and what computer facilities were available. This was followed by a practical demonstration of how to use these facilities after which course members were each allowed to work through a set of programmed exercises using the computer system.

3.4.2 Ethylene Plant Pre-commissioning

The Ethylene Plant technical, instrumentation and process sections each benefited from use of the computer facilities during the six months prior to plant commissioning.

The technical section used the computer for collecting data to check compressor characteristic curves and for logging turbine and compressor vibration measurements. The testing of the cracked gas compression and refrigeration turbines and compressors was one of the major plant precommissioning activities (11). The nature and size of axial and radial vibrations set up in the compressors and turbines were of particular concern and interest. It was important to measure vibrations as the machines were moved through their critical speeds. Vibration and thrust measurement equipment had been installed on the machines with analogue monitoring facilities in the Ethylene Plant control room. Manual logging of data proved inadequate and so use was made of the flexible trend logging facilities provided by the computer every 2 seconds. The scanning speed of 2 seconds was chosen, since it was compatible with the fastest speed the paper tape punch could output data.

The instrumentation section used the computer as a digital voltmeter to facilitate the checking and calibration of computer inputs. Every encouragement was given to the instrumentation section in this exercise, as the establishment of good instrument practice for the maintenance of computer inputs was essential to the success of the computer system. Calibration procedures were defined to cover the different types of inputs to the computer system and instruction was given to members of the instrumentation section in use of the procedures. As the majority of computer signals were shared with the control room instrumentation, the more accurate and stringent instrument calibrations required by the computer, had the effect of raising the overall standard of instrumentation on the plant.

The process operating section used this period to develop confidence in use of the display and logging facilities of the computer, thus ensuring that maximum benefit could be derived from use of the system at plant commissioning.

This period was also used by the author to complete preparation and checks of the computer software.

3.4.3 Ethylene Plant Commissioning

With the plant computer system fulfilling a complementary, rather than an essential role in the commissioning of the Ethylene Plant, it was expected that users of the computer system would be discerning in their use and application of the system. The computer system had to be seen to provide distinct advantages over the conventional control room facilities if it was to be successful.

The application of the computer system is discussed under the following three headings.

(i) Data Presentation.

(ii) Computer System Flexibility.

(iii) Flow Averaging.

(i) Data Presentation

Haalman (12) pointed out that the duplication of data by the computer and conventional instrumentation confuses plant operators and should be avoided. On the No. 2 Ethylene Plant Computer System over 85% of the basic plant data displayed by the computer system were obtained from signals shared with the conventional control room panel instrumentation. The remaining 15% of data, consisting mainly of resistance thermometer temperatures, originated from the second bulb of duplex resistance bulb installations. No confusion arose over the duplication of data presentation as provided by the computer and conventional instrumentation.

The computer digital presentation of data was accepted, in general, as more accurate and more convenient to read except in instances when an analogue trend of a plant measurement was required. The computer presentation helped the plant management philosophy of encouraging process operators to think of flows in terms of engineering units (i.e. Klb/h) rather than as dimensionless chart readings. The computer system was able to display all key plant flows in engineering units and as equivalent chart readings in the range 0 to 10. Control room process operators, when requiring to change settings on panel controllers, found it convenient to adjust the controllers according to the computer digitally displayed values of the measured data.

The computer system logs were found to offer the following advantages over conventional logging:-

(a) The computer logs were able to bring together all important data associated with a particular plant section and present it in a convenient form for analysis. The computer logs were either displayed on the visual display unit for immediate analysis, or printed on a teleprinter to be analysed at some later time. This alleviated problems caused by the positioning of control panel indicators and recorders at different places in the large Ethylene Control Room. For instance, the analyser display panel and the fractionation control panel were located at opposite ends of the control room, and certain fractionation temperatures were only available on a temperature indicator desk in the centre of the room.

(b) The computer logs contained data related to the same time or time period. Manual logging of a large number of instruments scattered about the large control room resulted in a significant time lapse between the first and last logged data. This often distorted and complicated any subsequent analysis of the data.

(c) The computer logs included derived data in addition to basic plant data. For instance, a reflux ratio as well as a reflux flow was logged.

(d) The computer was programmed to automatically output logs at pre-specified time intervals or at a pre-specified time. This facility was used extensively by technical personnel to gather data in trouble-shooting exercises during commissioning. The automatic production of a daily computer log containing all key plant production data eliminated the need to manually collect and to planimeter flow charts in order to provide measures of plant production.

(e) The computer removed the need to record manually large amounts of data on log sheets, and thus allowed personnel to concentrate on the problems of plant commissioning.

(ii) Computer System Flexibility

The flexibility of the computer system proved extremely valuable during the commissioning of the plant. Software provided the key to computer system flexibility. Whenever a particular section of the plant was experiencing difficulties, process operating staff were able to assign plant measurements, in the form of computer loops, to a computer trend log and to log automatically the points at a required frequency.

The adaptability of the computer system was demonstrated during commissioning, when surges of refrigerant were sent to flare. It was important to ensure that the flare line temperature did not drop too low and result in the freezing and subsequent blockage of the flare line. It was possible, within a matter of seconds, to put a computer low temperature alarm on the flare temperature. The computer immediately warned process operating staff if the flare line temperature fell too low, thus allowing corrective action to be taken.

Another example of the flexibility of the computer system occurred when it was necessary to use, temporarily, a different source of hydrogen in the C2 and C3 hydrogenation units of the Plant. It proved comparatively easy to modify the computer software and maintain the computer facilities provided for improved control of these sections of the Plant.

(iii) Flow Averaging

Soon after the start up of the Ethylene Plant the value of being able to average flow data using the plant computer system became apparent. Mass balance flows, averaged over 1 hour periods, aided process operating staff in their task of lining up and steadying the Plant. Meaningful plant material balances were being produced two days after start up.

The need was then recognised for flow data to be averaged over a longer time period. At the end of each 8 hour shift, averaged flows were entered on to a simple schematic material balance flow sheet of the Plant, and the data analysed. Analysis of the data highlighted possible sources of material hold-up and instrument errors. Faulty meters were identified with a reasonable degree of confidence and brought to the attention of the instrument section.

Shift flow data were used in the preparation of a daily summary of the Plant's production performance, which was discussed each day be senior plant management. It was later found necessary to introduce daily averaged flows in addition to shift averaged flows. These daily averaged flows formed the basis of the Plant's data reconciliation/production records reporting system.

3.4.4 Computer System Reliability

To complete this section on the application of the computer system, it is appropriate to comment on the reliability of the computer system during the period of the Ph.D project. Good system reliability was fundamental to the success of the project.

The reliability of the plant computer system during the Ph.D project is summarised in Fig. 3.9. The slightly inferior reliability figures for 1972 are mainly due to the development and de-bugging of software in preparation for Ethylene Plant commissioning in 1973. The reliability figures for 1973 reflect the value of the rigorous checking of computer hardware and software.

3.5 CONCLUSIONS

The conclusions drawn from the development and application of the No. 2 Ethylene Plant Computer System are as follows:-

FIG.3.9 RELIABILITY OF NO.2 ETHYLENE PLANT COMPUTER SYSTEM

Period	Number of Major System Failures				Total	Total Down Time (Hours)	Basic Availability %
	Hardware			Software			
	Core Store Blocks	CPU's	Power Supply Units				
1972	3	2	0	7	12	254	97.1
1973	2	0	0	3	5	27	99.7

Note: 1. A major system failure is defined as a fault in computer system hardware or software resulting in a total loss of computer facilities.

2. Basic Availability = $\frac{\text{(Run time - down time)}}{\text{Run time}} \times 100\%$

(i) The size and complexity of the No. 2 Ethylene Plant demanded a standard of plant performance monitoring which could not have been achieved without the plant computer system. This conclusion is endorsed by Sommer et al (13) who found that although it is difficult to justify economically on-line information systems for plants, such systems can greatly enhance plant operability and aid plant commissioning.

(ii) The reliability of the computer system hardware and software, was an important factor in establishing confidence in the computer system. Such confidence was important since it was identified at the beginning of the project that the complementary role of the computer system might make its acceptance and use more difficult to establish.

(iii) The computer system provided an incentive for maintaining a high standard of plant instrumentation for the whole plant.

(iv) Computer flexibility was the key to the success of the computer system during plant commissioning. Plant commissioning, by nature, can be an unpredictable and rapidly changing scene where unexpected problems have to be solved as quickly as possible. The ability to quickly assemble or modify computer loops, logs and alarms proved an invaluable aid over this period.

(v) The computer presentation of data was readily accepted by plant personnel and afforded distinct advantages over conventional control room data presentation facilities.

(vi) The good working relationship with the Ethylene Plant personnel, prior and during plant commissioning, ensured that computer system facilities met plant requirements and were effectively used.

(vii) With the computer system established as a reliable on-line plant information system it is possible to consider extending its function to improved computer control of certain key sections of the Ethylene Plant.

(viii) The plant computer system achieved its objectives during commissioning of the No. 2 Ethylene Plant.

CHAPTER 4

DATA RECONCILIATION

CHAPTER 4 - DATA RECONCILIATION

4.1 INTRODUCTION

The problem of reconciling data from a large industrial flow system such as found at Baglan Bay was introduced in Chapter 2. This chapter is concerned with the development of a data reconciliation technique and system for reconciling such data. Before proceeding with the evaluation of methods to reconcile the data, an analysis and estimation is made of the errors that exist in an industrial mass flow measuring system. A review is then given of the various techniques that have been used for reconciling inconsistent data from industrial systems. This is followed by an account of an investigation into the merits of different data reconciliation error criteria. The investigation used a simple computer model of industrial flow measurement errors to generate sets of typically measured raw data from an ideal set of flows. These data were used in the assessment of the data reconciliation error criteria. The Chapter proceeds to describe the selection of a data reconciliation technique for reconciling data from a large scale industrial mass flow measuring system. The technique must be capable of meeting the requirements specified in Chapter 2. The application of this technique to the reconciliation of data from the No. 2 Ethylene Complex is described. Features and limitations of the No. 2 Ethylene Data Reconciliation Model are discussed, and a description is given of the No. 2 Ethylene Reconciliation System implemented at Baglan Bay to collect, reconcile and report data. The Chapter ends with an assessment of a recently published work, which has employed a similar approach to data reconciliation.

4.2 ANALYSIS AND ESTIMATION OF ERRORS IN INDUSTRIAL MASS FLOW MEASURING SYSTEMS

An industrial mass flow measuring system consists predominantly of pressure differential type meters. The remainder of metering devices in the system are usually turbine flow meters, positive displacement meters and level gauges for measuring tank stock changes. It is convenient to include tank stock changes as part of the mass flow measuring system since they can be regarded as a form of mass flow measurement into or out of tanks. The following discussion of industrial flow measurement errors is mainly concerned with errors associated with this type of mass flow measuring system. Pressure differential meters are used as examples in the discussion but reference is made to other types of meters.

The likely size of a flow measurement error can be estimated, without experimentation, if:-

i) the various sources of error are considered.

ii) their separate numerical contributions are estimated on the basis of past experience.

iii) these contributions are combined together to give the required estimate of the overall error.

Each of these stages in the estimation of the total error is discussed in the following sections.

4.2.1 Nature of Errors

There are two distinct kinds of errors (14): those errors that determine the accuracy of a flow measurement and those that determine its reproducibility or precision.

i) Accuracy of Flow Measurement

Accuracy is defined as the degree of agreement between the apparent flow as measured by the flow meter and the actual flow obtained at the time or occasion of measurement. The estimation of the accuracy of a flow measurement consists in determining the likely magnitude of the difference between the apparent and actual flow. The estimation can apply both to a single measurement, or to the average of series of measurements.

All sources of error that may contribute to a difference between the apparent and actual flow, enter into the estimation of accuracy. Such component errors are called Systematic Errors because they result in a systematic bias of the apparent flow away from the actual flow. The bias may not necessarily be the same for all component errors and they may partially cancel out.

Different sources may or may not contribute systematic errors depending on the way in which the flow measurement has been carried out, e.g. a zero error on a differential pressure transmitter which is adjusted every two days would produce a systematic error on daily integrated flow measurements but may contribute only a negligible random error on monthly integrated flow measurements.

ii) Precision or Repeatability of Flow Measurement

Precision is defined as the degree of agreement between repeated determinations of the apparent flow, the actual flow being constant.

All sources of error whose magnitude can vary from one occasion to another and can produce variations in the apparent flow, enter into the estimation of precision. Such component errors are called Random Errors because both their magnitude and their sense varies from occasion to occasion.

Random errors provide a measure of the precision, or repeatability, of the measurement. If the error distribution has a Gaussian character the actual random error will be smaller than twice the standard deviation in 95% of all cases.

iii) Flow Measuring System Errors

The performance of a flow measuring device can be stated in terms of its Systematic Errors and Random Errors, normally expressed as a percentage of Nominal Value. Since these errors, in the case of differential pressure devices, become very large as the flow rate approaches zero, (flow is proportional to the square root of the pressure difference) it is common practice to state the error figures together with the measuring range within which they are expected to hold. This measuring range, called Rangeability, is an indication of the flexibility of the measuring device. Rangeability is defined as the ratio of the maximum meter reading to the minimum meter reading for which the error is less than a stated value. Turbine flow meters are inherently more accurate than differential pressure type meters and the accuracy limits over the usable flow range are independent of the flow rate. Likewise, tank stock changes, measured as the difference between two stock levels, have measurement errors independent of the stock change.

When a measuring system is composed of several instruments the total error is a combination of the errors of each instrument. The error of each instrument consists of a random error and a systematic error. For a group of instruments the systematic errors will be different for each instrument and must be considered as random for the group.

Systematic errors that exist in industrial flow measuring systems can be subdivided into Inherent Systematic Errors and Gross Systematic Errors. The inherent systematic errors are the systematic errors which are a function of system design and operation, whereas gross systematic errors are a function of system failure/availability, and the extent and quality of human intervention. Gross systematic errors are greater in magnitude than the maximum combined inherent systematic and inherent random errors of the meters.

4.2.2 Sources of Error

The errors associated with the industrial measurement of flows can be classified into three groups as follows:-

i) Inherent random errors.

ii) Inherent systematic errors.

iii) Gross systematic errors.

Sources of inherent random errors include:-

i) Ambient temperature changes.

ii) Changes in static line pressure.

iii) Fluid density changes due to variation in fluid pressure, temperature or composition.

iv) Changes in viscosity of fluid.

v) Hysteresis in elements of the measuring system, in particular the differential pressure transmitter.

vi) Faulty adjustment of elements of system during calibration checks.

Source of inherent systematic errors include:-

i) Incorrect construction of elements of measuring system e.g. orifice plate not machined correctly.

ii) Incorrect design or installation of elements of measuring system e.g. insufficient lengths of straight pipe up-stream or down-stream of primary element.

iii) Faulty adjustment of elements of system during calibration checks.

It should be appreciated, as stated earlier, that different sources of error may contribute either a systematic or random error effect on the measurement, depending on the way in which the flow measurement has been made.

Sources of gross systematic errors found in a typical computer based flow measuring system, such as at Baglan Bay, include:-

i) Failure of measuring system component e.g. differential pressure transmitter fails resulting in zero or full scale signal.

ii) Unavailability of measurement due to routine checking of instrument.

iii) Human errors - examples of such errors are:-

a) failure to update meter constants in computer flow calculations.

b) failure of instrument mechanic to re-initialise computer flow calculation after re-instatement of repaired or checked meter.

c) incorrect manual recording of measurements not automatically picked up by computer system. For instance, incorrect positioning of decimal point.

Industrial flow measurement systems are strongly characterised by the presence of gross systematic errors. In the case of a well maintained laboratory or pilot size plant undergoing strictly controlled experiments, the influence and occurrence of gross systematic errors can be reduced to an extent whereby they can be considered negligible. However, in a large scale industrial flow measurement system comprising several hundred instruments exposed to an environment which creates problems of corrosion, fluctuating ambient conditions, leaking flanges and valves, the occurrence of gross systematic errors is unavoidable. Lees et al (15) analysed the reliability of instruments working in a industrial environment and concluded that instrument reliability is strongly dependent on the severity of the environment. They stated that a severe environment could increase the instrument failure rate by a factor of up to 4. With the exception of on-line analysers, the failure rate of flow differential pressure transducers was greater than most other widely used measuring instruments examined in the survey.

A flow measuring system significantly dependent on human intervention is also likely to be characterised by gross systematic errors. The human traits of boredom, tiredness and absentmindedness are likely to give rise to human errors of the gross systematic type.

The occurrence of gross systematic errors can be reduced by:-

a) Efficient instrument maintenance practice. Regular checking and calibration of instruments will reduce the likelihood of instrument failure.

b) Minimising human intervention by automating the data acquisition and processing of flow data. It should be emphasised that expedient use of human interaction in such an automated system is still desirable to ensure that system performance is being maintained.

4.2.3 Estimation of Errors

Hop (16) has estimated the expected errors for a number of different types of flow measuring systems under industrial conditions, with fluid and ambient conditions changing. He did not consider the existence or effect of gross systematic errors in his survey of mass flow measuring systems. He quoted a maximum total error (% of nominal value) of between 2.3 and 3.3% for a flow measuring system comprised of a square edge orifice flow meter with two differential pressure transmitters and automatic flow integration. Other systems involving orifice type flow meters and automatic flow integration had maximum total errors between 1.7% and 3.2%.

An estimation of the gross systematic errors in an industrial flow measuring system can be made by defining:-

i) the probability of meters being affected by gross systematic errors during the flow integration period.

ii) of the meters affected by gross systematic errors, the probabilities that the gross systematic errors will produce:-

a) full scale flow readings

b) zero flow readings

c) flows between zero and full scale.

These probabilities can be estimated by examination of the flow meter data records from the industrial flow measuring system.

4.3 DATA RECONCILIATION TECHNIQUES AND ERROR CRITERIA

4.3.1 Review of Data Reconciliation Techniques

Since 1961 when Kuehn and Davidson (17) used the mathematical technique of the Lagrange method of undetermined multipliers for adjusting the flow and enthalpy measurements to satisfy heat and mass balances, a number of workers have shown interest in the problem and techniques of data reconciliation.

It is common practice in process calculations to adjust the measured data by small amounts so that discrepancies in heat and material balances are eliminated. Manual adjustment can be done intelligently by combining the knowledge that one may have regarding the accuracy of certain instruments and the nature of the process (e.g. stoichiometric ratios).

Kuehn and Davidson (17) set out to solve this problem of data reconciliation in a systematic way by considering the heat and mass balances as a set of simultaneous equations. Measurements are adjusted so that the set of equations balance. The data reconciliation error criterion was required to introduce larger percentage adjustments into those measurements that are prone to error and keep the total necessary adjustment to a minimum. Kuehn and Davidson used the classical Lagrange method of undetermined multipliers to obtain a solution, and selected a least squares error criterion for which the sum of squares of the individual adjustments to the data is a minimum. They believed the method to be beneficial, since advantage is taken of the redundancy in the measurements that are made in the plant in order to provide a more accurate estimate of actual plant conditions.

The problem in mathematical form is stated as follows:-

$$\text{Minimise } \phi(x_i) = \sum_{i=1}^{n} \left\{ \frac{1}{\sigma_i^2} (x_i - x_i^*)^2 \right\} \quad - (4.1)$$

subject to the constraints

$$\psi_j(x_i) = \sum_{i=1}^{n} a_{ij}\, x_i = 0 \quad j = 1,2\text{--}\, m \qquad - \quad (4.2)$$

where

x_i	=	the ith measurement when corrected (i.e reconciled)
x_i^*	=	the ith measurement as actually observed
σ_i^2	=	the error variance of the ith measurement
a_{ij}	=	the coefficient of the ith measurement in the jth material (or heat) balance equation
n	=	number of measurements
m	=	number of constraints

The method of Lagrange (undetermined multipliers) solves for the x.i's as the solution of the set of simultaneous equations.

$$\sum_{i=1}^{n} \frac{\partial}{\partial x_i} \left\{ \phi(x_i) + \sum_{j=1}^{m} \lambda_j \psi_j(x_i) \right\} = 0 \qquad - \quad (4.3)$$

$$\sum_{j=1}^{m} \frac{\partial}{\partial \lambda_j} \left\{ \phi(x_i) + \sum_{j=1}^{m} \lambda_j \psi_j(x_i) \right\} = 0 \qquad - \quad (4.4)$$

The solution of these above equations for x is given in matrix notation as follows:-

$$\bar{\lambda} = (\bar{A}\,\bar{C}\,\bar{A}^T)^{-1} \,.\, \bar{A}\,\bar{X}^* \qquad - \quad (4.5)$$

$$\bar{X} = \bar{X}^* - \bar{C}\,\bar{A}^T\,\bar{\lambda} \qquad - \quad (4.6)$$

where

$\bar{A}$ is the matrix (a_{ij})

$\bar{X}$ is the vector (x_i)

$\bar{X}^*$ is the vector (x_{i*})

$\bar{C}$ is the diagonal matrix with elements $1/2\sigma_i^2$

$\bar{\lambda}$ is the vector of undertermined multipliers (λ_i)

Details of the solution of these equations is given in (17).

Clementson (18) also recognised the need for a systematic approach for rationalising complicated and large configurations of mass balances. He pointed out that in the chemical and oil industries the majority of processes are operated continuously and in such processes there is no way of determining the exact quantity flowing in any line - all that can be obtained are estimates of the true flow using flow meters of varying accuracy and quality. He stated that a set of meter readings will not 'balance' because of the errors that existing in the readings. In a small plant it may be possible to obtain meaningful and consistent values by applying some logical rules. However, in a larger plant this becomes too complicated and the need for a systematic approach to the problem is evident.

Clementson suggested the application of the statistical method of regression analysis using a least squares error criterion as a solution to the problem of data reconciliation. The regression analysis technique is ideally suited, like the Lagrangian multiplier approach, for routine application on a digital computer. The technique he claimed offered the following advantageous features:-

i) it will cope with missing or incomplete data.

ii) the solution is consistent.

iii) the presence of accuracy estimates allows the detection of incorrect data.

The least squares error criterion used by Clementson in the regression analysis technique was the same as used by Kuehn and Davidson (i.e. it is the set of flows that give a minimum total square error between the corrected and uncorrected flows). As both the Lagrangian multiplier method and the regression analysis method attempt to minimise the same error criterion, provided the constraint equations and data are identical, it is inevitable that the resultant set of reconciled data should be the same. The methods differ only in the mathematical technique used to manipulate the system equations and data.

Ripps (19) showed that the Lagrangian multiplier technique of Kuehn and Davidson (17) worked well for data containing only small random type errors (i.e. no gross systematic errors). However, when the set of data contains gross systematic errors in addition to the random errors the technique is inadequate. Because the individual adjustments appear as the square, a high penalty is imposed on making any single large correction. Thus, a gross error present in one measurement is attributed to a series of small errors in each measurement. This distribution of the gross error has two disadvantages; it makes the data as a whole highly inaccurate, and it does not indicate which measurement had the gross error to guide instrument repair or similar corrective action.

Ripps proposed a method that permitted a distinction between the two major types of error (i.e. gross systematic and random) in process data. He modified the Lagrangian multiplier procedure to allow a certain number of the measurements to be discarded as gross errors. The measurements suspected as being in gross error are each discarded sequentially from the complete set of raw measurements and a 'least squares' analysis performed on the remainder of the data. Comparison of the resulting least squares error criterion should provide an indication of the meters with gross errors.

The chief disadvantages of this method are that it is iterative and strongly dependent on the subjective view of the analyst who must decide which measurements to discard or keep.

Meharg (20) saw data reconciliation primarily as a means of improving data for calibrating models of the plant. The technique used was the classical Lagrangian multiplier method using a least squares error criterion. Meharg made use of non-linear component balances involving analytical data, in addition to linear bulk flow material balances. This involved him in an iterative solution to the Lagrangian multiplier method. An additional use of data reconciliation suggested by Meharg was in the estimation of variables which cannot be measured (e.g. leaks from plant).

Nogita (21) was also aware of the limitations of the basic least squares error criterion in reconciling data containing both random and reconciled data. He, like Ripps (19) extended the basic Kuehn and Davidson (17) procedure to include use of a serial elimination algorithm for automatic selection of suspect measurements. Ripps (19) had relied very much on the subjective judgement of the analyst in selecting suspect measurements.

Recently, Mathiesen (22) has used a modulus error criterion and the linear programming method for adjusting inconsistent sets of measurements. He did not restrict the method to mass flow measurements but considered it generally applicable to all types of measurements (i.e. flows, pressures, concentrations, temperatures etc.). His approach was to take a set of equations that describe the system under consideration and linearise the equations about an operating point. Application of the linear programming method to the set of linear equations and measured data would result in the adjustment of inconsistent data.

The work of Mathiesen (22) is discussed further in Section 4.5 in the light of experiences of data reconciliation at Baglan Bay.

4.3.1.1 Conclusions

Workers involved with the reconciliation of plant data have mainly concerned themselves with the minimisation of a least squares error criterion using either the Lagrangian multiplier or regression analysis techniques. Although some workers considered the simultaneous reconciliation of mass and heat data it is felt that there is no incentive for introducing heat balances into the reconciliation of flow data from industrial mass flow measuring systems. In an industrial environment, estimates of heat flows are considerably less accurate than the estimates of mass flows, and unmeasured heat losses and gains are very prevalent. The inclusion of heat balance data would produce a significant degradation of the quality of the data used to reconcile the mass flows.

Component mass balances require accurate measurements of stream concentrations to be worthy of inclusion in the reconciliation of mass flow data. Otherwise, inaccurate concentrations will, like heat balance data, degrade the overall quality of data.

Ripps and Nogita were very much aware of the inadequacy of the least squares criterion in its ability to reconcile data with gross systematic errors in addition to random errors. They both suggested interative procedures to improve this situation. Ripps approach was strongly dependent on the subjective judgement of the analyst performing the reconciliation whilst Nogita proposed the application of a serial elimination algorithm to avoid having to depend on the subjective views of the analyst. Mathiesen, using a modulus error criterion, has recently applied the technique of linear programming to the adjustment of inconsistent data.

4.3.2 Evaluation of Data Reconciliation Error Criteria

4.3.2.1 Introduction

Data reconciliation techniques are strongly characterised by the error criteria used to reconcile the data. It has been shown in the previous section that the development and refinement of data reconciliation techniques has centred upon adaptations of a 'least squares' error criterion. The analysis of errors in industrial mass flow measuring systems identified the existence of gross systematic errors in addition to inherent random type errors. Gross systematic errors have a probability distribution which is akin to a rectangular distribution. For such a distribution, a 'modulus' criterion would seem to be the most appropriate error criterion. It is the intention of this investigation to show whether the 'modulus' error criterion (i.e. minimisation of a sum of the moduli of the adjustments to the flows) is better suited than the 'least squares' error criterion (i.e. minimisation of a sum of the squares of the adjustments to the flows) for reconciling industrially measured flow data.

An analysis of the types and sources of error that exist in flow data obtained from an industrial flow measuring system was described in Section 4.2. From such an analysis a mathematical model of the errors can be formulated which can be used to generate sets of typical 'raw' industrial flow data from an ideal set of flows. The characteristics of the 'raw' industrial flow data generated by the model will depend on the settings of model parameters.

To facilitate the assessment of data reconciliation test criteria it is convenient to select a simple flow system, incorporating the main features of typical industrial flow systems. Data reconciliation can be carried out on this system using sets of typical 'raw' industrial flow data generated using the error model. With the true and 'raw' values of the flows known, performance criteria can be defined to measure the success of the data reconciliation error criteria in adjusting the 'raw' flow data.

4.3.2.2 Model of Errors in Industrial Flow Data

A Fortran program which models the errors in industrial flow data was written on the ICL 1904 computer. A simple flow chart and listing of the program are given in Appendix 2. The program produced sets of typical 'raw' flow data from an ideal set of flows.

The program contained the following features:-

i) A pseudo-random number generator was used to produce random variables. The subroutine used to generate the random numbers had been used extensively by the Operational Research Section, Baglan Bay. It was shown to repeat itself after 40000 numbers.

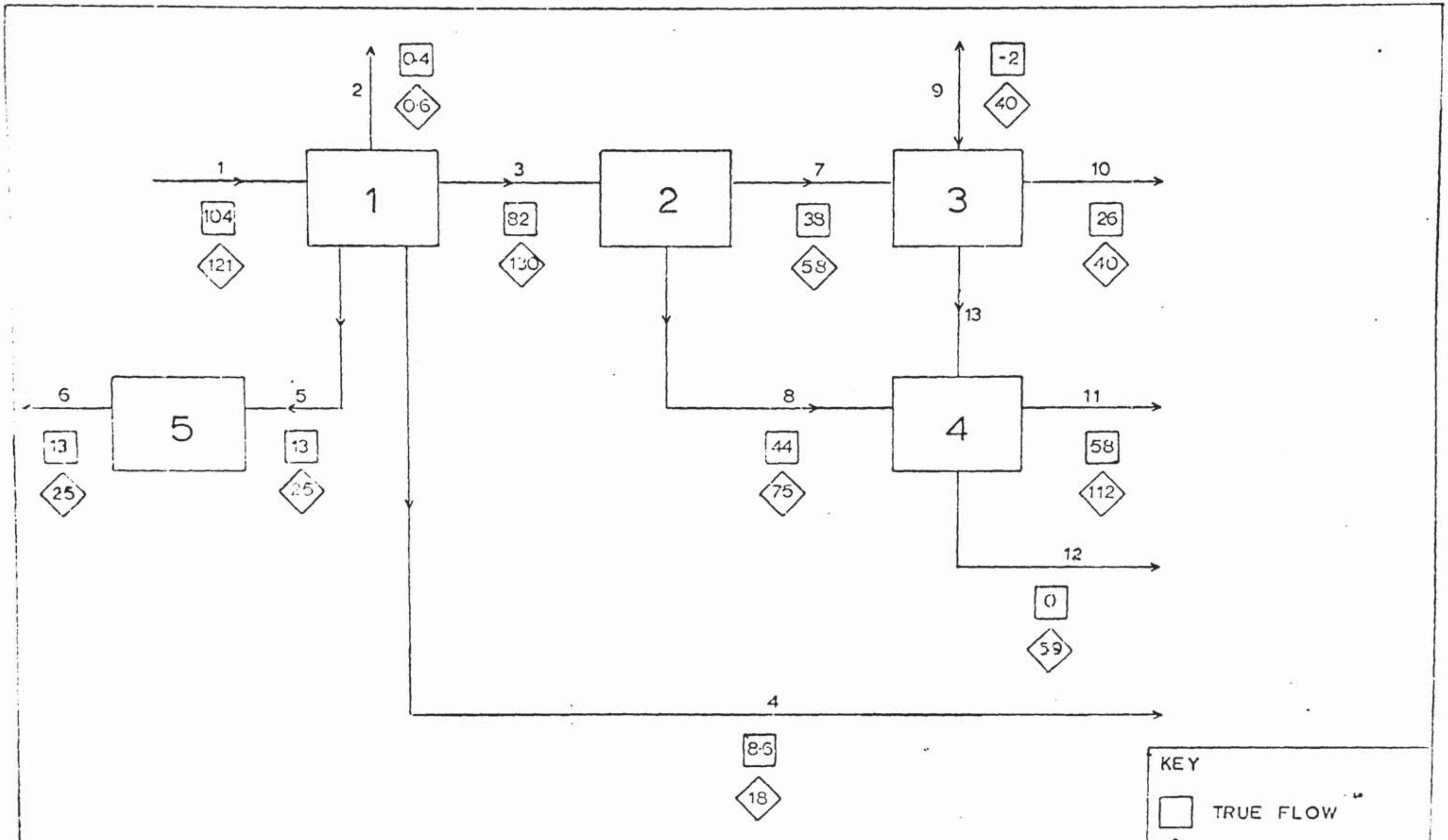
ii) The sum of the inherent random and inherent systematic errors for the set of meters comprising the flow measuring system was considered as having a normal Gaussian distribution. The combined inherent random and inherent systematic error for a particular meter was determined by sampling the normal distribution. A maximum total error of 3% (twice the standard deviation), based on Hop's (16) analysis of flow meter systems, was taken as being the combined inherent random and inherent systematic error for a computer based industrial flow measuring system comprising mainly of orifice plate type meters.

iii) The occurrence and nature of gross systematic errors was determined by defining the probability of meters being affected by gross systematic errors during the flow integration period, and the probabilities that the systematic errors would produce zero or full scale flows. The errors were produced by repeated sampling of a rectangular probability distribution. Analysis of the flow data obtained from plant records provided estimations of the probabilities of gross systematic errors.

4.3.2.3 Experimental

The investigation into the evaluation of data reconciliation error criteria involved a computer program (23) that used the Lagrangian method of undetermined multipliers for minimising a 'least squares' error criterion, and an iterative Lagrangian procedure for minimising the modulus error criterion. Modifications were made to the program to improve the iterative Lagrangian procedure; to enable repeated sets of data to be run; and to enable performance criteria to be calculated from the data reconciliation results.

The flow system selected for the investigation is shown in Fig. 4.1. It comprises of 5 balances and 13 flows. The linking of the flows is shown in Fig. 4.1 with flow 9 representing a stock change. Also shown are the true flows and flow ranges of the meters used in the investigation. The raw data sets generated by the error model and used in the investigation are given in Appendix 3. The appendix also



DATA RECONCILIATION TEST SYSTEM (FIG 4-1) contains a typical set of results produced by the reconciliation program (Data Set 1, Run 1). The investigation examined the performance of the least squares and modulus error criteria in reconciling flow data containing:-

i) only inherent random and systematic errors. A total error of 3% nominal value was used in the investigation.

ii) only gross systematic errors. The probability of meters being affected by gross systematic errors was set at 0.1. This produced, on average, one gross systematic error per run in the simple flow system used in the investigation.

iii) errors that exist in industrial flow measuring systems. A total of 3% nominal value was used for the inherent type errors. The probabilities of gross systematic errors were derived from an analysis of industrial flow data (see Fig. 4.2).

The effect of different weighted error criteria in reconciling data was also considered in the investigation. The weighting functions considered were unity weights, weights inversely proportional to the raw flows and weights inversely proportional to the flow ranges of the meters used to measure the flows. The investigation did not include the effect of the different inherent accuracies of the flow meters. Inherent meter accuracies can be conveniently introduced into data reconciliation by using weights in the error criterion that are inversely proportional to the meter accuracies. Such weights would bias the reconciled results towards the measurements of the more accurate meters, but would not invalidate the findings of this investigation.

For each data reconciliation error criterion and data type, reconciliation was carried out on 20 sub-sets of data and the mean

FIG. 4.2 SUMMARY OF FLOW METER FAULTS

TAKEN FROM PLANT RECORDS

Total Number of Meters = 92

PERIOD (7 days)	METER FAULTS*			TOTAL
	Zero flow	Full Scale Flow	Error $\pm 5\%$ of nominal value	
1	3	5	18	26
2	4	2	16	22
3	4	1	9	14
4	4	1	10	15
5	3	2	7	12
6	3	1	13	17
7	5	3	14	22
8	4	2	13	19
9	4	2	15	21
AVERAGE	4	2	13	19

*Errors identified using data reconciliation model and confirmed by meter calibration checks.

Probability of gross systematic error $= \frac{19}{92} \simeq 0.2$

Probability of gross systematic error producing zero flow $= \frac{4}{19} \simeq 0.2$

Probability of gross systematic error producing full scale flow $= \frac{2}{19} \simeq 0.1$

performance criteria calculated.

4.3.2.4 Performance Criteria

Data reconciliation, as well as producing reconciled data that satisfy material balances and are technically meaningful, must also attempt to ensure that the reconciled data are more 'correct' (i.e. closer to the true set) than the raw data. As there exists no unique measure of 'correctness' of data, a set of performance criteria (Fig. 4.3) were defined in order to assess the merits of the data reconciliation error criteria in reconciling the raw data.

A set of linear and quadratic performance criteria were used in the investigation. With reference to Fig. 4.3, performance criteria nos. 7 to 12 are the quadratic equivalents of the linear criteria nos. 1 to 6. The performance criteria calculate the absolute and normalised differences between the true, raw and reconciled flows.

The normalised performance criteria, in which the flow differences are divided by the full scale ranges of the meters, reflect the undesirability of introducing large changes in flows that have small flow ranges.

Performance criteria 1, 3, 7 and 9 can be regarded as measures of the error in the data before reconciliation, while performance criteria 2, 4, 8 and 10 provide measures of the error in the data after reconciliation. The differences between these corresponding criteria give measures of the improvement in the data caused by data reconciliation.

Performance criteria 5 and 11 provide checks that the relevant data reconciliation error criteria are minimised. The modulus error criterion should always be smaller than the least squares for performance criterion 5 and conversely for performance criterion 11.

FIG. 4.3 LINEAR AND QUADRATIC DATA RECONCILIATION PERFORMANCE CRITERIA

NO.	MNEMONIC NAME	MATHEMATICAL DEFINITION	DESCRIPTION	FUNCTION
1	AVM(RAW-TRU)	$\frac{1}{N}\sum_{i=1}^{N}\left\lvert Fi_{Raw} - Fi_{Tru}\right\rvert$	Average modulus of difference between raw and true flows.	Provides an absolute measure of original error in raw data.
2	AVM(REC-TRU)	$\frac{1}{N}\sum_{i=1}^{N}\left\lvert Fi_{Rec} - Fi_{Tru}\right\rvert$	Average modulus of difference between reconciled and true flows.	Provides an absolute measure of error in reconciled data.
3	PAVM(RAW-TRU)	$\frac{1}{N}\sum_{i=1}^{N}\left\lvert \frac{Fi_{Raw} - Fi_{Tru}}{Fi_{Range}}\right\rvert \times 100$	Normalised average modulus of difference between raw and true flows.	Provides a weighted measure of original error in raw data.
4	PAVM(REC-TRU)	$\frac{1}{N}\sum_{i=1}^{N}\left\lvert \frac{Fi_{Rec} - Fi_{Tru}}{Fi_{Range}}\right\rvert \times 100$	Normalised average modulus of difference between reconciled and true flows.	Provides a weighted measure of error in reconciled data.
5	AVM(RAW-REC)	$\frac{1}{N}\sum_{i=1}^{N}\left\lvert Fi_{Raw} - Fi_{Tru}\right\rvert$	Average modulus of difference between raw and reconciled flows.	Provides a check on data reconciliation error criteria and provides a weighted measure of flow changes induced by reconciliation.
6	PAVM(RAW-REC)	$\frac{1}{N}\sum_{i=1}^{N}\left\lvert \frac{Fi_{Raw} - Fi_{Rec}}{Fi_{Range}}\right\rvert \times 100$	Normalised average modulus of difference between raw and reconciled flows.	Provides a weighted measure of the flow changes induced by reconciliation.
7	AVS(RAW-TRU)	$\frac{1}{N}\sum_{i=1}^{N}(Fi_{Raw} - Fi_{Tru})^2$	Average square of difference between raw and true flows.	Provides a weighted measure of original error in raw data.
8	AVS(REC-TRU)	$\frac{1}{N}\sum_{i=1}^{N}(Fi_{Rec} - Fi_{Tru})^2$	Average square of difference between reconciled and true flows.	Provides a weighted measure of error in reconciled data.
9	PAVS(RAW-TRU)	$\frac{1}{N}\sum_{i=1}^{N}\left\{\frac{Fi_{Raw} - Fi_{Tru}}{Fi_{Range}}\right\}^2 \times 100$	Normalised average square of difference between raw and true flows.	Provides a weighted measure of error in raw data.
10	PAVS(REC-TRU)	$\frac{1}{N}\sum_{i=1}^{N}\left\{\frac{Fi_{Rec} - Fi_{Tru}}{Fi_{Range}}\right\}^2 \times 100$	Normalised average square of difference between reconciled and true flows.	Provides a weighted measure of error in reconciled data.
11	AVS(RAW-REC)	$\frac{1}{N}\sum_{i=1}^{N}(Fi_{Raw} - Fi_{Rec})^2$	Average square of difference between raw and reconciled flows.	Provides a check on data reconciliation error criteria and provides a weighted measure of flow changes induced by data reconciliation.
12	PAVS(RAW-REC)	$\frac{1}{N}\sum_{i=1}^{N}\left\{\frac{Fi_{Raw} - Fi_{Rec}}{Fi_{Range}}\right\}^2 \times 100$	Normalised average square of difference between raw and reconciled flows.	Provides a weighted measure of flow changes induced by reconciliation.

KEY
N - Number of flows
Fi_{Raw} - Unreconciled raw measurement of i^{th} flow
Fi_{Tru} - True value of i^{th} flow
Fi_{Rec} - Reconciled value of i^{th} flow
Fi_{Range} - Flow range of meter measuring i^{th} flow

4.3.2.5 Discussion of Results

The results of the investigation are summarised in Fig. 4.4. Columns 1 to 6 contain values of the linear performance criteria and columns 7 to 12 contain values of the quadratic performance criteria, as defined in Fig. 4.3. Improvements of reconciled data over raw data can be assessed by comparing columns 2 with 1, 4 with 3, 8 with 7 and 10 with 9.

The following observations can be made from the results in Fig. 4.4.

i) Data containing only inherent random and systematic errors (Data Set 1 - Rows 1 to 6 (Fig. 4.4)

Both the least squares and modulus error criteria applied to data containing small random type errors produced reconciled data closer to the true data. The least squares criterion always produced a greater improvement than the modulus criterion except when unity weights were used. In this instance, the resulting normalised error in the reconciled data (row 1, columns 4 and 10) was greater than the original error in the data (row 1, columns 3 and 9). This is attributed to the unity weights in the error criterion not discouraging large flow changes in flows which have small flow ranges.

ii) Data containing gross systematic errors (probability of systematic error = 0.1) (Data Set 2 - Rows 7 to 12 (Fig. 4.4))

The only criterion to produce an improved set of reconciled data, as measured by both linear and quadratic performance criteria, was the modulus criterion with the weights inversely proportional to the flow range (row 12). It is interesting to note the marked deterioration in the reconciled data produced by the modulus error criterion with weights inversely proportional to the raw flows (row 10).

FIG. 4.4

SUMMARY OF DATA RECONCILIATION ERROR CRITERIA INVESTIGATION RESULTS

DATA SET	DATA TYPE	ERROR CRITERION WEIGHTS	ERROR CRITERION FUNCTION	rows \ columns	LINEAR PERFORMANCE CRITERIA AVM (RAW-TRU)	AVM (REC-TRU)	PAVM (RAW-TRU)	PAVM (REC-TRU)	AVM (RAW-REC)	PAVM (RAW-REC)	QUADRATIC PERFORMANCE CRITERIA AVS (RAW-TRU)	AVS (REC-TRU)	PAVS (RAW-TRU)	PAVS (REC-TRU)	AVS (RAW-REC)	PAV[illegible] (RAW-[illegible]
					1	2	3	4	5	6	7	8	9	10	11	12
1	Contains only Inherent Random and Systematic Errors	Unity	Least Squares	1	0.6840	0.5928	1.1672	5.9988	0.4944	5.9079	1.0755	0.6603	2.2293	481.48	0.4152	482.[illegible]
			Modulus	2		0.6377		5.2241	0.4181	4.8700		0.7631		429.28	0.5086	429.[illegible]
		Raw Flows	Least Squares	3		0.4505		0.9225	0.4920	0.7656		0.4163		1.5305	0.6599	1.0[illegible]
			Modulus	4		0.5048		0.9758	0.4583	0.5856		0.5351		1.7432	0.9556	1.31[illegible]
		Flow Range	Least Squares	5		0.4646		0.9346	0.4623	0.8201		0.4516		1.5041	0.5152	1.0[illegible]
			Modulus	6		0.5071		1.0055	0.4204	0.5480		0.5478		1.9005	0.8443	1.2[illegible]
2	Contains Only Gross Systematic Errors	Unity	Least Squares	7	3.1773	5.0659	4.3813	80.480	4.0016	79.159	195.64	137.77	245.87	228055.0	57.884	227839[illegible]
			Modulus	8		3.4295		89.449	3.0894	89.081		112.21		376720.0	74.39[illegible]	376758[illegible]
		Raw Flows	Least Squares	9		6.7634		13.198	5.5273	11.793		268.30		821.8	151.63	758.[illegible]
			Modulus	10		7.0024		8.5564	5.6611	6.8039		509.94		600.96	379.60	495.[illegible]
		Flow Range	Least Squares	11		3.8734		7.6824	4.0718	7.2570		70.512		219.55	92.744	168.[illegible]
			Modulus	12		1.0778		2.4651	3.0939	3.4193		31.843		110.66	185.50	159.[illegible]
3	Typical Industriel Flow Data	Unity	Least Squares	13	4.2359	5.4309	7.4096	42.874	3.9384	41.325	141.98	102.90	323.55	35051.7	39.080	35101[illegible]
			Modulus	14		4.0654		28.5612	3.0625	27.172		78.65		21709.0	53.397	21719[illegible]
		Raw Flows	Least Squares	15		6.9045		11.7923	4.9730	8.3715		210.95		42[illegible].76	11[illegible].0[illegible]	25[illegible]
			Modulus	16		6.4874		9.6295	4.6583	6.3394		264.31		413.[illegible]	122.81	[illegible]5.0[illegible]
		Flow Range	Least Squares	17		4.9079		9.1276	3.7527	6.4524		90.331		244.[illegible]	46.934	[illegible]0.3[illegible]
			Modulus	18		3.2981		6.0242	3.0700	4.2585		75.445		204.91	83.890	121.7[illegible]

This can be explained by the reluctance of the error criterion to correct a flow which has a large true flow, but due to the presence of a gross systematic error, has a small raw flow and hence large weight in the error criterion.

iii) Industrial Flow Type Data (Data Set 3 - Rows 13 to 18 (Fig. 4.4))

For data which are characteristic of industrial flow systems and contain both small random-type errors and gross systematic errors, it can be seen that the modulus criterion with weights inversely proportional to the flow range (row 18) produced the best improvement in the raw data. The least squares error criteria were not successful in producing improved sets of reconciled results.

The results showed that, in general, the modulus error criterion is more suitable than the least squares error criterion for reconciling data containing gross systematic errors. This can be explained by examining the forms of the criteria.

i) Modulus Error Criterion

$$\text{Minimise} \sum_{i=1}^{n} w_i \left| Fi_{REC} - Fi_{RAW} \right| \qquad - \qquad (4.7)$$

ii) Least Squares Error Criterion

$$\text{Minimise} \sum_{i=1}^{n} w_i \left(Fi_{REC} - Fi_{RAW} \right)^2 \qquad - \qquad (4.8)$$

$$\text{or Minimise} \sum_{i=1}^{n} w_i' \left| Fi_{REC} - Fi_{RAW} \right| \qquad - \qquad (4.9)$$

$$\text{where } w_i' = w_i \left| Fi_{REC} - Fi_{RAW} \right| \quad - \quad (4.10)$$

The least squares error criterion as defined by equation 4.9 can be regarded as a pseudo weighted modulus criterion where the weights are proportional to the adjustments to the flows. By weighting large flow adjustments more than small adjustments, the least squares criterion will always encourage small changes in a large number of flows rather than large changes in few flows, in order to satisfy the material balance constraints. Therefore, any gross systematic error in a single flow measurement will tend to be distributed amongst neighbouring flows.

The modulus error criterion attempts to satisfy the material balance constraints by selecting as few flows as possible that reduce the material imbalances and minimise the weighted error criterion. This, normally, has the effect of identifying and correcting flows that have gross systematic errors.

The investigation showed that it was possible for reconciled flows as produced by the Lagrangian method to reverse direction and represent an infeasible solution. It is difficult to prevent this effect using the Lagrangian method.

4.3.2.6 Conclusions

It can be concluded from the investigation that the modulus criterion with weights inversely proportional to the flow range is more suitable than any least squares criteria for reconciling industrial flow data containing gross systematic errors. The modulus criterion with weights inversely proportional to the flow range, was the only criterion tested that produced reconciled flows closer to the true flows when applied to industrial type flow data.

The modulus criterion with weights inversely proportional to the raw flows proved inadequate in reconciling data containing gross systematic errors.

There is little to choose from a practical viewpoint, between the modulus and least square criteria for reconciling data containing only random type measurements. The least squares criterion is marginally better and statistically more valid.

4.3.3 Selection of Data Reconciliation Technique

It was demonstrated experimentally in the previous section that the linear modulus error criterion is more suitable than the 'least squares' error criterion for the reconciliation of industrial flow data. The Lagrangian multiplier technique, which was used to test the error criteria, was not capable of preventing infeasible flows. Constraints to prevent flows from becoming infeasible cannot easily be introduced into the method. However, since a linear error criterion was shown to be suitable for reconciliation of industrial flow data it is possible to exploit the powerful and versatile technique of linear programming in reconciling data.

Linear programming (LP) has the following features important in its application to data reconciliation:-

i) Standard Packages are available for applying the technique on most computers

This ensures that development problems are minimised. The standard formulation of LP problems requires definition of a matrix with the columns representing the system variables to be minimised and the rows the system constraints. Such a formulation of the problem facilitates the initial structuring and any subsequent re-structuring of the system under consideration. Advantage may also be taken of any matrix generators and report writers that are in existence.

ii) <u>The linear objective function (i.e. the data reconciliation error criterion) can conveniently be subjected to inequality as well as equality constraints</u>

Data reconciliation equality constraints involve the system mass balances. Inequality constraints allow the system to be described in terms of technically feasible operating conditions. Inclusion of process yield and efficiency inequality constraints ensure that the reconciled data are technically feasible as well as mathematically feasible. Inequality constraints also provide a convenient means of handling unmeasured material loss flows.

iii) <u>The variables in the objective function can be bounded</u>

The linear programming feature of bounding variables can be used in data reconciliation to prevent reconciled solutions with infeasible negative flows. One of the major limitations of the Lagrangian method was the difficulty in preventing infeasible negative flows from being produced in certain situations. Bounding can also be used to restrict loss flows.

The linear programming technique is able to satisfy the requirements demanded of a data reconciliation technique, as defined in Chapter 2.

The formulation of a data reconciliation model using the linear programming technique is described in Appendix 4. A simple single material balance system is selected to illustrate features of the linear programming technique as applied to data reconciliation. The definition and development of data reconciliation models for the No. 2 Ethylene Complex are described in the next section.

4.4 DEVELOPMENT OF THE NO. 2 ETHYLENE DATA RECONCILIATION SYSTEM

4.4.1 Definition of No. 2 Ethylene Data Reconciliation Models

The No. 2 Ethylene Data Reconciliation System includes:-

i) No. 2 Ethylene Plant

ii) No. 2 Butadiene Plant

iii) No. 2 GTU Plant

iv) No. 2 Ethylene Fuel Gas System.

Details of the No. 2 Ethylene Data Reconciliation System including schematic data reconciliation models of each of the Plants are given in (24). The schematic representation of the No. 2 GTU Plant data reconciliation model is shown in Fig. 4.5A, as an example, and a summary of the No. 2 Ethylene Data Reconciliation data and material balances is given in Fig. 4.5B.

The flow data for data reconciliation fall into three categories:

i) Flows automatically logged by the plant computer.

ii) Flows which are metered but are not automatically logged by the plant computer.

iii) Flows which are not metered but whose values can be estimated.

The majority of flow data are plant computer inputs since the requirement to be able to produce plant and sectional material balances was recognised when the computer system was specified.

In defining the data reconciliation models it was realised that fairly comprehensive sectional material balances could be specified for the No. 2 Ethylene Plant. The most ill-defined sectional balances involved the compression and pre-fractionation sections of the plant, as the only direct measurement of main plant throughput after the furnace feed flows, was provided by the demethaniser feed flow. A noticeable feature of the data reconciliation model of the Ethylene Plant is the

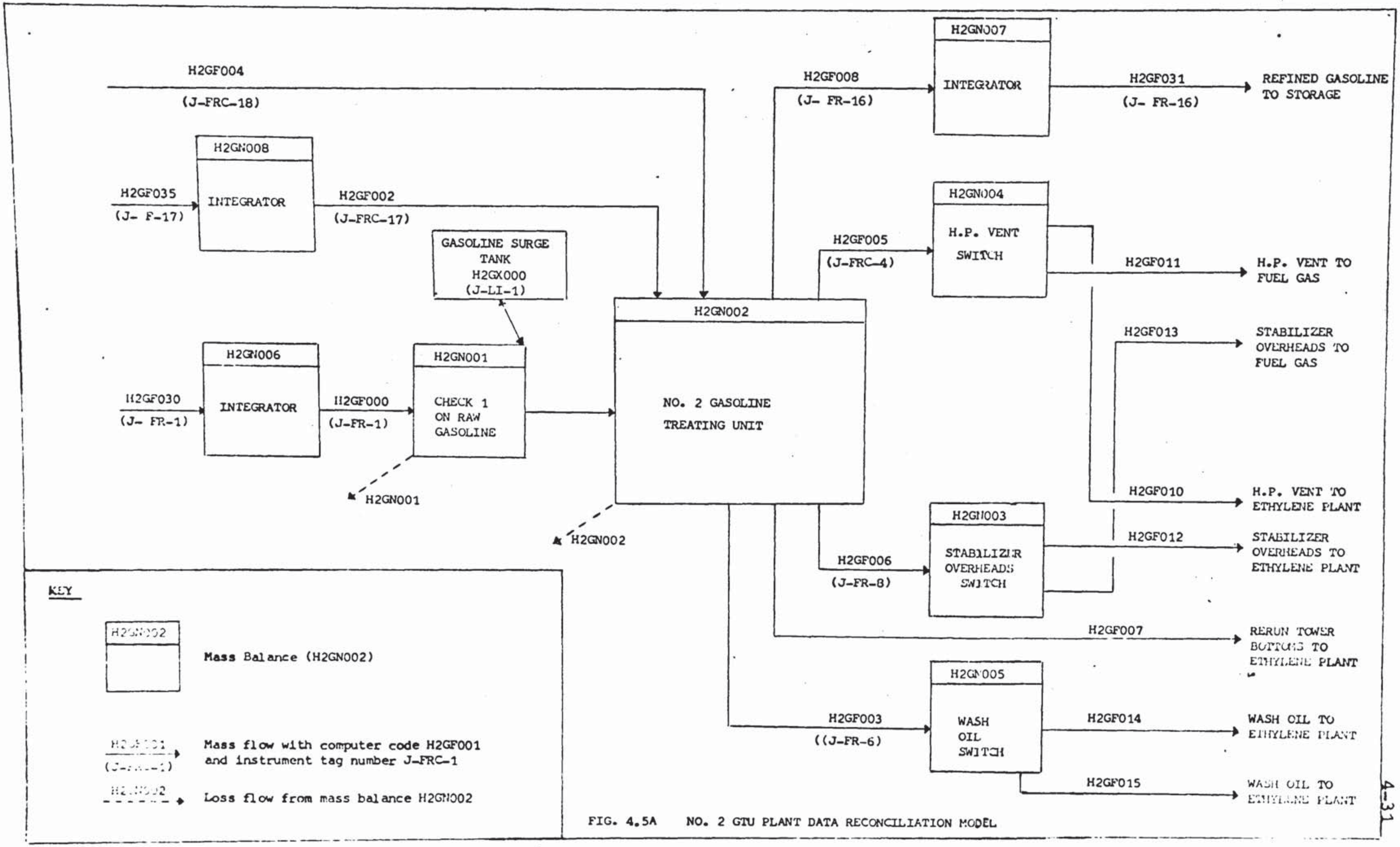


FIG. 4.5A NO. 2 GTU PLANT DATA RECONCILIATION MODEL

FIG. 4.5B SUMMARY OF NO. 2 ETHYLENE DATA RECONCILIATION DATA AND MATERIAL BALANCES

	BASIC PLANT DATA				
Plant	Meter + Computer Logged	Metered (Includes panel flow integrators)	Estimated (Includes loss and flare flows)	Total	Material Balances
Ethylene	98	21	29	148	48
Butadiene	8	0	10	18	7
G.T.U.	10	3	8	21	8
Others *	–	2	–	2	2
TOTAL	116	26	47	189	65

Note : Fuel Gas Data Reconciliation System is not shown separately as it mainly consists of flows originating from the Ethylene, Butadiene and GTU plants. In the above table, specific fuel gas system flows and balances have been included in the Ethylene Plant figures.

* Others include raw and refined gasoline stock changes.

number of direct meter checks that exist on key battery limit flows including naphtha import, gasoline product, C4 product and fuel oil. Loss flows are included only where there exists a physical possibility of material loss. For example, a loss flow is not included between 2 meters in the same flow line, but loss flows are defined for sectional material balances where material could leave the system un-monitored such as through relief safety valves.

As the No. 2 Ethylene Plant is closely linked to the No. 2 Fuel Gas System through production and use of fuel gas, it was expedient to specify and develop the Ethylene and Fuel Gas data reconciliation models in parallel. The metering on the No. 2 Fuel Gas system allows an overall fuel gas balance to be defined, together with a number of check balances.

The data reconciliation model of the relatively smaller and simpler GTU Plant consists of an overall plant balance incorporating battery limit flows. A feature of this model is the alternative switching of streams dependent on plant operation. Switch balances are included in the data reconciliation model to accommodate these situations e.g. the stabiliser column overheads from the GTU plant can be returned to the compression section of the Ethylene Plant or sent to Fuel Gas. The GTU Plant is linked to the Ethylene Plant in the data reconciliation models via raw gasoline and hydrogen production.

It was necessary to simplify the data reconciliation model of the Butadiene Plant, since the complex solvent recovery system of the plant, which had a significant number of unmeasured flows, made a more detailed model unsuitable for reconciliation.

The linear programming (LP) representation of the data reconciliation models is an LP Matrix. The columns of the matrix consist of the flows to be reconciled and the rows of the matrix consist of equality and inequality constraints. The plant section material balances form the equality constraints. The inequality constraints in the matrix can be divided into two main types:-

i) Loss Constraints

ii) Performance and Yield constraints.

i) Loss Constraints

The plant section loss flows are constrained to lie between fixed percentages of flows associated with the plant sections. The lower limit is zero and the upper limit is normally about 3 percent of the total mass flow to the plant section. These figures are based on experience of ethylene plant operations over a number of years. In addition, the Ethylene Plant loss, i.e. the sum of the individual plant section material losses, has an upper limit expressed as a per cent of the naphtha feed. Loss flows also have a facility to include absolute bounds i.e. loss flows can be constrained to lie between upper and lower absolute values rather than as a percentage of throughput.

ii) Yield Constraints

Yield constraints were specified for each Ethylene Plant product and are used to ensure that reconciled data are technically valid. For each product the sum of flows representing the recovery of the product are constrained to lie between fixed percentages of the naphtha and ethane feeds to the cracking furnaces, e.g. the gasoline yield constraint ensures that the reconciled gasoline flow lies between 18% and 33% of the total naphtha flow to the furnaces.

4.4.2 Testing of No. 2 Ethylene Data Reconciliation Model

The combined LP data reconciliation model of the Ethylene, Fuel Gas and GTU Plants was tested using flow data collected by the Ethylene Plant computer system. The testing revealed the need to improve the model. The improvements included:-

i) The Introduction of Flare Flows into the Model

In periods of plant upsets, flows can be diverted from various parts of the Ethylene Plant to flare. The points in the process where flows are sent to flare depend on the nature of the plant upset, e.g. operational problems on the C2 hydrogenation system might result in the total overheads flow from the de-ethaniser tower being flared.

Flare flows represent abnormal loss flows. Before the introduction of flare flows into the model, grossly distorted results were produced when reconciling data over periods when there had been appreciable flaring. Data reconciliation was unable to completely remove, by adjustment of the normal loss flows, the large material imbalances due to flaring. Therefore, the remainder of the imbalances were distributed between the internal plant section flows.

In the absence of flaring, flare flows are fixed at zero. In periods when flaring occurs, estimates are specified of the maximum and minimum values of the flare flows. These values are derived from knowledge of plant section throughput and the length of time flaring occurs. The data reconciliation model arrives at flare flows between these limiting values.

ii) The Introduction of Plant Status Information to Supplement Flow Data

Plant status information is required to enable estimates to be made of data reconciliation flows that are not metered. Unmetered flows include flare flows. Meaningful estimates of these flows can be made if the times when the flows exist are recorded.

Plant status information is also needed to establish the routes of flows which have alternative destinations depending on the mode of plant operation. For instance, under normal operation GTU vents are recycled to the cracked gas compression system of the Ethylene Plant. During a plant upset there is often a need to divert these vents to the Fuel Gas System. Status information, covering the times when streams are temporarily diverted, is needed for data reconciliation purposes.

A status report log sheet was designed to meet data reconciliation requirements. As part of the routine operation of the data reconciliation system, the sheets are completed by process operating personnel on a daily basis, and supplement the daily production records log produced by the plant computer system. Routine operation of the data reconciliation system is described in Section 4.4.3.

Testing of the data reconciliation model also revealed the following characteristics of the model and raw data.

i) Data Reconciliation Time Periods

As the time periods become less, the effect of unmeasured changes in material hold-up in the plant becomes significant. In the Ethylene Plant, while gaseous hold-up is only of the order of a few hours, liquid hold-up in the prefractionation section is of the order of a couple of days. This effect of hold-up is accentuated by unsteady plant operation especially at low plant throughputs. Unsteady plant operation is caused by plant operational difficulties and when plant throughput is changed (for example, when an additional furnace is brought on-stream).

The No. 2 Ethylene data reconciliation model proved successful in reconciling raw data over time periods greater than a day. However, it was concluded that data reconciliation over periods less than a day was unreliable, and was considered not worth implementing on a routine basis.

ii) Weighted Data Reconciliation Error Criterion

The weighting factors initially used in the data reconciliation modulus error criterion were calculated according to the equation

$$\text{Weighting Factor} = \frac{1000}{(\text{Raw Flow}) \times (\text{Measurement Accuracy})} \quad - \quad (4.11)$$

i.e. the weighting factors were inversely proportional to the raw flows and the measurement accuracies.

Data reconciliation accounts for the different accuracies of the measured data by adjusting the measurement accuracies and hence weighting factors in the error criterion. The measurement accuracies used for routine operation of data reconciliation are given in Fig. 4.6.

The weighting factors defined by equation 4.11 were used in the No. 2 Ethylene data reconciliation model before the investigation, described in Section 4.3.2, showed that a more satisfactory weighting factor equation was:-

$$\text{Weighting Factor} = \frac{1000}{(\text{Flow Range}) \times (\text{Measurement Accuracy})} \quad - \quad (4.12)$$

i.e. flow range should be substituted for raw flow in equation 4.11.

This does not mean that the No. 2 Ethylene data reconciliation model results produced using the modulus error criterion, with weighting factors defined by equation 4.11, were inferior to the raw unreconciled data. Experience in using the No. 2 Ethylene data reconciliation model with this weighted error criterion found it necessary to re-run the model, usually one or two times, before a

FIG. 4.6 MEASUREMENT ACCURACIES USED IN NO. 2 ETHYLENE DATA RECONCILIATION MODEL

Measurement Type	Measurement Accuracy
Tank Farm Stock Charge	0.5
Turbine Flow Meter	1.0
Orifice Plate Flow Meter with Density Correction	3.0
Orifice Plate Flow Meter without Density Correction	6.0
Flow Integrators	10.0
Good Manual Estimates of Data	15.0
Poor Manual Estimates of Data	30.0
Data Unavailable	99999.0

satisfactory set of reconciled data was produced. This iterative procedure was necessary to nullify the effect of gross systematic errors, which distorted the reconciled results. Such errors were nullified by giving flows containing the errors very small weighting factors. It was not always possible after one run of the model to identify all flows containing gross systematic errors. However, the raw data used in the final run of the model would contain essentially only inherent random type errors for which the weighted error criterion used was adequate.

Use of the weighted modulus error criterion with weighting factors defined by equation 4.12 resulted in improved identification and correction of gross systematic errors.

iii) Model Sensitivity

The LP data reconciliation technique was designed, through the setting of large objective function weighting factors, not to change zero raw flow measurements. In general, this is desirable since a significant number of raw flow measurements have genuine zero flows. However, it was discovered that a faulty zero flow measurement could cause the data reconciliation model to produce a meaningless set of results.

The model reconciled a set of raw data, containing a faulty zero measurement of the hydrogen flow to the GTU Plant, by reducing most of the Ethylene Plant flows to zero. This effect was attributed to the way in which inequality constraints were defined in the model. The hydrogen flow was ratio constrained with the gasoline flow to the GTU Plant, to lie between fixed limits. Similarly, the gasoline flow and other Ethylene Plant product flows were ratio constrained with the total naphtha flow to the Ethylene Plant. Since the reconciliation model regarded zero flows as virtually fixed, (i.e. the GTU hydrogen flow was held at zero), this combination of inequality constraints could only be satisfied by reducing most of the Ethylene Plant flows to zero.

The form of the LP solution allows a faulty flow measurement of this kind to be easily traced, by examination of the shadow prices associated with the inequality constraints in the LP matrix. The shadow price of a constraint is defined as the value to the objective function of 'slackening' the right hand side of the constraint by unity. The offending constraint will have the largest shadow price. It is comparatively easy to then identify the offending flow in the constraint.

However, the situation concerning the faulty hydrogen flow to the GTU plant did highlight how the indiscriminate use of inequality performance constraints can create problems whereby faulty measurements of relatively unimportant flows can cause the data reconciliation results to become meaningless.

iv) Combined Flows

If two or more flows connected the same two material balances in the data reconciliation model, it was found expedient to represent the flows as a single combined flow with an average weighting factor. If this was not done, the LP data reconciliation technique would always select and change only one of the flows connecting the balances, (the flow with the smallest weighting factor), in order to satisfy the material balances. With the combined flow representation, the reconciled values of the combined flows are divided proportionately amongst the individual flows constituting the combined flows. This was considered to be a more realistic approach to data reconciliation rather than assigning the entire error to one flow which has the largest inherent error.

4.4.3 Operation of No. 2 Ethylene Data Reconciliation System

The No. 2 Ethylene Data Reconciliation System involves the collection, reconciliation and reporting of data. Although the System was designed to derive maximum benefit from the Factory On-line Computer System, implementation of the data reconciliation system had to proceed without the availability of the message switching computer facilities. The No. 2 Ethylene Data Reconciliation System, as well as functioning as a system in its own right, forms a major part of the Baglan Bay Factory Data Reconciliation System, which has the same principles of operation. It is convenient to describe the No. 2 Ethylene Data Reconciliation System, for which a schematic flow chart is shown in Fig. 4.7, in three stages:-

i) Data Collection

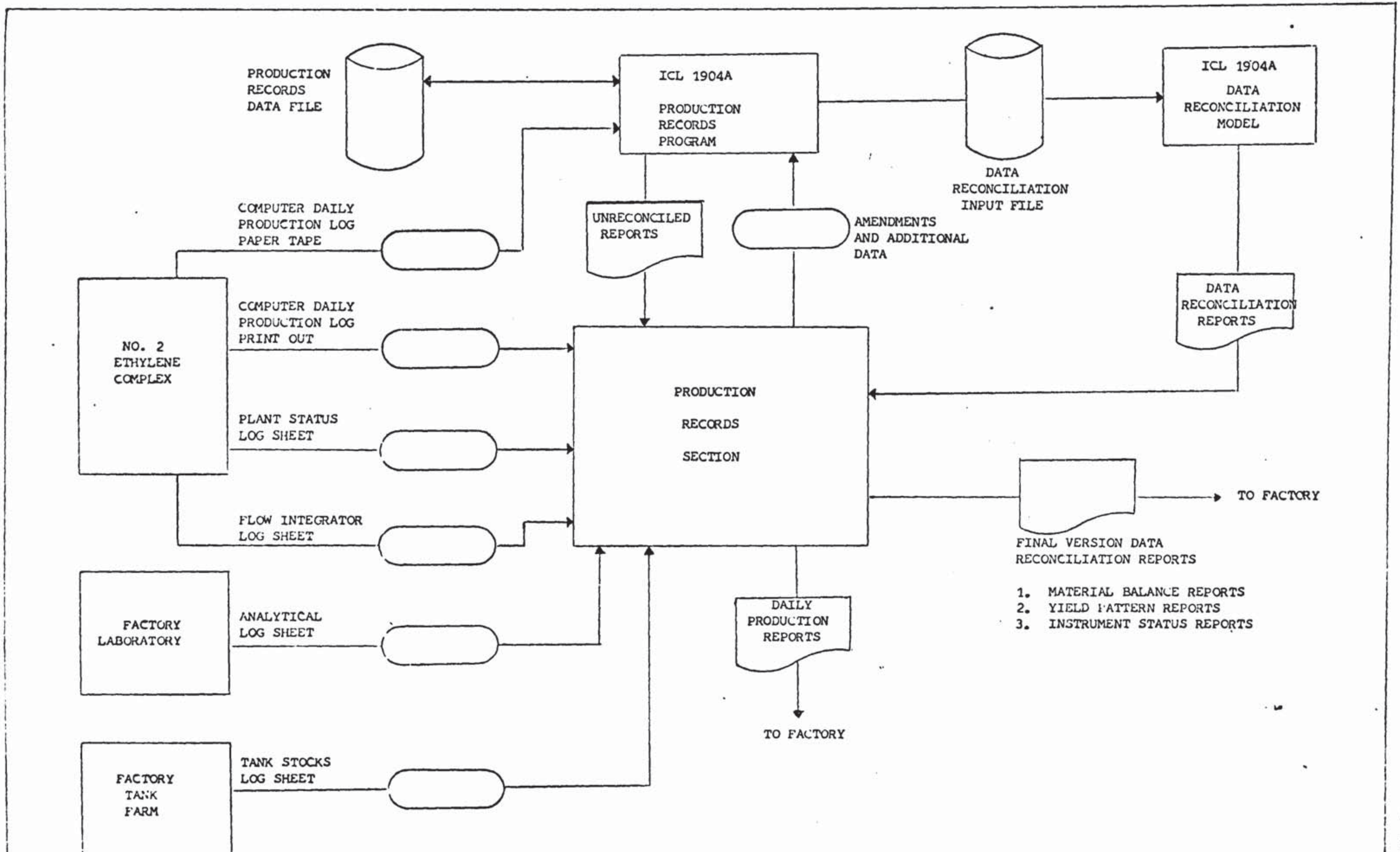
ii) Data Reconciliation

iii) Data Reporting

i) Data Collection

Data originate from the No. 2 Ethylene Complex, Factory Laboratory and Factory Tank Farm.

The majority of data from the No. 2 Ethylene Complex, are collected by the plant computer system. Each day a paper tape computer log is produced containing the daily flows of all battery limit and plant sectional accounting streams. The paper tape computer log is input directly to the central computer system and used to update the production records data file. Supplementing the computer log is a plant status log sheet and flow integrator log sheet. The plant status log sheet, which was referred to in section 4.4.2, contains information on plant operations which are needed for data reconciliation e.g. plant flaring. The status information is interpreted by the Production Records



NO. 2 ETHYLENE DATA RECONCILIATION SYSTEM (FIG. 4.7)

Section before being used to update the production records data file. Control room panel flow integrator readings are logged daily as part of the data reconciliation standby system. These data are used in event of failure of the plant computer system.

Analytical data from the Laboratory are used only in the reporting of data while tank stock data are used in data reconciliation to provide accurate checks on certain important battery limit flows (e.g. naphtha and gasoline).

ii) Data Reconciliation

The data reconciliation input data file is created from the production records data file. The No. 2 Ethylene Data Reconciliation model, which is run on the central ICL 1904A computer, is used to reconcile weekly and monthly data. More frequent reconciliation of data is not practical until the availability of the message switching computer system. It is often necessary to re-run the model to adjust measurement accuracies before a satisfactory set of reconciled data are produced.

iii) Data Reporting

Reconciled results are issued each week to Ethylene Complex and Factory management. The reports comprise of:-

a) comprehensive and summary plant material balance reports

b) a furnace yield pattern report

c) an instrument status report.

A set of reports are given in Appendix 5. The material balance reports show both the reconciled and unreconciled data. The instrument report, which is of particular value to the Ethylene instrumentation section, highlights those flow meter measurements that data reconciliation has found necessary to change by a significant amount, and thus suggested to be in error.

The report is divided into two sections:

Section 1 - meters unavailable i.e. those meters for which a measured value was not available

Section 2 - meters whose values data reconciliation has changed greater than 5 percent.

The instrument report forms the basis of the formalised procedure for checking flow instrumentation on the No. 2 Ethylene Complex.

Daily production reports are issued by the Production Records Section using unreconciled data from the daily computer log, which have been manually checked for obvious inconsistencies. This is an interim procedure until automatic daily data reconciliation is implemented.

In event of computer system failure, the manually recorded flow integrator readings are substituted for the computer derived flows for use in the data reconciliation model. Flows for which panel integrator readings are not available are estimated using the previous day's data. If plant operation remains steady such estimates are fairly accurate. The accuracies and hence weighting factors in the data reconciliation model are adjusted to reflect the degree of confidence that can be placed on the measurements.

4.5 COMMENTARY ON WORK OF MATHIESEN (22)

After the experience of using linear programming for reconciling data at Baglan Bay, it is appropriate to comment on the work of Mathiesen (22). Mathiesen has recently used a modulus error criterion and linear programming method for adjusting inconsistent sets of data. His conclusions, in general, endorsed the use of linear programming for data reconciliation. The main points and conclusions arising from

Mathiesen's work are discussed in the following sections.

i) Suitability of Linear Method for adjusting inconsistent data

Mathiesen concluded that the linear method was more useful in practice than quadratic methods for adjusting inconsistent sets of data. He also recognised that a great advantage of the linear programming method was that inequality constraints could easily be included amongst the system equations.

It was shown experimentally in section 4.3.2 that a modulus error criterion was more suitable than a quadratic error criterion for reconciling industrial flow data containing gross systematic errors. Also, one of the important features of linear programming, in its application to data reconciliation, was identified in section 4.3.3 as being the use of inequality constraints. These conclusions are in agreement with the conclusions of Mathiesen.

ii) General Application of Linear Method

Mathiesen suggested that the method be generally applicable to all types of measurements. His approach was to take a set of equations that describe the system under consideration and linearise the equations about an operating point. He suggested that application of the linear programming method to the set of linear equations and measured data would enable the measurements that are in gross error to be identified. He recognised that the linearisation of the system equations may introduce additional errors and suggested that such linearisation errors may be eliminated by successive re-linearisations.

At Baglan Bay, the linear method was restricted to the reconciliation of mass flow data. It was recognised, as stated in

Section 4.3.1.1 that the introduction of either heat balances or component mass balances could degrade the overall quality of the data used to reconcile mass flows. This is because enthalpy and component concentration data are notoriously less accurate than mass flow data. Component concentration data were, however, effectively used in inequality constraints to define process yield and efficiency limits.

iii) Rectangular Error Distribution of Instrument Error

Mathiesen considered that it is more correct to assume that instrument errors have a rectangular rather than a normal distribution.

In the investigation into data reconciliation error criteria, described in Section 4.3.3, two main types of instrument errors were recognised. Inherent instrument errors were represented by a normal distribution while gross systematic errors, which are caused by instrument failure, human error etc., were represented by a rectangular distribution.

iv) Limitation on number of adjusted measurements

Mathiesen considered the adjustment of a redundant set of m measurements which were subjected to p linear equality constraints and q linear inequality constraints. He pointed out that the linear programming method would divide the m measurements into (m - p) measurements that are not adjusted, and would adjust a sub-set of the remaining p measurements.

This statement of Mathiesen's is not strictly correct, since for each inequality constraint that becomes "tight," it is possible to adjust an extra measurement in addition to the p measurements corresponding to the number of equality constraints. However, this limitation on the number of adjusted measurements, means that the linear programming method is not suitable for the data reconciliation of mass flow data involving a large number of flow measurements but few constraints (e.g. material balances). The quadratic or 'least squares' method could be used for such data only if the measurement errors have a normal distribution.

In the No. 2 Ethylene data reconciliation model, there exist a satisfactory ratio of equality constraints to flow measurements. The No. 2 Ethylene data reconciliation LP matrix consists of:-

165 variables (includes flows defined as combined flows)

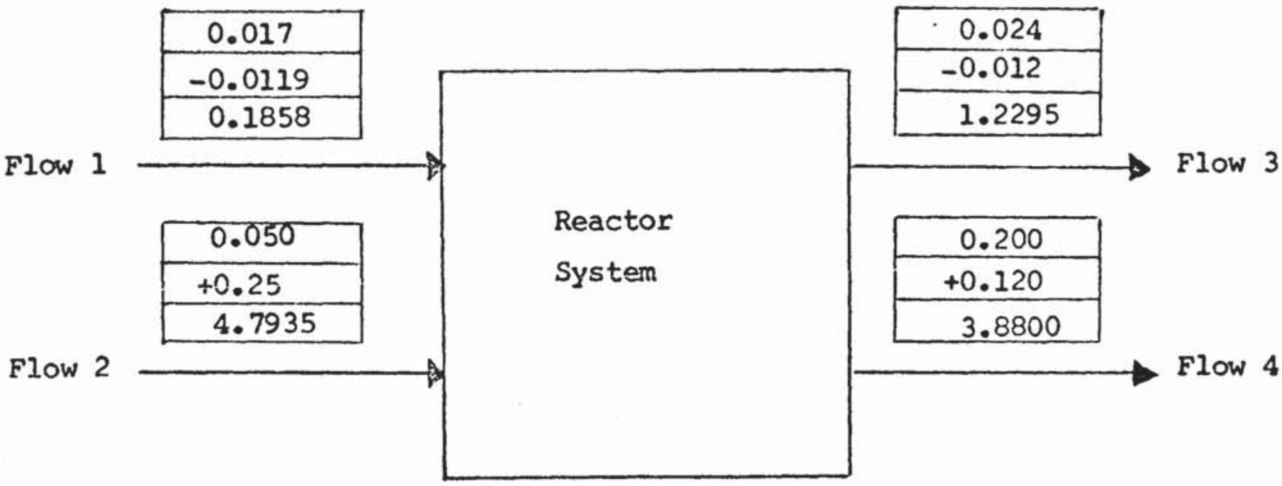
64 equality constraints (material balances)

52 inequality constraints (yield and loss constraints etc.).

The ratio of total constraints to variables is 0.703. The ratio of equality constraints to variables (i.e. 64/165 = 0.39) is approximately the same as used in the data reconciliation test system in section 4.3.2. The test system comprised of 5 mass balances and 13 flows giving a ratio of 0.38.

v) Adequacy of Linear Method for directly identifying gross measurement errors

Mathiesen concluded that the linear method is able to identify the existence of gross systematic errors in the data set, but is inadequate in directly identifying the measurements containing the errors. To demonstrate this effect he employed the same simple numerical example used by Ripps (19) and summarised in Fig. 4.8. The example involved four measured mass flows (measurements, $m = 4$) two entering and two leaving a chemical reactor. Three elemental material balances (e.g. a carbon balance) were defined in terms of the four flow measurements (equality constraints, $p = 3$). In order to identify the measurements in gross error, Mathiesen suggested that it was necessary to discard measurements one at a time from the data set, and to observe the values of the



KEY

Standard Deviation S_i
Absolute Error E_i
Measured Flow F_i

Elemental Mass Balances

$$0.1\,F_1 + 0.6\,F_2 - 0.2\,F_3 - 0.7\,F_4 = 0$$

$$0.8\,F_1 + 0.1\,F_2 - 0.2\,F_3 - 0.1\,F_4 = 0$$

$$0.1\,F_1 + 0.3\,F_2 - 0.6\,F_3 - 0.2\,F_4 = 0$$

Weights

Weights, W_i = 1/Standard Deviation, S_i

FIG 4.8 EXAMPLE USED BY MATHIESEN

data reconciliation error criterion. This approach was similar to that used by Ripps (19) and Nogita (21) in identifying and eliminating gross errors.

Data reconciliation at Baglan Bay has shown that the modulus error criterion and linear programming method are, in general, able to adequately identify and correct gross systematic errors. The trivial example used by Mathiesen was not typical of data reconciliation at Baglan Bay. The No. 2 Ethylene data reconciliation model was defined using equality constraints consisting of only bulk mass balances. As the LP matrix coefficients of these constraints are all unity, the choice of which variables are adjusted (i.e. enter or leave the LP basis) is determined solely by the size of the mass balance errors and the weights used in the error criterion objective function. The inclusion of component or elemental mass balances, as used in the example of Mathiesen, affects the selection of which variables are to be adjusted. The coefficients of the component or elemental balances decide which variables leave the LP basis and thus act as pseudo weighting factors.

In the example of Mathiesen, inlet flow no. 2 and outlet flow no. 4 each contained large positive absolute errors compared with small absolute errors in the other two flows. Thus, whereas the total material balance was only 0.1302 units, the sum of the errors in the flow measurements was 0.3939 units. To make the smallest linear change in a system consisting of 4 measurements and 3 equality constraints, a maximum of 3 measurements will be adjusted. The four possible combinations of flow changes which the linear method might select in Mathiesen's example are shown in Fig. 4.9. The particular combination of flow changes chosen depends on the weights used in the error criterion. For instance, with equal weights combination No. 4 would be selected, while for the

Flow No. (F_i)	Absolute error in Flows (e_i)	Weights used by Mathiesen (W_i)	Combination of linear flow changes (ΔF_i) 1	2	3	4
1	-0.0119	58.8	0	-0.0205	-0.0100	-0.0170
2	+0.25	20.0	+0.5947	0	+0.3001	+0.0987
3	-0.012	41.7	+0.0711	-0.0724	0	-0.0486
4	+0.120	5.0	+0.3934	-0.0783	+0.1598	0
Error Criterion		$\sum$ Mod (ΔF_i)	1.0592	0.1712	0.4699	0.1642
Error Criterion		$\sum$ Mod ($W_i \Delta F_i$)	16.825	4.615	7.387	4.999

FIG. 4.9 POSSIBLE COMBINATION OF FLOW CHANGES IN EXAMPLE OF MATHIESEN

weights used in Mathiesen's example, combination No. 2 was selected. However, since the elemental balance equations can be satisfied by making total flow changes that are significantly smaller than the original sum of errors in the flow measurements (i.e. 0.3939), unless the weights reflect the size of the errors in the measurements, the adjusted set of results is likely to fail to identify the errors in the data. This is what happened in Mathiesen's example. Similar effects occurred in data reconciliation at Baglan Bay, but were found to be the exception rather than the rule. The fallibility of data reconciliation is discussed in the last paragraph of this section.

The way in which the modulus criterion is able, at Baglan Bay, to identify gross flow measurement errors can be demonstrated by considering the simple 2 balance system (equality constraints, $p = 2$), with 3 flows (measurements, $m = 3$), shown in Fig. 4.10. If the true flows are 10 units, consider a gross error in flow 2 producing a measured flow of 5 units. The modulus data reconciliation mathematical definition of the system with equal weights applied to the measurements is:

$$
\begin{array}{llll}
\text{Minimise} & \left| \Delta F_1 + \Delta F_2 + \Delta F_3 \right| & & \text{(Error Criterion)} \\
\text{subject to} & \Delta F_1 - \Delta F_2 & = -5 & \text{(Balance 1)} \\
 & \qquad + \Delta F_2 - \Delta F_3 & = +5 & \text{(Balance 2)}
\end{array}
$$

where $\Delta F_i, i = 1$ to 3 represent the flow adjustments.

It is obvious that the linear programming method would select flow 2 and change it by 5 units (i.e. $\Delta F_2 = +5$) to make the smallest linear change to satisfy the material balances. Hence it has identified and corrected the gross error in stream 2. Similarly, if a gross error existed in either stream 1 or 3 the LP technique would identify and correct the stream in error.

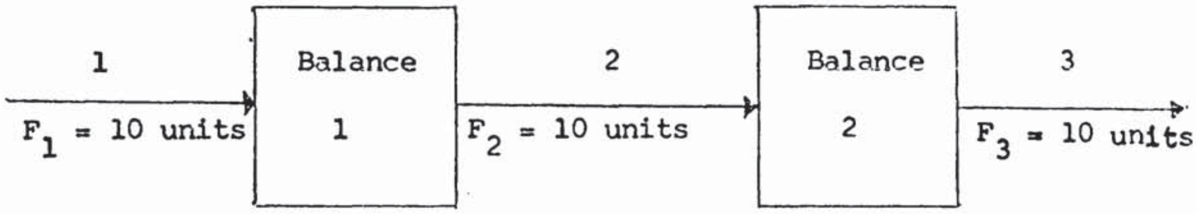


FIG.4.10 Simple mass flow measuring system used to demonstrate how modulus error criterion identifies gross meter errors.

However, data reconciliation is not fool-proof. It depends greatly on the values of the weights used in the error criterion, since it is through the judicious selection of weights that the user of data reconciliation is able to reflect his own judgement and any additional information about the quality of the raw unreconciled data. For instance, if it is known in advance that a raw measurement has a gross error, then the lack of confidence in the measurement can be reflected in the data reconciliation model by the use of a small weight. However, since the weights in the weighted error criterion normally reflect the inherent errors associated with the measuring instruments, it should not be surprising if the method proves unsatisfactory in cases where an inherently accurate meter has a large gross systematic error. It is a matter of whether the supporting evidence of inherently less accurate but consistent measurements is greater than the weighted contribution of the inherently accurate measurement with the gross error. In such cases it is often necessary to apply a small weight to the faulty measurement and re-run the data reconciliation model.

4.6 CONCLUSIONS

Consistent manual adjustment of data from a large scale industrial mass flow measuring system, such as found at Baglan Bay, is not feasible. Automatic data reconciliation is a consistent method for reconciling such data. However, skilful human intervention is required to ensure that maximum benefit is derived from the data reconciliation technique. Human intervention normally involves the setting of measurement accuracies that reflect the confidence in the raw measured flow data.

From an analysis and estimation of the errors that exist in industrial flow data it was seen that it is the gross systematic errors that dominate and present the major data reconciliation problems. It was demonstrated that a linear modulus data reconciliation error criterion was more suitable than quadratic criteria for reconciling industrial flow data. Consequently, it was possible to use the versatile and well proven technique of linear programming for reconciling data. A standard and robust LP package was available, thus ensuring that development problems were minimised. An important feature of linear programming in its application to data reconciliation is the use of inequality constraints. The inclusion of process yield and efficiency constraints ensures that reconciled data are technically feasible as well as mathematically feasible. Although data reconciliation is able to identify and correct faulty data, and provide estimates for unavailable data, it must not be regraded as a panacea for poor quality data.

The work of Mathiesen endorses the use of linear programming for data reconciliation. It was shown, however, that some of the conclusions he drew from an example used to demonstrate the technique, cannot be generalised.

A data reconciliation system for the No. 2 Ethylene Complex was successfully developed and implemented. The system, which involves the collection, reconciliation and reporting of data, provides Factory management with high quality consistent data upon which decisions can be made. The data reconciliation system also provides an incentive for maintaining a high standard of flow instrumentation.

CHAPTER 5

MODELLING AND SIMULATION OF THE COLD END OF AN ETHYLENE PLANT

CHAPTER 5 - MODELLING AND SIMULATION OF THE COLD END OF AN ETHYLENE PLANT

5.1 INTRODUCTION

This Chapter describes how systems engineering was applied to the analysis, modelling and simulation of a large scale industrial process system in the form of the Cold End of the No. 2 Ethylene Plant.

First, general systems engineering concepts, which were based on the work of Jenkins (2), are introduced. How these concepts were applied to the analysis, modelling and simulation of the Cold End is described in the subsequent sections of the Chapter. In establishing a performance criterion for the Cold End, reference is made to Chapter 1, which describes the Ethylene Plant and Cold End as systems, and to Chapter 2 which contains a preliminary analysis of these systems. Chapter 2 identified characteristic features of the Cold End and presented a case for its modelling and simulation. Having defined a performance criterion, and decided that the operation of Cold End compressors and turbines are prime factors in the determination of this criterion, a section briefly describes the characteristics and operation of centrifugal compressors.

The Chapter then proceeds to describe the development of the Cold End models. The initial objective of the modelling work is defined and the Cold End systems are further analysed for the purpose of modelling. The approach to modelling is discussed and the computer structure and formulation of the models are described from a systems engineering viewpoint. Points arising from the verification of the models are discussed and examples are given showing how the models were used to simulate the behaviour of the Cold End system and sub-systems.

Finally, the value of using systems engineering in the study is assessed, and recommendations are made as to how future Cold End modelling work should proceed.

5.2 SYSTEMS ENGINEERING CONCEPTS

Systems engineering is concerned with the interactions between units within a larger system, and with how these units should be designed and operated so that the performance of the whole system can be improved.

It is appropriate to define some properties of an industrial process system of which the No. 2 Ethylene Plant is an example.

An industrial process system:-

i) is a grouping of process units.

ii) may be broken down into sub-systems which may interact with one another.

iii) will usually form part of a hierarchy of such systems.

iv) has an objective.

v) should be designed and operated in such a way that it will achieve its objective.

The normal stages through which a systems engineering study can pass are:-

i) Establishment of Criteria.

ii) Model Building.

iii) Simulation.

iv) Optimisation.

v) Control and Implementation.

5.2.1 Establishment of Criteria

To set a problem in its proper perspective the type of questions to be ased are (2)

i) What is the problem?

ii) What is the system?

iii) What is the wider system of which this system forms part?

iv) What is the objective of the wider system?

v) What is the objective of the system?

vi) What is the relevant performance criterion for measuring the efficiency with which the system can achieve its objective?

5.2.2 Model Building

A model of a system has been described by Jenkins (2) as a quantitative description of the behaviour of the system which can be used to predict system performance over a relevant range of operating conditions. A model need only describe the system in sufficient detail to give acceptable accuracy in the performance criterion over this range of operating conditions.

Model building is an iterative or adaptive process in which one moves from a state of little knowledge to one of greater knowledge. Experience and judgement are needed to decide which type of model should be used for a particular situation. In general, modelling in systems engineering requires that one should start with whatever knowledge of the system is available, and how one builds on this is dictated by time, resources and the accuracy required by the model. During model building it is necessary to find out:-

i) which variables are important

ii) why and how such variables influence the performance of the system.

Model building is concerned with ways in which local models, which describe the behaviour of sub-systems, can be linked together to form a global model which can then be used to examine overall system performance. The importance of being able to estimate overall system performance is essential to avoid what is called sub-optimisation. Optimisation of each sub-system independently does not necessarily lead to a system optimum. In building local models, one should concentrate on those aspects which are important to the objective of the global model.

5.2.3 Simulation

Once a model of a system has been built it can be used to simulate the behaviour of the system when subjected to:-

i) realistic inputs typical of those which the system experiences in practice.

ii) realistic disturbances which will cause the behaviour of the system to fluctuate from its steady state performance.

If the simulation is accurate, data generated from the simulation should agree closely with data from the operational system.

5.2.4 Optimisation

Equipped with a model which can predict system performance, it is possible to calculate a systems performance criterion (e.g. minimise utility cost or maximise throughput) for different modes of operation. Finding a set of operating conditions which result in the most favourable value of the performance criterion is what is meant by optimisation.

5.2.5 Control and Implementation

Following optimisation it is necessary to examine how the system can be controlled so that the optimised conditions can be achieved in practice. In order to justify the appropriate degree of sophistication in the control system, the cost of control must be balanced against the cost of deterioration in the performance criterion.

The final stage of the study is the implementation of the findings arising from the study.

The following sections will describe how systems engineering was applied to the analysis, modelling and simulation of the Cold End of the No. 2 Ethylene Plant.

5.3 ESTABLISHMENT OF CRITERIA

In establishing a performance criterion for the system under examination (i.e. the Cold End of the No. 2 Ethylene Plant) it is necessary to refer to previous chapters of the thesis.

5.3.1 The Problem

A concise statement of the problem and motivation behind the work was that a need was recognised (1) for some form of mathematical aid/models of the Ethylene Plant and other key plants in the Baglan Bay Factory, in order to assist management in decision taking at the supervisory control level. Reasons why the operation of the No. 2 Ethylene Plant would benefit from the availability of such models were discussed in Chapter 2.

5.3.2 The Wider System and System

The wider system and system under examination were defined as

i) The Wider System - No. 2 Ethylene Plant.

ii) The System - Cold End of No. 2 Ethylene Plant.

5.3.2.1 The Wider System (No. 2 Ethylene Plant)

The function of the No. 2 Ethylene Plant is to produce, by the steam cracking of naphtha, and to recover, olefinic type products. The No. 2 Ethylene Plant was described in Chapter 1. The Plant was divided into its component sub-systems, as shown in Fig. 1.4, and the function of, and interactions between, the sub-systems described. The two major sub-systems of the Plant were identified as the Hot End and the Cold End. Selection of the Cold End, as the system to be examined in detail, was a consequence of:-

i) the natural division of the Plant into two main systems (i.e. Hot End and Cold End).

ii) the confidentiality of Hot End furnace information.

5.3.2.2 The System (Cold End of No. 2 Ethylene Plant)

The function of the Cold End is to recover the olefinic products produced by the steam cracking of naphtha. The Cold End is comprised of the following three sub-systems.

i) Cracked gas compression.

ii) Process fractionation.

iii) Refrigeration.

Fig. 5.1 shows the principal material and energy flows between these sub-systems. In Chapter 2, a preliminary systems analysis of the Cold End sub-systems identified:-

i) features of these sub-systems which characterised the performance of the Cold End.

ii) the need for modelling the Cold End.

From this analysis it was recognised that the cracked gas compression system, process fractionation system and the refrigeration

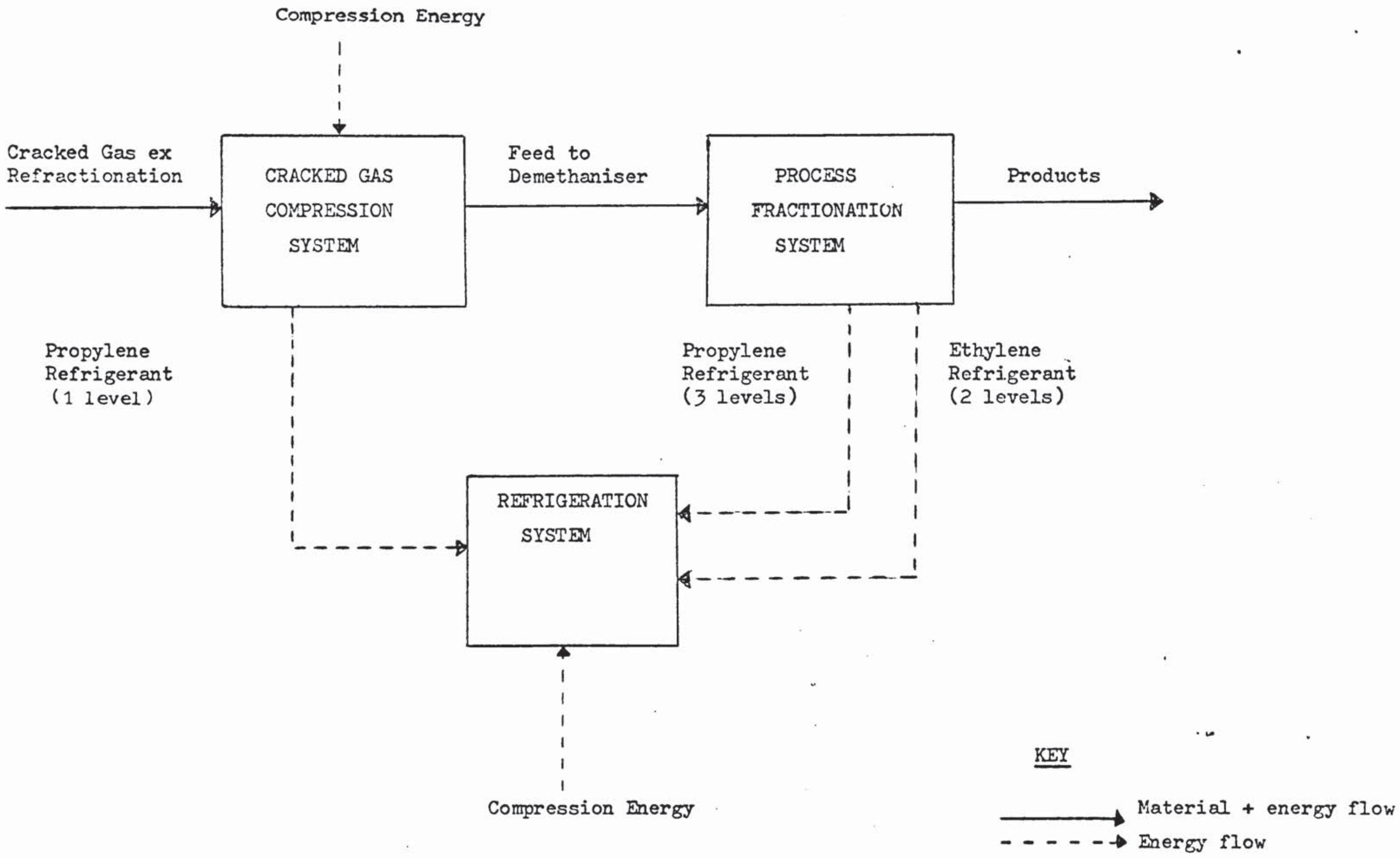


FIG. 5.1: PRINCIPAL MATERIAL AND ENERGY FLOWS BETWEEN COLD END SUB-SYSTEMS

system are complex systems possessing a high degree of interaction with one another.

5.3.3 System Performance Criterion and Objectives

An appropriate criterion for measuring the economic operating performance of the Cold End is cash surplus, as defined by the following equation:-

i.e. Cash Surplus = Value of Products - Cost of Feed - Cost of Utilities

(Utilities consist of steam, cooling water, power for compressors and pumps etc.).

The cash surplus equation takes account of the major cash flows entering and leaving the Cold End. The costs included in the equation are variable processing costs which are functions of plant operation. Fixed costs such as plant depreciation and plant overheads can be regarded as independent of plant operation. The cash surplus performance criterion can be expressed algebraically as follows:-

$$C = F\ (P_2 \cdot y + P_3 \cdot (1 - y)) - F \cdot P_1 - F \cdot P_4 \qquad - \quad (5.1)$$

where

C = Cash Surplus (£/unit time)

F = Flow of cracked gas to the Cold End (mass/unit time)

P_1 = Unit value of cracked gas feed to the Cold End - fuel gas value (£/unit mass)

P_2 = Unit value of cracked gas based on product values of components (£/unit mass)

P_3 = Unit value of fuel gas (£/unit mass)

P_4 = Unit utility cost for cracked gas at throughput F (£/unit mass)

y = efficiency factor (0 to 1) which takes into account two effects:

i) slippage of high value products into lower value products and fuel gas, i.e. recovery efficiency of Cold End.

ii) production and recovery of products in excess of market limits. The price structure for a typical cracked gas product is shown in Fig. 5.2

Substitution, into equation 5.1, of unit values and costs which are relatively correct and are based on the design performance of the plant would produce an expression of the form

$$C = F\,(25y + 10\,(1 - y)) \;-\; F.10 - F.3 \qquad - \qquad (5.2)$$

Products Feed Utilities

The efficiency factory, y, will normally lie between 0.90 and 0.99. From equation 5.2 it can be seen that the upgrading in value of the cracked gas by the Cold End (value of products - value of feed) is approximately 5 times as great as the utility costs incurred in processing the gas. Hence, the effect of utility costs on cash surplus is of secondary importance compared with achieving the required plant throughput and recovery of products. It is important to ensure that any reduction of utility costs does not jeopardise plant reliability and consequently affect plant production.

The relative effects of throughput, product recovery and utility consumption on the cash surplus (performance criterion) are reflected in the evolving objectives of Ethylene Plant and Cold End operation. These objectives were defined as:-

i) during commissioning - to establish reliable operation.

ii) post commissioning - to establish production levels and product recoveries.

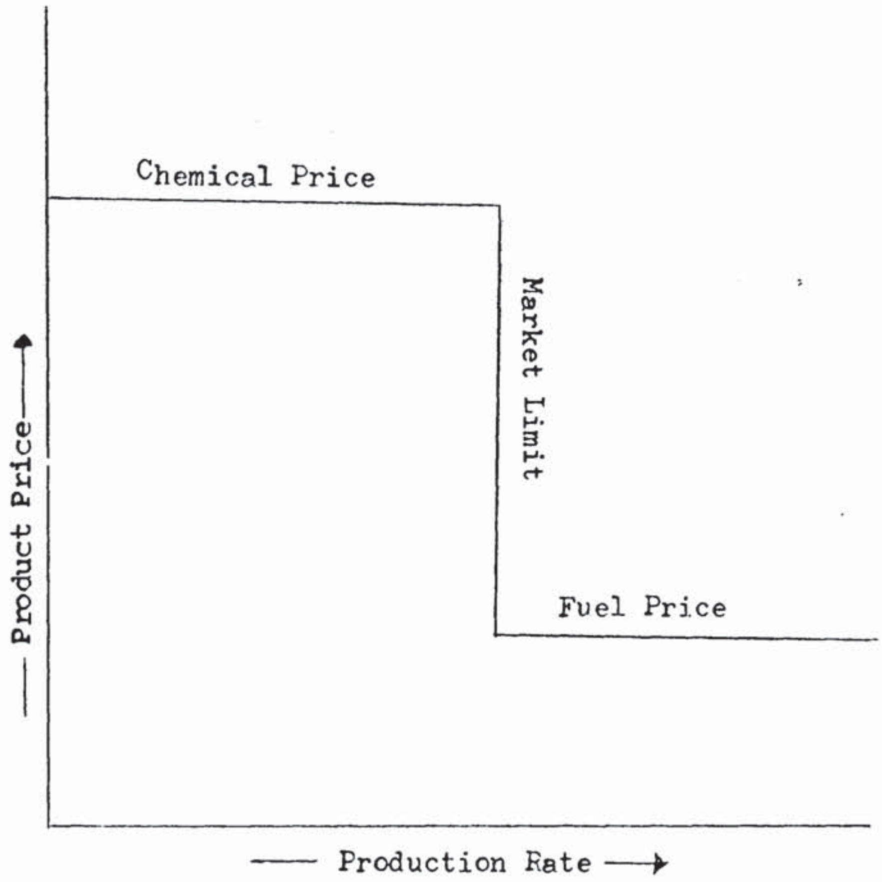


FIG.5.2 Product Price Versus
Production Rate

iii) subsequent operation - to achieve production requirements at minimum cost.

The timing and priorities of the Ethylene Plant objectives were reflected in the objectives of the Cold End modelling work. The modelling objectives were defined as:-

i) to provide an understanding of the interactions that exist between the refrigeration, compression and fractionation systems.

ii) to provide a measure of the effect of such interactions on Cold End system performance.

iii) to examine the optimal operation of the Cold End System.

iv) to contribute to the optimal operation of the wider system i.e. Ethylene Plant.

5.3.4 System v Sub-System Performance

If a particular sub-system is found to be dominating system performance, the optimisation of that sub-system will improve the overall system performance. For the Cold End System, the sub-systems involving the large centrifugal compressors are the dominant sub-systems.

5.3.4.1 Cold End Compressors as a Measure of System and Sub-System Performance

The major Cold End equipment items that are primary factors in the determination of Cold End processing capacity and utility consumption are the cracked gas and refrigerant compressors/turbines. They account for approximately 15 percent of the total Ethylene Plant capital cost, govern plant throughput, and consume 30 to 40 per cent of the total energy demand. It is important that the Cold End is operated to derive maximum benefit from the compressor/turbine installations and that optimal compressor loadings be established. Hence, both Cold End system and sub-system performance were studied initially in terms of the performance of the cracked gas and refrigerant compressors.

A brief description of the factors affecting the performance of centrifugal compressors is given in the following section. The main performance variables of interest are summarised and the performance of the cracked gas and refrigerant compressors are discussed.

5.4 CENTRIFUGAL COMPRESSORS

5.4.1 General

A multistage centrifugal compressor consists of a stationary casing and a rotor which is comprised of a series of rotating blades (wheels) mounted on a single shaft. The casing serves to guide the gas to and from the rotor and to convert the kinetic energy of the gas leaving the rotor into pressure. The function of the wheels is to generate fluid energy or head which averages about 10,000 ft. of fluid flowing per wheel.

The rotary centrifugal cracked gas and refrigerant compressors are operated to maintain fixed pressure ratios by adjustment of the compressor machine speeds. The performance curves shown in Fig. 5.3 define the characteristics of a compressor stage in a multistage compressor. To maintain a fixed pressure ratio for different volumetric flow rates, the compressor machine speed changes along a horizontal line on the compressor characteristic curves. Each compressor stage has capacity constraints. The upper capacity constraint is the series of maximum volumetric throughputs which the stage is capable of processing at fixed pressure ratios. The lower capacity constraint, known as the surge limit, are the volumetric flows below which compressor operation is unstable. Below the surge limit the unstable pulsating operation is

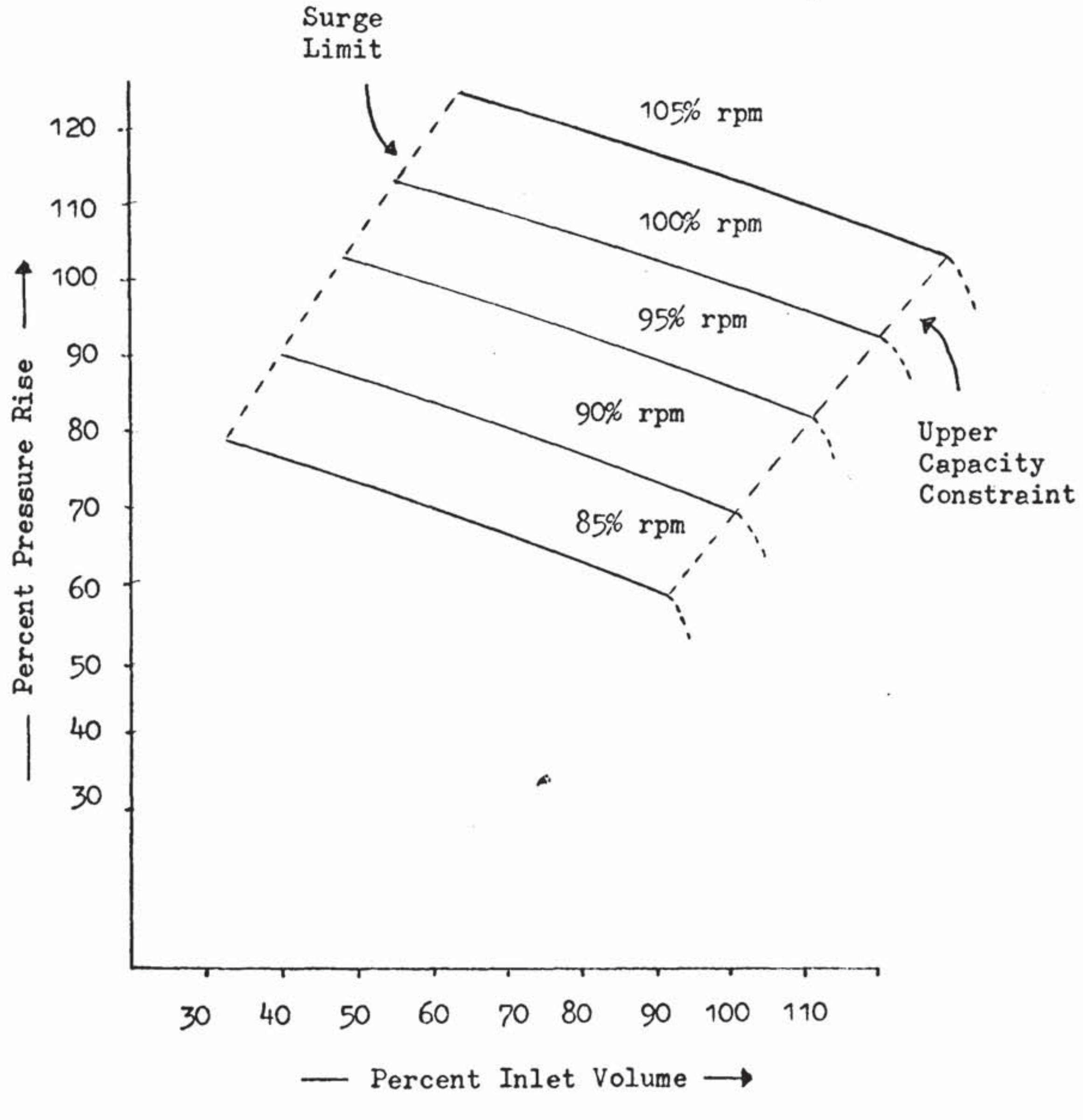


FIG. 5.3 VARIABLE SPEED PERFORMANCE CURVES FOR CENTRIFUGAL COMPRESSOR STAGE.

called surge. Surge is caused by collapse of the flow pattern in the impellers and normally occurs at about 45 to 55% of the compressor stage design flow. The compressor control system prevents surging by directly recycling vapour from the discharge to the suction of the compressors when the volumetric flow through the compressor falls below a certain value. Both the upper capacity and the surge limits are functions of the compressor speed and are determined by the type and size of the compressor frame.

Approximately half the cost of a compressor installation is the driver. The steam turbines used to drive the compressors must have a good speed match with the compressors. A turbine usually drives a series of compression stages thus making the performance of the compressor stages highly interdependent. The turbine capacity constraint is the maximum compression energy that can be transferred from the turbine to the compressor. This limit is determined by the mechanical design of the turbine.

To understand which variables influence compressor capability it is necessary to examine the head/pressure relationship for a compressor stage. Each compression stage has a design capability, normally expressed as ft/lb/lbs, or more commonly as 'feet of head'. The head/pressure relationship may be expressed as follows:

$$H_p = T_i \frac{1544}{MW} Z \frac{n}{n-1} \left\{ \left(\frac{P_2}{P_1} \right)^{\frac{n-1}{n}} - 1 \right\} \qquad - \qquad (5.3)$$

where

H_p = Polytropic head (ft/lb/lbs)

T_i = Inlet temperature to the compressor stage (^{o}F)

$\frac{1544}{MW}$ = R_1 the gas constant

MW = Mole weight of the gas

n = Polytropic factor ($n = E \times k$)

E = Polytropic efficiency (72 to 88%)

k = specific heat ratio

Z = compressibility factor

P_2 = discharge pressure (psia)

P_1 = suction pressure (psia)

The polytropic head is related to compressor brake horsepower (b.h.p.) as follows:

$$\text{b.h.p.} = 5.05 \times 10^{-5} \; \frac{W}{E} \; H_p \qquad - \qquad (5.4)$$

where W = Pounds per hour of gas

It can be seen from equations 5.3 and 5.4 that the compression energy (b.h.p.) is a function of the inlet temperature and molar flow of the gas (molar flow equals mass flow divided by mole weight). In practice, it is expedient to manipulate the temperature and molar flow of the gas in order to reduce the compression energy and polytropic head of the stage, whilst still ensuring that the required pressure rise is achieved.

5.4.2 Cold End Cracked Gas and Refrigerant Compressors

During the simulations of the Cold End system and sub-systems, as described in Section 5.6, the main performance variables examined were those that described the performance of the Cold End compressors. These variables included:-

i) Compression energy

ii) Compression stage flow rates

iii) Compression stage inlet temperatures

iv) Molecular weights of flows to compression stages

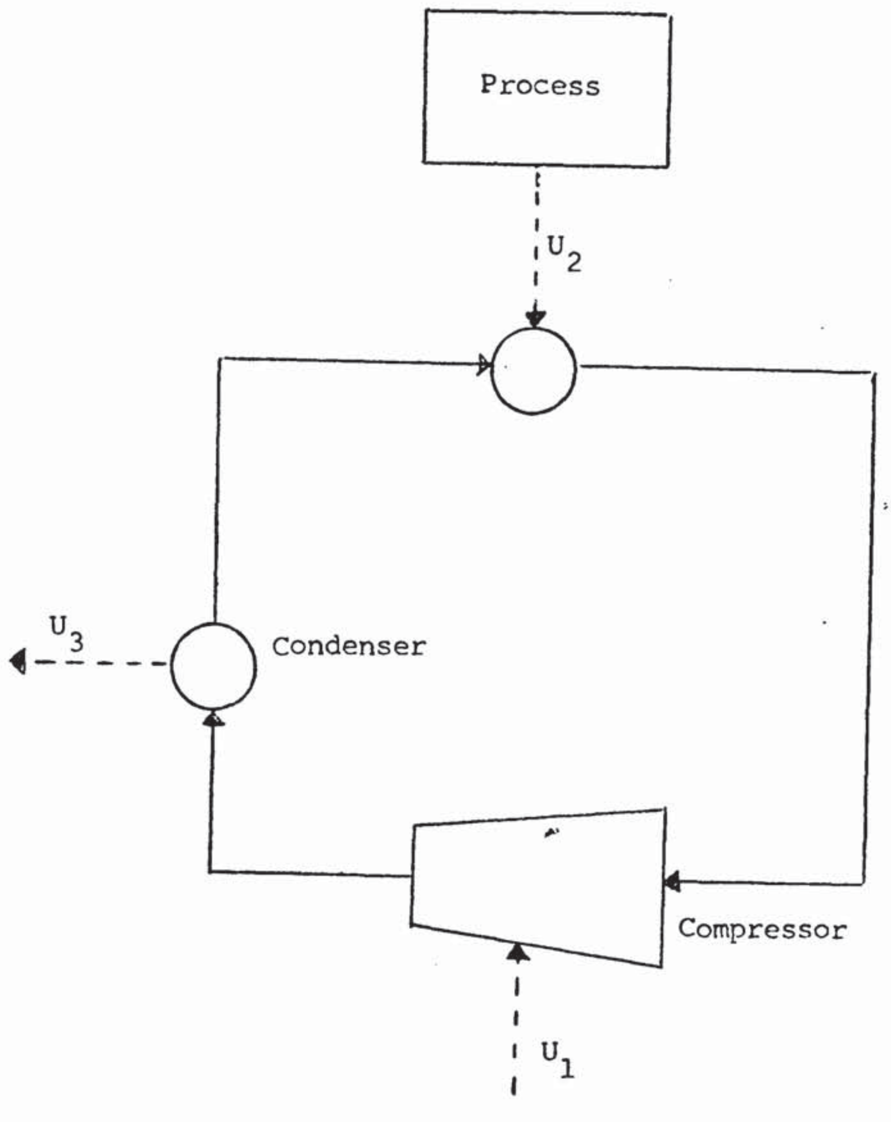
v) Compressor speed.

5.4.2.1 Cracked Gas Compressors

In Section 5.4.1 it was shown that the compression stage inlet temperatures and molar flows are important variables in the determination of compression energy. Control of the inlet temperatures of the cracked gas to the compression stages of the cracked gas compressors is achieved by adjusting the cooling water flows to the aftercoolers. However, a change in inlet temperature is accompanied also by a change in the molar flow of the cracked gas. This effect is due to the temperature change altering the complex vapour/liquid hydrocarbon splits in the interstage separators. Therefore, if optimal operation of the cracked gas compression system is to be achieved, judicious selection of after-cooler temperatures is required whilst ensuring that turbine, compressor and aftercooler constraints are not violated.

5.4.2.2 Refrigerant Compressors

The two key equipment items in the refrigeration system are the compressor/turbine installation and the refrigerant condenser. If the refrigeration system, as shown in Fig. 5.4, is examined in its simplest form, it is evident that the condenser must be capable of removing an energy load equivalent to the sum of the energy of compression and the net energy removed from the process. Thus, either the condenser, compressor or turbine can directly limit the refrigeration capacity of the system. The refrigeration compressors, unlike the cracked gas compressors compress a single component fluid. Their performance is closely involved with the process fractionation system since interstage cooling is achieved by the process streams. It should be the aim of the process fractionation



$U_3 = U_1 + U_2$

where

U_1 is the compression energy

U_2 is the net energy removed from the process systems

U_3 is the energy removed in condensing the refrigerant.

FIG. 5.4 REFRIGERATION SYSTEM

system to maximise the refrigeration recovery from the process streams whilst achieving the desired separation and recovery of cracked gas products.

5.5 COLD END MODEL BUILDING

5.5.1 Objective of Modelling Work

The objectives of the modelling work to satisfy the Cold End System requirements were stated in 5.3.3 as:-

i) to provide an understanding of the interactions that exist between the refrigeration, compression and fractionation systems.

ii) to provide a measure of the effect of such interactions on Cold End System performance.

iii) to examine the optimal operation of the Cold End System.

iv) to contribute to the optimal operation of the wider system i.e. Ethylene Plant.

Initially, modelling work was confined to the first two of these objectives. Thus the objective of the modelling work in this study was:-

to develop models in order to explore and understand the interactions that exist between and within the Cold End sub-systems, and to relate the effect of such interactions on Cold End System performance.

5.5.2 Approach to Modelling

i) Parsimonious Approach

It was important to adopt a parsimonious approach to the Cold End modelling work in order to assess which sub-units must be modelled accurately and which need only be crudely represented. If such an approach had not been taken, much time and effort may have been wasted in building accurate models in areas which have little influence on the performance of the system, and where the crudest models would have sufficed.

Thus, simple model representations were used initially to describe the performance of the process units. The depth of detail included in the models was determined by their adequacy to simulate the principal flows of material and energy between and within the Cold End sub-systems, and to enable estimations of cracked gas and refrigerant compressor performance to be assessed. The parsimonious approach to the formulation of the Cold End models is discussed in Section 5.5.5.

ii) <u>Modular Approach</u>

It was found expedient through careful division of the Cold End into a number of sub-systems, and through an appreciation of the material and energy links between these sub-systems, to model and simulate individual sub-systems separately and then, whenever suitable, merge together the sub-system models. The major Cold End sub-systems were:-

a) Cracked gas compression

b) Process fractionation

c) Refrigeration.

For instance, although the refrigeration energy links between the process and refrigeration systems are extensive, it is shown in Section 5.5.5, how it was possible to 'un-couple' these systems, model them separately, and then merge them as part of the global steady state Cold End model.

This modular approach had the advantage of:-

a) enabling modelling effort to be directed first towards those sections of the Cold End where there existed a greater incentive for the development of a model.

b) enabling individual sub-system models to be checked and verified before being merged together. The size and complexity of the systems under examination made this checking of sub-system models virtually essential.

c) providing greater understanding of the Cold End sub-systems and of their contribution to overall Cold End performance.

A summary of the stages in the development of the global Cold End model from the individual local sub-system models is shown in Fig. 5.5 Three basic models were developed comprising of a cracked gas compression model, process fractionation model and a refrigeration model. The cracked gas compression and process fractionation models shared many common features since both were concerned with the processing of streams containing complex mixtures of hydrocarbons. A fundamental requirement of the models was the determination of vapour/liquid splits for these hydrocarbon mixtures. Section 5.5.5 discusses features of the models and demonstrates how systems engineering was used in the formulation of the models.

5.5.3 Definition of Cold End Sub-Systems for Modelling

This section introduces operating and design features of the Cold End sub-systems (i.e. Cracked Gas Compression, Process Fractionation and Refrigeration Systems) relevant to the Cold End modelling work and discusses how the Cold End can be divided into a series of interlinking systems for the purpose of Cold End modelling. Fig. 5.1 is a block

FIG. 5.5 DEVELOPMENT OF COLD END MODEL

ACT.	MODEL	DESCRIPTION OF MODEL	PURPOSE OF MODEL
1	Cracked Gas Compression System	Model of cracked gas interstage system involving:- i) mass balances ii) heat balances	i) to establish a set of K value/enthalpy data sufficient to reflect plant operation. ii) to explain the plant operational data. iii) to examine the distribution of loading on each compressor stage.
2	Cracked Gas Compression System	Extension of Model to include:- i) improved representation of compression stages.	i) extension of above in certain areas.
3	Refrigeration System	Model of propylene compression with single 'lumped' representation of heat exchangers at each of the three refrigerant levels.	i) to examine sensitivity of compressor operation and interstage flows to changes in refrigerant loads. ii) to evaluate adequacy of compressor model.
4	Process Fractionation System	Comprises all key process units directly affected by the propylene refrigeration system. i.e. Cracked gas chilling Demethaniser De-ethaniser Ethylene Tower	i) to establish energy demands upon the propylene refrigeration system for various process conditions.
5	Process Fractionation System ⇠ - - ⇢ Refrigeration System	Combined simulation of process fractionation and refrigeration systems. The refrigeration system contains a simple linear representation of the ethylene refrigeration system.	i) to examine the combined effect of the process fractionation and refrigeration systems.
6	Cracked Gas Compression System → Process Fractionation System; Cracked Gas Compression System ⇠ - - ⇢ Refrigeration System; Process Fractionation System ⇠ - - ⇢ Refrigeration System	Combined simulation of the process fractionation, refrigeration and cracked gas compression systems.	i) to examine interactions between three systems.

KEY ——→ Material Flow

- - - -→ Energy Flow

diagram showing the main material and energy links between the three principal Cold End sub-systems, while Fig. 5.6 shows how these systems can be further sub-divided for the purpose of Cold End modelling.

5.5.3.1 Cracked Gas Compression System

The cracked gas compression system, which is shown schematically in Fig. 1.4, accounts for between 15 and 20 per cent of the total energy consumption of the Ethylene Plant. It consists of two sets of parallel compressor trains, each train having an independent cracked gas interstage system for cooling and separating the vapour/liquid phases of the compressed cracked gas. However, both trains share the same condensate stripper. Compression is achieved, for each train, by two separate machines; a low pressure two stage turbo compressor set which has a condensing turbine, and a high pressure two stage turbo compressor set with a back pressure turbine.

The main material and energy connections between the cracked gas compression system and the other Cold End sub-systems are through the demethaniser feed flow and propylene refrigerant which is used for cooling the cracked gas. Minor vent streams are also recycled from the fractionation system to the cracked gas compression system.

Hence any modelling and simulation of the cracked gas compression system must take account of these interactions with the other Cold End systems.

5.5.3.2 Process Fractionation System

The process fractionation system of the Cold End is shown schematically in Fig. 5.7. It is possible to divide the system into two sub-systems for the purpose of the Cold End modelling.

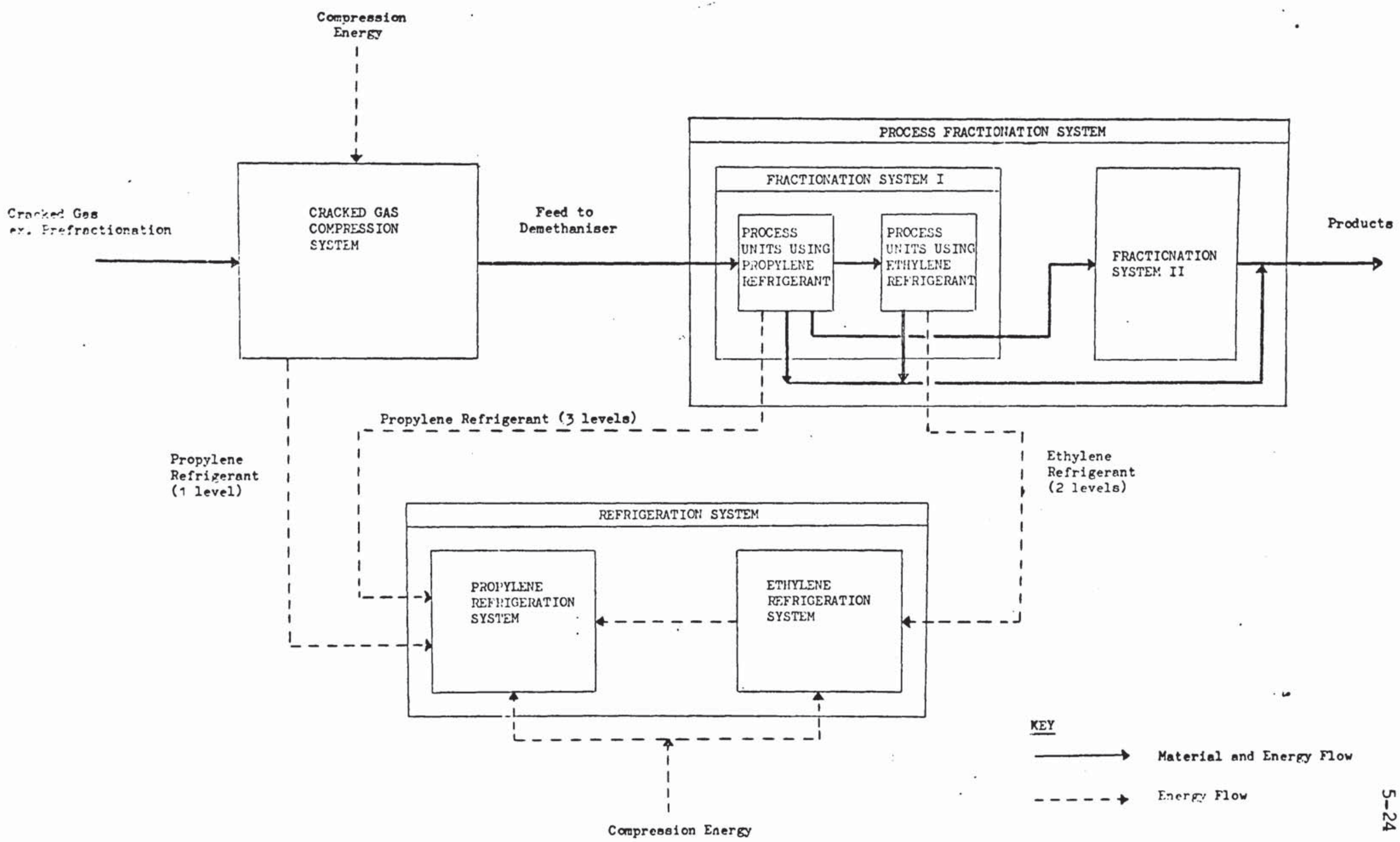
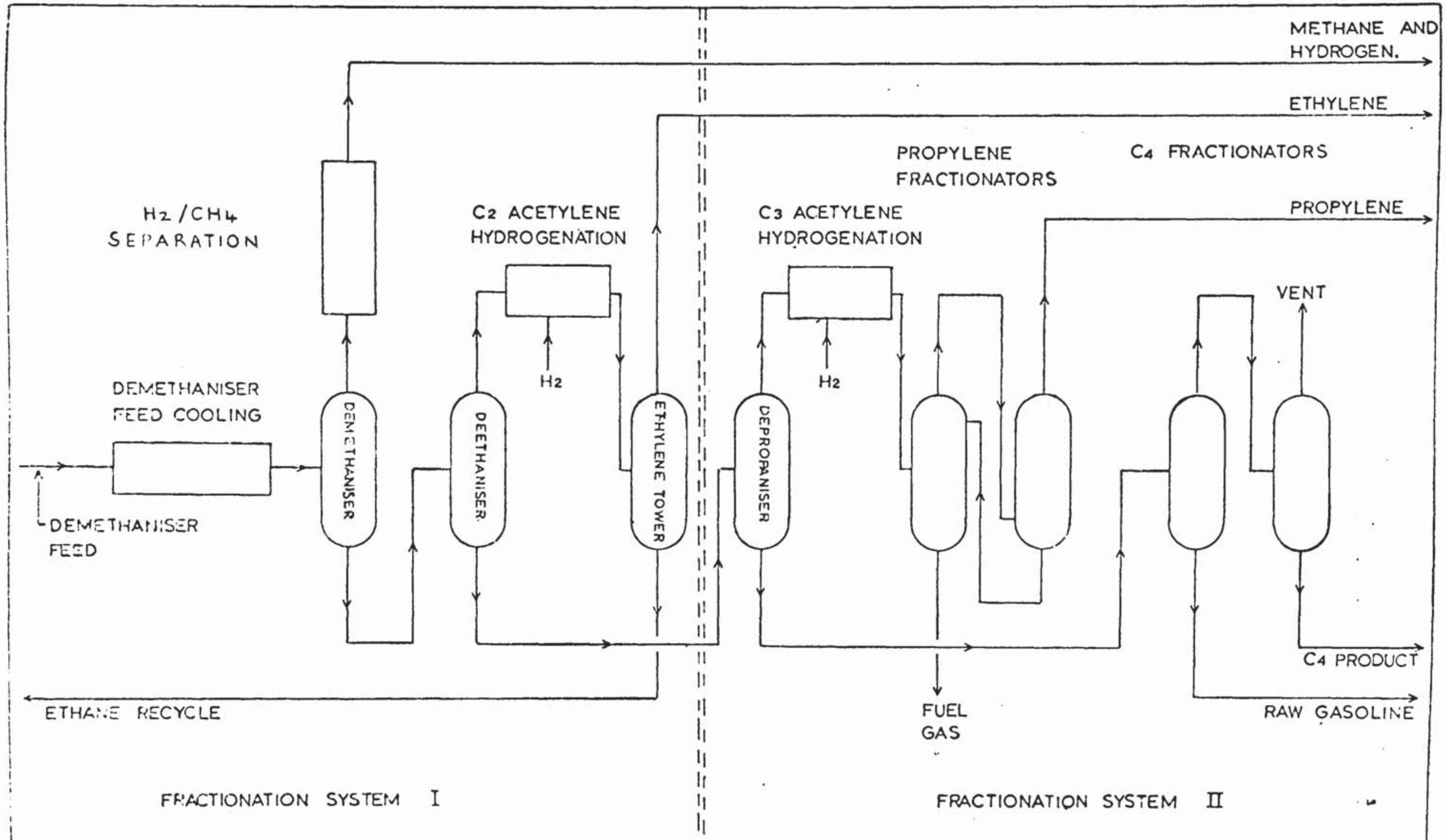


FIG. 5.6 SUB-DIVISION OF COLD END SUB-SYSTEMS FOR MODELLING PURPOSES



PROCESS FRACTIONATION SYSTEM (FIG 5-7)

i) Fractionation System I

Which comprises of all key process units directly affected by the propylene and ethylene refrigeration systems (i.e. demethaniser feed pre-cooling, demethaniser, de-ethaniser, ethylene tower and the demethaniser overhead system). These process units are concerned with the recovery of the lighter cracked products (i.e. hydrogen, methane, ethylene and ethane).

Five temperature levels of refrigerant are used at various points in the fractionation system, and process streams are involved in 3 types of energy exchange with refrigerant:-

a) vapourising refrigerant is used to cool or condense process streams

b) process streams are used to sub-cool liquid refrigerant

c) condensing refrigerant is used as a heating medium in the ethylene tower reboiler.

By far the dominant and most extensive form of energy transfer is type (a) in which refrigerant loses its latent heat of vapourisation. Type (b) involves sensible heat transfer while type (c) is used only at one point in the process.

Also, it was recognised that since the use of ethylene refrigerant is localised to the demethaniser overhead system and to the cooling of liquid ethylene product, it is possible to model and examine the process units concerned with propylene refrigerant apart from the units that use ethylene refrigerant (i.e. fractionation system I can be further sub-divided for modelling purposes).

The recovery of refrigeration energy from the process streams is centred upon the cooling of the cracked gas feed to the demethaniser. Liquid ethylene and ethane product are recycled and vapourised in de-methaniser feed pre-cooling exchangers, and a fraction of the cracked gas is cooled against low temperature hydrogen/methane product streams.

The distribution of refrigerant between the major process sections is shown in Fig. 5.8. It is interesting to observe that the refrigeration energy is shared fairly evenly between the process sections.

ii) Fractionation System II

Includes the remainder of the process fractionation units which are involved in the recovery of the heavier cracked gas components (i.e. from propylene to gasoline). As the separation of these components does not require such low temperatures, the operation of fractionation system II does not directly depend on the refrigeration system. Instead, steam and water are used as conventional heating and cooling utilities.

As fractionation system II does not contain a high degree of interaction with the other Cold End systems it contributes negligible effect to the performance of the other systems (see Fig. 5.6) and can be modelled separately at some later stage.

Thus the process fractionation system, which has the main material link with the cracked gas compression system, and which is closely involved with the refrigeration system through five temperature levels of refrigerant, can be divided into sub-systems to suit the requirements of Cold End modelling.

5.5.3.3 Refrigeration System

Refrigeration is supplied to the process by a cascade propylene/ethylene refrigeration system. Although refrigeration demand

APPROXIMATE

FIG. 5.8 : DISTRIBUTION OF REFRIGERATION BETWEEN PROCESS SECTIONS

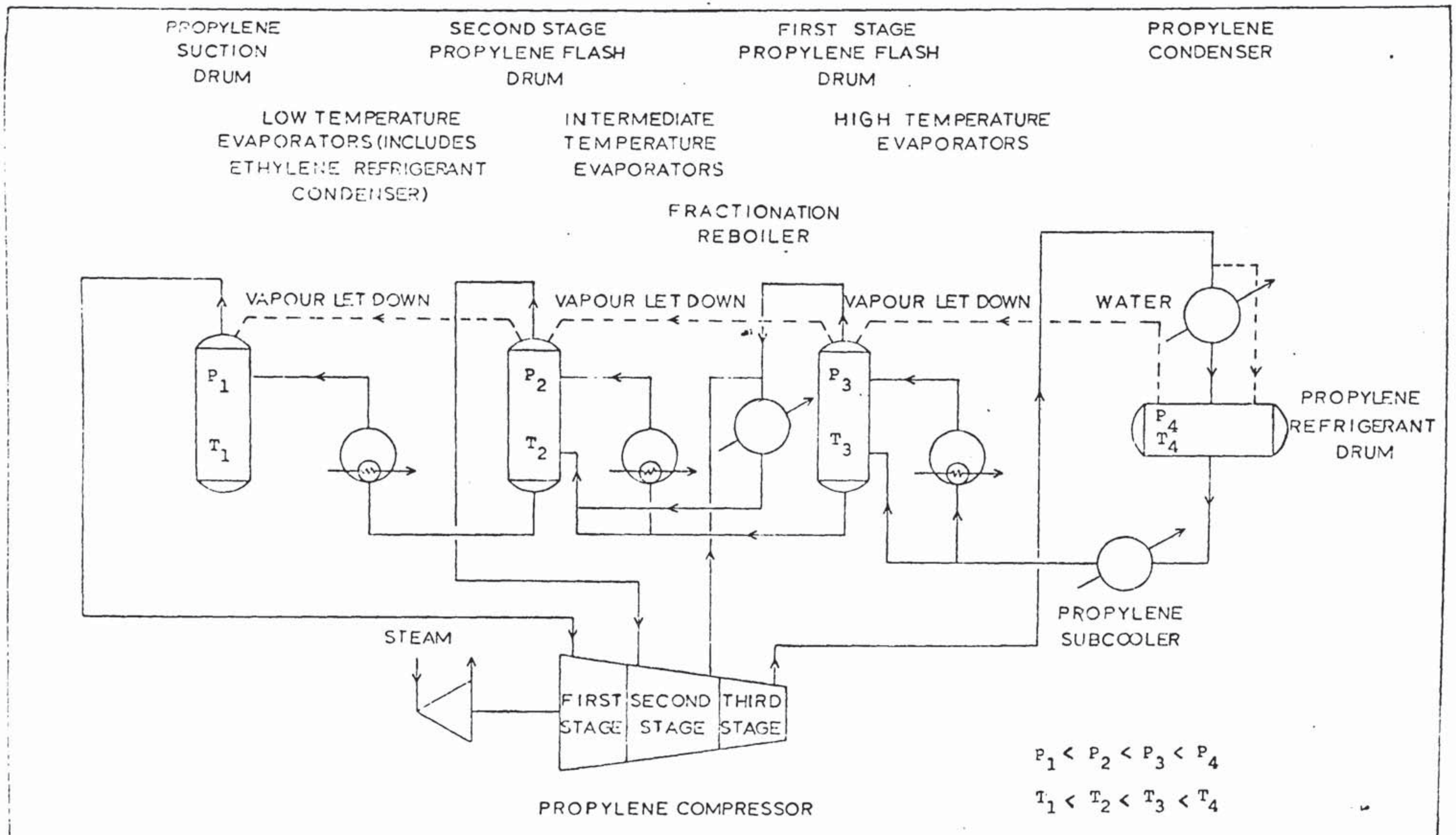
PROCESS SECTION	PER CENT REFRIGERATION
Cracked Gas Compression Cooling	20
Demethaniser Feed Pre-cooling	15
Demethaniser overheads system	25
De-ethaniser	20
Ethylene Tower	20
	100.0

is high, refrigeration compression energy can be saved provided the system is designed and operated to minimise thermodynamic irreversibilities. In part, this is accomplished through the multiple levels of evaporation and the efficient refrigeration recovery from process sections. Three temperature levels of propylene refrigerant and two temperature levels of ethylene refrigerant are employed. To maintain satisfactory control of the heat transfer between the process and refrigerant streams it is important that the temperature of the vapourising refrigerant remains steady at each refrigerant temperature level. As the vapourisation temperatures of pure propylene and ethylene refrigerant are solely a function of pressure, it is necessary to maintain steady pressures in the interstage flash drums of the refrigeration system.

i) Propylene Refrigeration System

The propylene refrigeration system is shown schematically in Fig. 5.9. Circulation of propylene refrigerant is maintained by two equal sized, three stage, steam turbine driven compressors, operating in parallel and each capable of slightly over half the total duty. The temperature of the cooling water used to condense the propylene, determines the third stage discharge pressure.

The propylene refrigeration system maintains fixed pressures in the interstage flash drums by allowing propylene vapour to be pressure let down between the drums. The refrigeration system has been designed such that when the process refrigeration requirements at each of the three refrigerant temperature levels produce propylene vapour flows that exactly satisfy the performance characteristics (see Fig. 5.3) of each of the three compression stages, there should exist no vapour let down between the flash drums. In practice, however, process refrigerant loadings occur which produce vapour flows that do not exactly satisfy the



PROPYLENE REFRIGERATION SYSTEM (FIG 5-9) performance characteristics of each compression stage. This imbalance results in propylene vapour being let down between the flash drums to maintain drum pressures, and the control system ensures that the turbine speed, which is directly controlled by the propylene vapour flow to the 1st stage compression, is adjusted if necessary. Thus, the operation of the propylene refrigeration system is closely dependent on the operation of the propylene refrigerant compressors and control system. A brief description of the theory of centrifugal compressors was given in section 5.4.

ii) Ethylene Refrigeration System

The ethylene refrigeration system which has two temperature levels of refrigerant, is similar, but basically simpler than the propylene refrigeration system. As low temperature propylene refrigerant is used to condense ethylene refrigerant, the operation of the ethylene refrigeration system is dependent on the propylene refrigeration system. Ethylene refrigerant is compressed by two equal, two-stage steam turbine compressors operating in parallel. The ethylene refrigeration system does not require pressure let-down flows between the flash drums, since the process refrigerant duties at each of the ethylene refrigerant temperature levels change proportionately with plant throughput.

The propylene and ethylene refrigeration systems are linked, through energy exchange, with one another and with the other Cold End systems (see Fig. 5.6). Both systems are directly linked with the fractionation system whereas only the propylene refrigeration system has a direct link with the cracked gas compression system.

Thus, by examining the Cold End systems using the systems approach, one has been able to establish the extent and nature of the major material and energy links between the sub-systems and identified where modelling effort should be concentrated.

5.5.4 Computer Program Structure of Models

The computer models of the Cold End sub-sytems were written according to the BP Chemicals specification for steady state process simulation (25). This specification adopted the basic concept of modularity in defining the structure of steady state process simulation models, and reflected, through a series of interlinking modules, each with a definite purpose, a distinct systems approach to steady state modelling. Adherence to this specification ensured compatibility between the Cold End sub-systems models. The modular structure of a computer simulation model is shown in Fig. 5.10.

The hub of the model is the module linking program which controls the flow of data and order of calculation of the simulation modules. Its form is determined by the structure of the process being simulated. The simulation modules are generalised program subroutines capable of performing appropriate modelling or mathematical calculations, responding to system control directives and performing input/output operation in a format compatible with the module linking program and other modules.

The following categories of simulation modules were used in the modelling of the Cold End:-

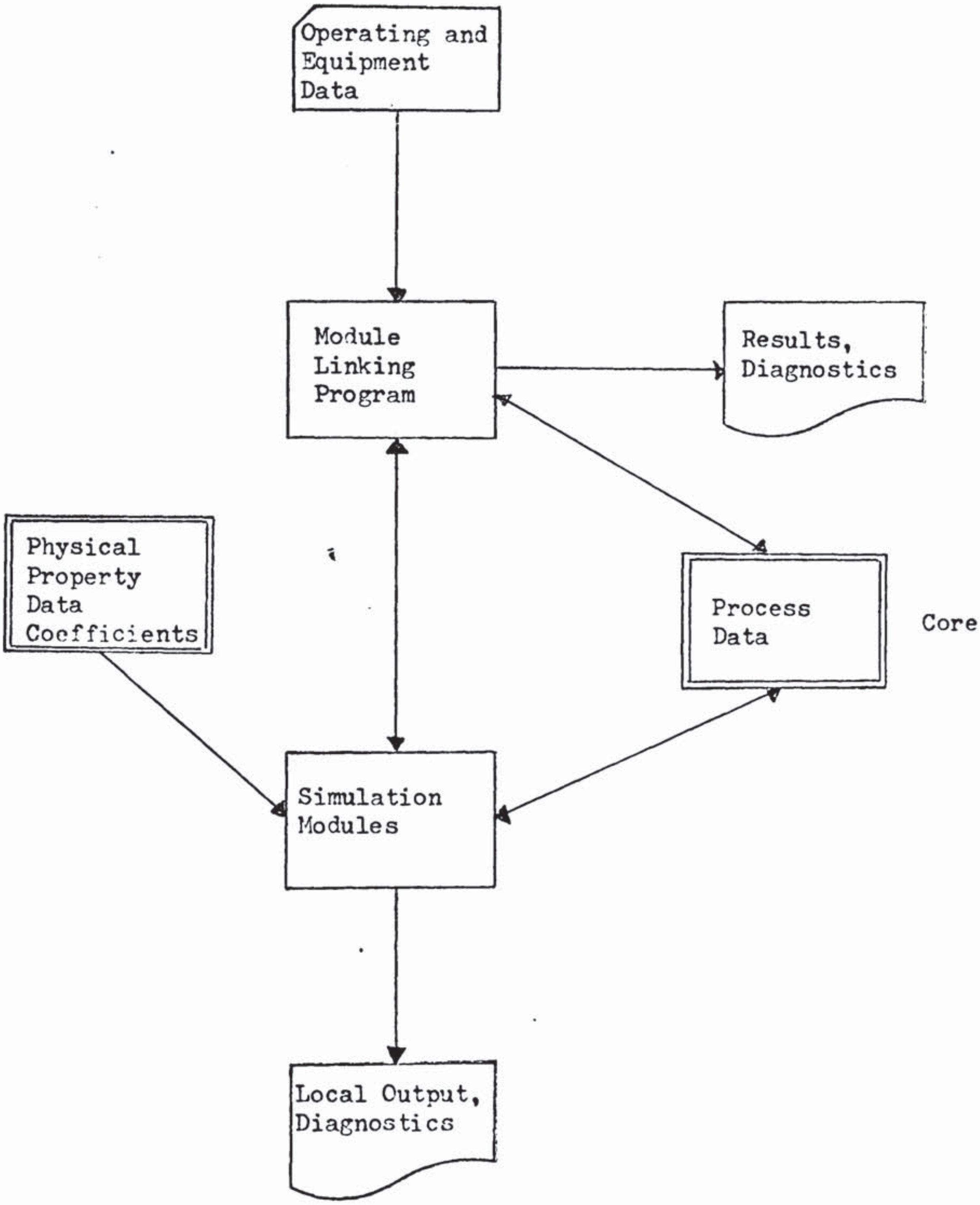


FIG.5.10 SIMULATION MODEL SCHEMATIC

i) Process Modules

These simulate the operation of plant equipment items or plant sections.

ii) Convergence Modules

These force convergence of recycle loop streams.

iii) Control Modules

These perform steady state process control functions to ensure specified plant conditions are met.

iv) General Modules

These include subroutines for data input/output, calculations of physical properties etc. General input/output subroutines for accepting module operating data and for printing the input data and model results were already in existence at the start of the Cold End modelling work.

The main groups of data used in the simulation were:-

i) Process Description Data

Since the model structure is contained within the module linking program, the process description data consist only of stream array data, i.e. the initial values of input stream paramters comprising of the temperature, pressure and component flow rates. The other streams are calculated, during the simulation, by the process modules, in the order defined by the module linking program.

ii) Process Operating Data

The process operating data are contained in a process module parameter list which contains the operating and design conditions for the process modules, e.g. reflux ratio of a distillation tower. Similar lists are used by the convergence, control and general modules.

iii) Physical Property Data

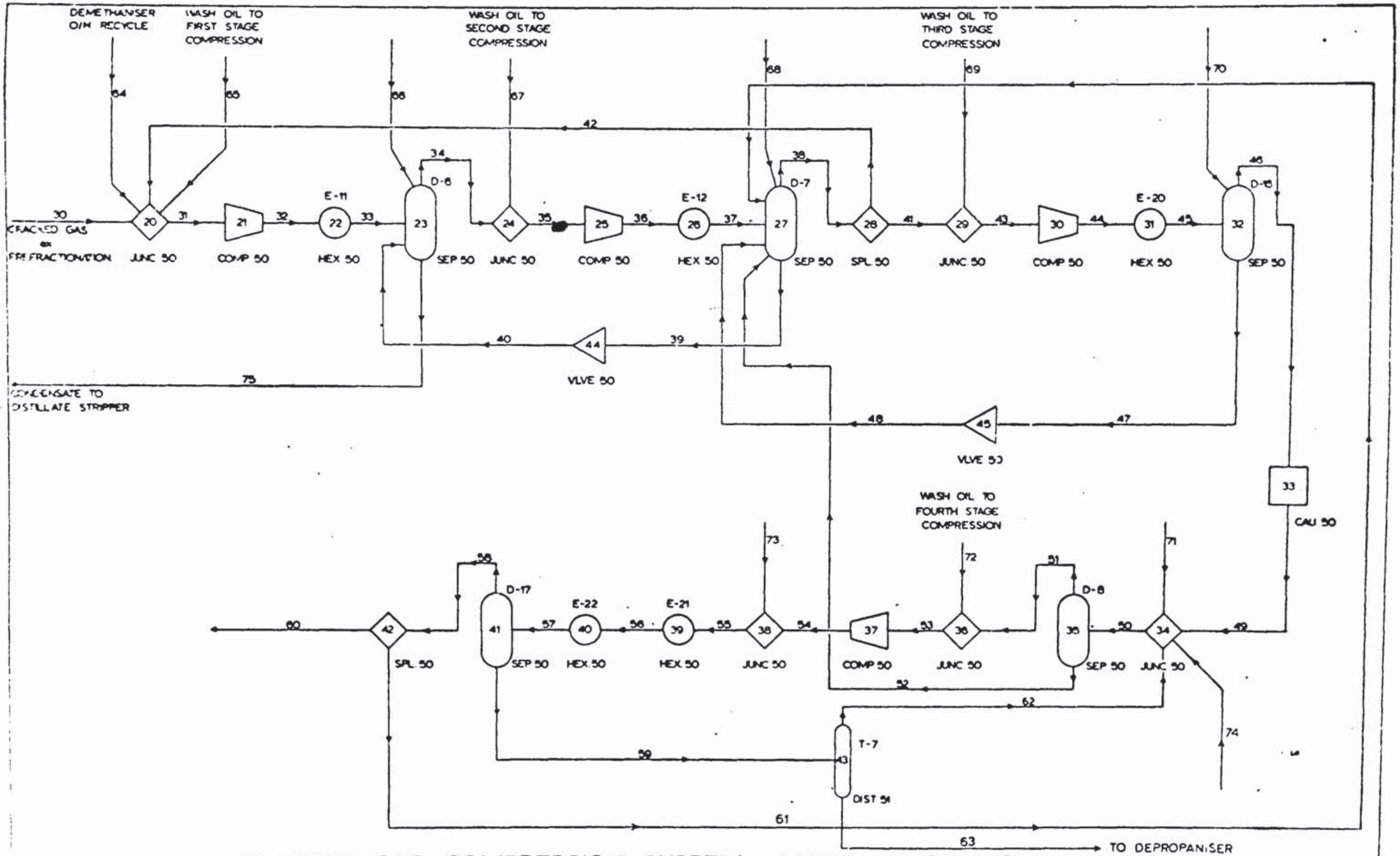
The physical property data array consists of groups of co-efficients used by general purpose subroutines (e.g. liquid enthalpy sub-routine) to calculate physical properties on demand from the process modules.

Annotated computer listings of the module linking program and a typical process module used in the Cold End Model are given in Appendix 7. The module linking program consists essentially of a series of sub-routine CALL statements which control the order in which the simulation modules are calculated. A complete set of annotated computer Fortran listings of the simulation modules used in the Cold End Model are contained in (26). Model flowsheets of the cracked gas compression, fractionation and propylene refrigeration systems are shown in Figs. 5.11 to 5.13 respectively. All process streams are identified by unique numbers, while each process module on the flow sheet is identified by a name and a unique number.

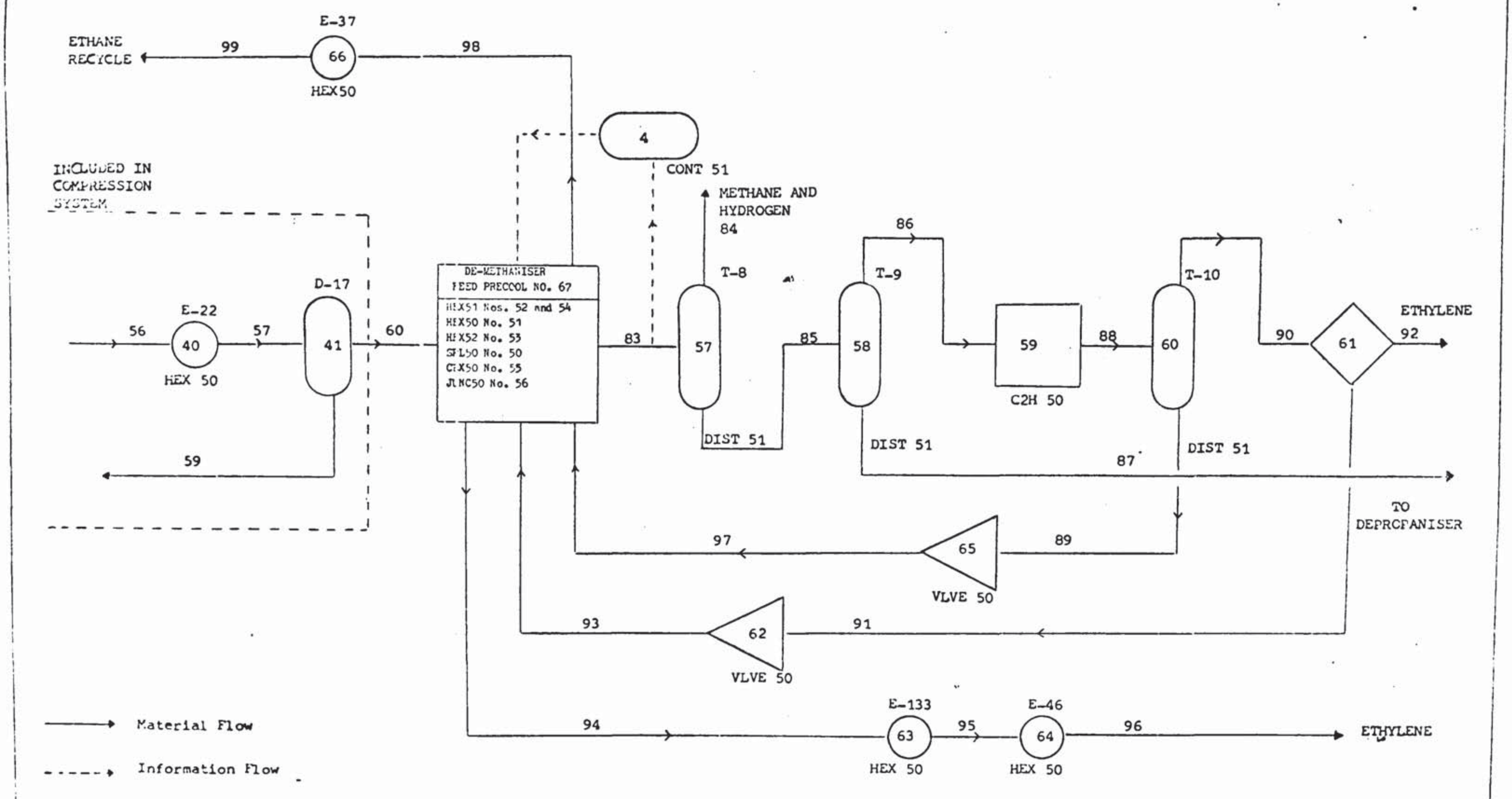
For instance, in Fig. 5.11, which is the cracked gas compression model flowsheet, the 1st cracked gas compression stage has a process module name COMP50 and equipment number 21. The equipment number is unique to the 1st compression stage, whilst the process module name COMP50, refers to the computer program subroutine used to represent the equipment in the model. (A computer listing of COMP50 is contained in Appendix 7) COMP50 is used also to represent the 2nd, 3rd and 4th compression stages which have equipment numbers 25, 30 and 37 respectively. The first compression stage is referred to in the module linking program by the following subroutine CALL statement.

```
CALL COMP50 (21, 31 - 32)
```

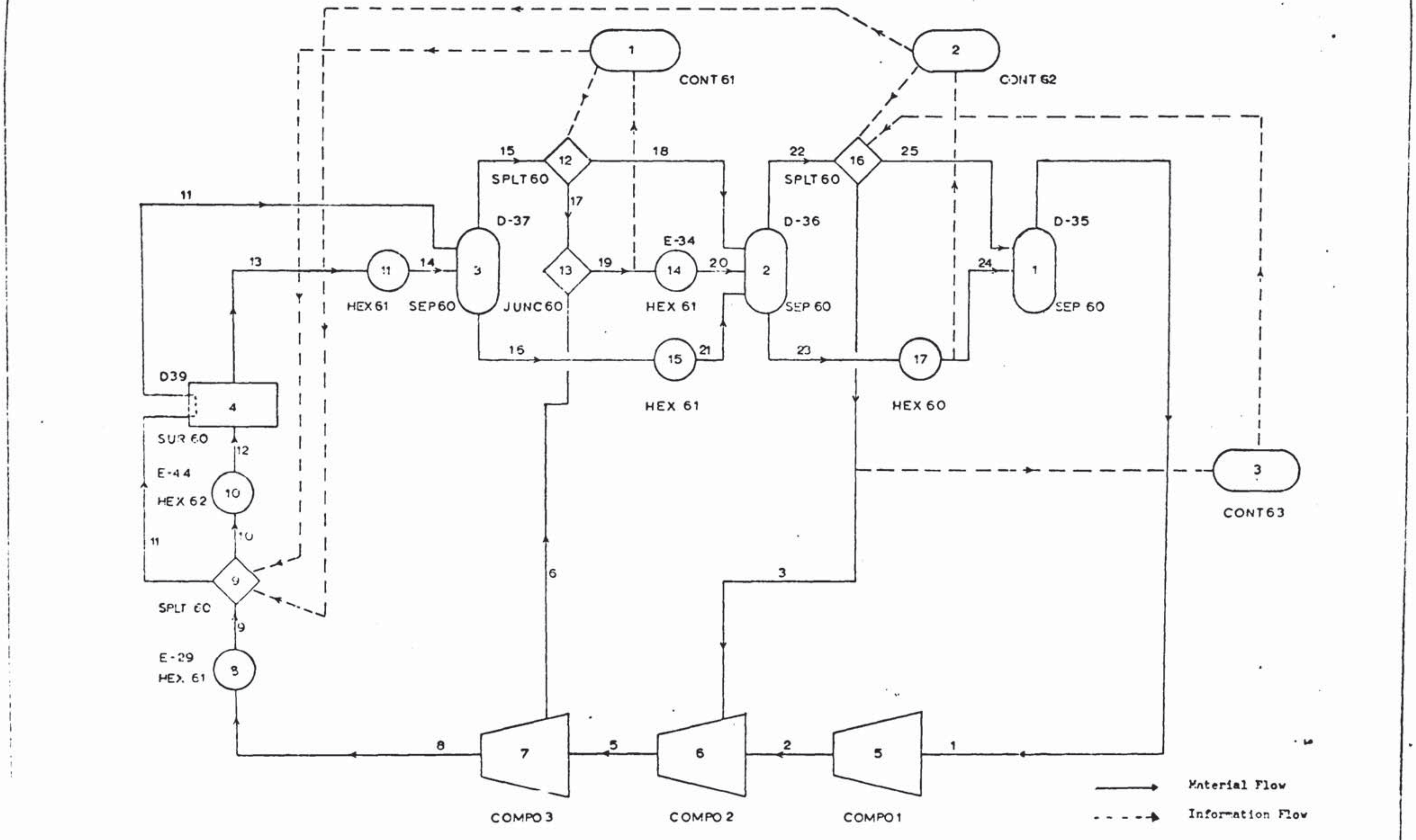
where 21 is the 1st compression stage process module equipment number



CRACKED GAS COMPRESSION SYSTEM - MODEL FLOWSHEET (FIG 5-11)



FRACTIONATION SYSTEM I - MODEL FLOWSHEET (FIG. 5-12)



PROPYLENE REFRIGERATION SYSTEM - MODEL FLOWSHEET (FIG 5-13)

31 is the number of the inlet stream

-32 is the number of the outlet stream

The first number in the subroutine argument list refers to the equipment number, while all subsequent positive numbers are the numbers of streams entering the equipment and all negative numbers are the numbers of streams leaving the equipment.

During the description of the Cold End models in the following sections, a process equipment module is referred to by its program subroutine name and equipment number. For example, in Fig. 5.12, the demethaniser tower, T-8, would be referred to as process module DIST51, No. 57.

5.5.5 Description of Models

5.5.5.1 Definition of Stream Components in Models

Twenty components were used to define the composition of the hydrocarbon process streams used in the cracked gas compression and fractionation models. The list of components is given in the module linking program listing in Appendix 7. The components were selected to give almost a one-to-one correspondence with the twenty components used in the Ethylene Plant design calculations. This grouping enabled direct comparisons of the model results with design data.

Preliminary runs of the cracked gas compression model using a reduced set of ten 'lumped' components revealed that the grouping of components can significantly affect the vapour/liquid splits of the hydrocarbon mixtures. The ten and twenty stream component definitions produced between 3 to 10% differences in the liquid/vapour molar splits at the compression system interstage drums. This suggests that care must be taken in defining a reduced set of 'lumped' components to describe the cracked gas compression system in any future modelling work requiring a smaller grouping of components.

Water was not included as a stream component in the models. Water is progressively removed from the hydrocarbon streams at each of the cracked gas compression interstage separators, and is only present in significant amounts during the first two stages of compression. (The hydrocarbon flow to the 1st stage contains approx. 5 wt% water while at the 3rd stage inlet the water content is less than 1 wt%). All traces of water are removed in the dehydrators after the 4th compression stage. As water and hydrocarbons form immiscible liquid phases, the partial pressure of the water in a liquid/vapour mixture is equal to its vapour pressure at the system temperature. This means that the presence of water in the hydrocarbon mixture affects the hydrocarbon vapour/liquid separations, by only marginally reducing the partial pressure of the hydrocarbon vapour phase by an amount equal to the vapour pressure of water. This effect was easily accounted for in the cracked gas compression model by subtracting the vapour pressure of water from the system pressure. Although the water contributes slightly to the compression loading of the 1st and 2nd compression stages and the cooling duties of the corresponding after-coolers, it was acceptable to ignore the presence of water until more detailed representations of the cracked gas compression stages are included in the model.

5.5.5.2 Physical Property Data

The establishment of a set of physical property data to adequately reflect plant operation was fundamental to the Cold End modelling work.

A computer program (28), developed by BP Sunbury, was used as a source of physical property data for the compression and fractionation models. Appendix 6 refers to the methods used to generate the vapour/liquid equilibrium and enthalpy physical property data for the process hydrocarbon streams, and describes how the data were stored and generated in the simulation models. A comparison of the K-value vapour/liquid equilibrium data used in the model and the physical property data used at the design stage are also discussed in Appendix 6.

Physical property data for the refrigeration model were obtained from Canjar (27). Propylene thermodynamic data were regression fitted on the Honeywell computer time sharing link and stored in the model in the form of regression equations. The regression equations and coefficients used in the propylene refrigeration model are summarised in Fig. 5.14. It proved necessary to fit data for the specific volume of superheated propylene, as a function of temperature and pressure, over 3 separate ranges to achieve the required accuracy for the propylene refrigeration model. The 3 ranges covered the operating conditions of the compression stages of the propylene refrigerant compressor. This was an example of the iterative and parsimonious nature of the model building where a single range covering the full compressor operating range proved inadequate for the purposes required.

5.5.5.3 Cracked Gas Compression Model (Fig. 5.11)

The cracked gas compression model was, basically, a simulation model of the cracked gas interstage system. The model contained simple representations of the plant equipment, sufficient to enable heat and mass balances to be performed. A schematic flowsheet of the model showing a single compressor train is contained in Fig. 5.11. As the configurations of both compressor trains are the same, the compression system was examined by modelling a single compressor train. Dual compressor train operation was simulated by doubling the capacity of the single train. Until more

FIG. 5.14 SUMMARY OF THERMODYNAMIC PROPERTY CORRELATIONS

USED IN PROPYLENE REFRIGERATION MODEL — REFERENCE : CANJAR (27)

NO	COMPUTER PROGRAM MODULE NAME	FUNCTION	REGRESSION EQUATION FORM	REGRESSION CONSTANTS	TEMPERATURE AND PRESSURE RANGE FITTED
1	VOSAT(TEMP)	Specific Volume of Saturated Vapour as function of temperature	$\text{Log } V = a + \frac{b}{(T+460)} + c(T+460)$	a = -2.43464 b = 2558.28 c = -0.00548945	-40 to 140°F
2	TLSAT(ENTH)	Temperature of Saturated Liquid as function of enthalpy	$T = \frac{(H - a)}{b}$	a = 295.45 b = 0.575236	-40 to 140°F
3	HLSAT(TEMP)	Enthalpy of Saturated Liquid as function of temperature	$H = a + bT$	a = 295.65 b = 0.575236	-40 to 140 F
4	TVSAT(ENTH)	Temperature of Saturated Vapour as function of enthalpy	$T = \frac{(H - a)}{b}$	a = 468.221 b = 0.157655	-40 to 140°F
5	HVSAT(TEMP)	Enthalpy of Saturated Vapour as function of temperature	$H = a + bT$	a = 468.221 b = 0.157655	-40 to 140°F
6	TFNPSAT(PRES)	Temperature of Saturated Vapour as function of pressure	$T = \frac{b}{(\text{Log }(P + 14.7) - a)} - 460$	a = 12.6164 b = 4024.91	-40 to 140°F 20 to 370 psig
7	HVSUP(TEMP, PRES)	Enthalpy of Superheated Vapour as function of temperature and pressure	$H = a + \frac{b}{(T+460)} + c(T+460) + d(P+14.7)$	a = 46.8813 b = 66682.8 c = 0.611919 d = -0.0842073	-40 to 200°F
8	TVSUP(TEMP, PRES)	Temperature of Superheated Vapour as function of enthalpy and pressure	(As for 7) Solved implicitly using Newton's method.	(As for 7)	(As for 7)
9	VOSUP(TEMP, PRES)	Specific Volume of Superheated Vapour as function of temperature and pressure.	$V = \frac{c + T}{aP + b}$	a = 4.10396 b = -5.05909 c = 432.639	-40 to 20°F 14.7 to 50 psi
				a = 3.62634 b = -21.4715 c = 335.832	60 to 100°F 50 to 100 psia
			(3 Ranges)	a = 3.47555 b = -22.0703 c = 291.171	-40 to 200°F 14.7 to 250 psia

KEY

TEMP	- Temperature (°F)	T	- Temperature (°F)
PRES	- Pressure (psig)	P	- Pressure (psig)
ENTH	- Enthalpy (Btu/lb)	H	- Enthalpy (Btu/lb)
		V	- Specific Volume (ft 3/lb)

accurate and detailed representations of plant equipment are included in the model there is little to be gained in the explicit representation of the two compressor trains. The model included all minor fractionation recycle streams and compressor wash oil injections so that it could be verified and compared with design data. All equipment modules used directly, or indirectly, general isothermal and adiabatic flash subroutines to determine either the temperature, enthalpy, or the vapour/liquid splits of the hydrocarbon streams.

The model representations of the process equipment are discussed as follows:-

i) Centrifugal Cracked Gas Compressors

The cracked gas compressors were represented as four independent compression stages (process modules COMP50 Nos. 21, 25, 30 and 37 in Fig. 5.11). Each stage was defined by specifying a design polytropic compression factor. This enabled the compression stage discharge temperature to be calculated for a specified discharge pressure according to the equation

$$T_2 = T_1 \left(\frac{P_2}{P_1} \right)^n \qquad - \; (5.5)$$

where T_1 = inlet temperature (^oR)

T_2 = discharge temperature (^oR)

P_1 = inlet pressure (psia)

P_2 = discharge pressure (psia)

n = polytropic compression factor

It is arguable that this representation is an over-simplification of the compressors since no account was taken of the interdependence of the compression stages. As the 1st and 2nd compression stages are driven by the same steam turbine, any change directly affecting one stage will be shared between the two stages through adjustment of the intermediate pressure (i.e. the 1st stage discharge pressure) and hence polytropic heads of the stages. The same applies to the 3rd and 4th compression stages. However, it was decided that the simple compression stage representation used in the model was adequate for the initial examination of the hydrocarbon flows through the system and was capable of providing meaningful estimations of compression duties. Future modelling work would require more detailed compressor representations. The true benefit of introducing improved model representations of the cracked gas compressors, which include the compressor characteristics and couple the performance of the compressor stages, would not be evident until compressor characteristics that reflect actual compressor operation have been established.

ii) Aftercooler heat exchangers

The process module HEX50, which was a simple general purpose heat exchange module, represented the aftercooler heat exchangers (Nos. 22, 26, 31, 39 and 40) and calculated the cooling water heat duties, in terms of MBTU/H, to cool the cracked gas to specified exchanger outlet conditions. This implied no heat transfer limitation for the exchangers.

iii) Condensate Stripper

The condensate stripper (process module DIST51 No. 43 in Fig. 5.11) was assumed to be capable of achieving a design separation as defined by specifying the percentage of upper and lower key components in the overhead product. This assumption acknowledged that the operation of the condensate stripper is to design standards and is not limiting.

iv) Other process equipment represented in the model included the interstage separator drums (process module Nos. 23, 27, 32, 35 and 41

SEP50), valves (process module VLVE50, Nos. 44 and 45) and general purpose junction and splitter modules. The modelling of the interstage separator drums is discussed in section 5.5.6.1. The caustic scrubbing system which had little effect on cracked gas flow was represented by a trivial process module (CAU50 No. 33) which accounted for slight changes in the temperature and pressure of the gas leaving the caustic scrubber.

A simple repeated substitution convergence routine, which was used in the serial convergence of two convergence loops, proved adequate in arriving at a model solution. The calculation order and convergence loops defined in the model are contained in the listing of the module linking program in Appendix 7. There was no incentive at this stage in the modelling work to incorporate improved methods of convergence.

5.5.5.4 Uncoupling of Process Fractionation and Refrigeration Systems

Although the refrigeration and process fractionation systems are, through energy exchange, highly interlinked systems, it was possible, by using a fundamental fact concerning the energy transfer between the process and refrigerant streams, and a basic assumption about the refrigerant heat exchangers, to uncouple the systems and simplify their modelling. This meant that the modelling of the fractionation and refrigeration systems could proceed independently. The uncoupling of these systems can be explained by first describing the calculation of refrigeration energy required by the fractionation system and then describing the transfer of this energy between the fractionation and refrigeration systems.

i) Calculation of Refrigeration Energy required by Fractionation System

The basic assumption used in the modelling of the refrigerant heat exchangers was that the rate of heat transfer in the exchangers was not limiting. It was assumed that the refrigeration exchangers, involving either sensible heat transfer or vapourisation heat transfer, were capable of maintaining the process streams at design conditions of temperature. The refrigerant exchanger model representation, (process module HEX50), used in the fractionation model, calculated the refrigeration energy duties in terms of MBTU/H taking only the process stream conditions into account. No account was taken of the temperature difference between the process and refrigerant streams in the exchangers, the heat transfer area of the exchangers or the heat transfer coefficients of the exchangers. This exchanger model representation was adequate for the initial purpose of exploring the energy interaction between the Cold End systems and was consistent with the parsimonious approach to modelling. Improved model representations of the exchangers, which reflect their true operating performance, are required at a later stage in the modelling work when it has been established which exchangers are heat transfer limiting and which exchangers have performances which vary significantly at different operating conditions.

ii) Transfer of Energy between Fractionation and Refrigeration Systems

It was shown in section 5.5.2 that the energy transfer between the process and refrigerant streams is of 3 types:-

a) vapourising refrigerant is used to cool and condense process streams.

b) process streams are used to sub-cool liquid refrigerant leaving the interstage flash drums.

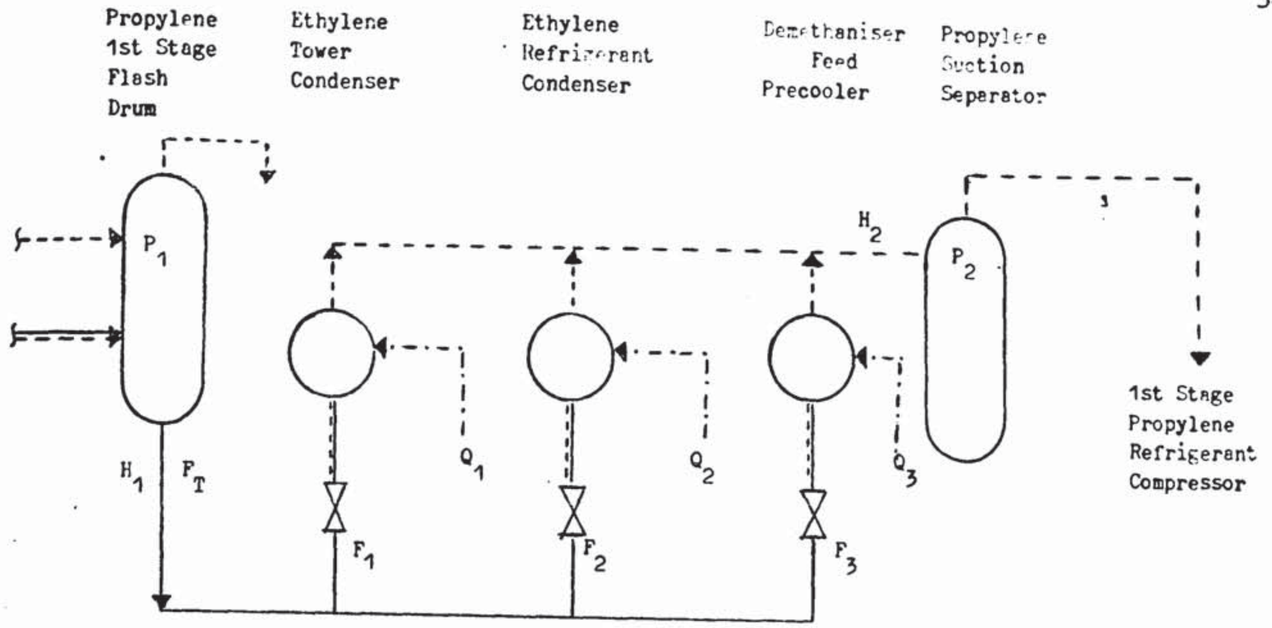
c) condensing propylene refrigerant is used as a heating medium in the ethylene tower reboiler.

Type (a) is by far the most prevalent and important form of energy transfer accounting for approximately 75% of the total propylene refrigeration energy transfer between process and refrigerant streams. Type (b) involving sensible heat transfer, accounts for 5% of the total whilst type (c), which is confined to one point in the process, accounts for 20% of the energy transfer.

Thus, the main form of energy transfer between the process and refrigerant streams is type (a) involving the release of the latent heat of vapourisation of the refrigerant at constant temperature. Since the energy transferred during vapourisation is a function of the amount of fluid vapourised, it can be stated as a fundamental fact, to be used in the modelling of the energy transfer between the refrigeration and fractionation systems, that the flow of refrigerant to the vapourising exchangers is defined by the amount of energy transferred between the process and refrigerant streams.

Therefore, at each refrigerant temperature level where there exists a series of vapourising refrigerant exchangers, operating in parallel, the flow of refrigerant to each exchanger is defined by the amount of energy transferred from the process stream to the refrigerant stream at each exchanger. The refrigerant used in the vapourising refrigerant exchangers exists either as saturated liquid or saturated vapour. For instance, if one examines the case of low temperature propylene refrigerant, as shown in Fig. 5.15, which is part of the propylene refrigeration system, it can be seen that the flows of refrigerant to each exchanger and subsequently to the 1st stage of compression are functions of the low temperature refrigeration duties. The refrigeration energy duties Q_1, Q_2 and Q_3 are calculated by the refrigeration exchangers in the fractionation model.

Thus, the link between the propylene refrigeration and fractionation models was through the refrigerant exchangers in the fractionation system model calculating the refrigerant heat duties,



KEY

Saturated Propylene Liquid

Saturated Propylene Vapour

Refrigerant Duty (BTU/H)

P_1 = Pressure in propylene 1st Stage Flash Drum (psia)

P_2 = Pressure in propylene suction separator (psia)

H_1 = Enthalpy of saturated propylene liquid at pressure P_1 (BTU/lb)

H_2 = Enthalpy of saturated propylene vapour at pressure P_2 (BTU/lb)

Q_1, Q_2, Q_3 = Refrigerant duties required by refrigerant exchangers (BTU/H)

F_1, F_2, F_3 = Refrigerant flows to exchangers (lb/hr)

$F_T = F_1 + F_2 + F_3$

$Q_T = Q_1 + Q_2 + Q_3$

The relationships between the refrigerant flows and refrigerant heat duties are as follows:

$$F_1 = \frac{Q_1}{H_1 - H_2} \text{ lb/h} \qquad F_2 = \frac{Q_2}{H_1 - H_2} \text{ lb/h} \qquad F_3 = \frac{Q_3}{H_1 - H_2} \text{ lb/h}$$

$$F_T = \frac{Q_T}{H_1 - H_2} \text{ lb/h}$$

FIG.5.15 LOW TEMPERATURE SECTION OF PROPYLENE REFRIGERATION SYSTEM expressed in MBTU/H, and conveying these duties, via a refrigeration heat duty interface, to the refrigerant exchangers in the refrigeration model, as shown in Fig. 5.16. It was convenient to sum the energy duties at each propylene refrigerant temperature level and use a 'lumped' representation of refrigerant exchangers in the propylene refrigeration model.

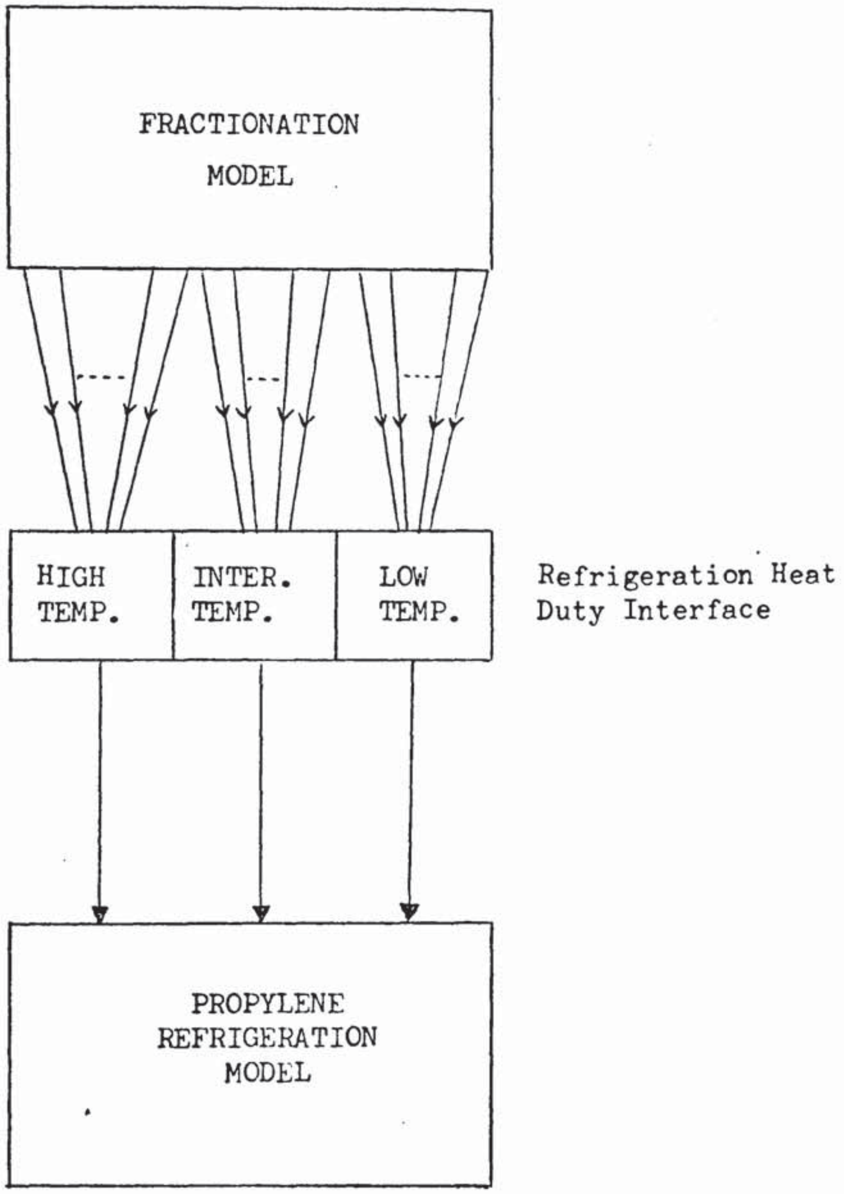
Although it was possible to model the ethylene refrigeration system in the same way as the propylene refrigeration system, it was expedient to use an extremely simple ethylene refrigeration model at this stage of the modelling work, as is described in Section 5.5.5.6.

Thus, it has been shown that by the use of a refrigeration heat duty interface it is possible to uncouple the refrigeration and fractionation systems. When more detailed representations of the exchangers are used in the modelling work this interface will have to include temperatures in order to calculate refrigeration heat duties. Descriptions of the fractionation and refrigeration models are contained in the following sections.

5.5.5.5 Fractionation Model (Fig. 5.12)

The fractionation model, which is shown in the form of a schematic flowsheet in Fig. 5.12, was a representation of fractionation system I, which was defined in section 5.5.3. The model contained a series of basic heat exchanger and distillation tower process modules.

Heat exchanger process module HEX50 was used to represent the majority of propylene refrigerant exchangers and calculated the propylene refrigerant heat duties required to attain design process outlet temperatures. Recovery of refrigeration energy from the ethane and ethylene product recycle streams, which were used to cool the demethaniser feed, was represented by process modules HEX51 Nos. 52 and 54 in Fig. 5.12. These



KEY

→ Energy Flow (MBTU/H)

FIG.5.16 INTERFACE BETWEEN PROPYLENE REFRIGERATION AND FRACTIONATION MODELS process modules assumed complete vapourisation of the recycled ethane and ethylene products in calculating the process outlet temperatures. The distillation tower modules (DIST51 Nos. 57, 58 and 60), which were specified by defining for each tower the reflux ratio and percentage of the upper and lower key components in the overhead distillate product, calculated the reboiler and condenser heat duties.

A control module (CONT51) adjusted the refrigerant duty on the demethaniser feed heat exchanger E-26 (process module HEX52, No. 53) to maintain a fixed inlet temperature to the demethaniser. No explicit representation of the demethaniser overheads recovery system, which is the main user of ethylene refrigerant, was included in the fractionation model. However, the effect of the system was accounted for in the ethylene refrigeration model which is discussed in section 5.5.5.6.

Trivial process modules were used to represent the C2 hydrogenation system (process module C2H50, No. 59), which has insignificant effect on the refrigeration energy interaction between the process and refrigeration systems, and the section of the demethaniser used to cool the demethaniser feed (process module CBX50 No. 55). This section, which consists of a series of efficient heat exchangers designed to maximise the recovery of refrigerant energy from the low temperature process streams, was assumed to operate at design performance.

The solution of the fractionation model involved a single convergence loop which used a simple repeated substitution routine to achieve convergence.

5.5.5.6 Refrigeration Model

The refrigeration model included representations of both the propylene and ethylene refrigeration systems. The propylene refrigeration system was modelled in greater depth than the ethylene refrigeration system for the following reasons:-

a) the propylene refrigeration system is the more important and dominant of the two refrigeration systems. The availability of propylene refrigerant is essential to the operation of the ethylene refrigeration system and the Ethylene Plant.

b) the distribution of propylene refrigerant loads is of a more complex nature.

c) the ethylene refrigeration system is simpler and its refrigerant loading and performance have a linear relationship with plant throughput.

i) Propylene Refrigeration Model

A flowsheet of the propylene refrigeration model is given in Fig. 5.13. It was shown in section 5.5.3 how the operation of the propylene refrigeration system is closely dependent on the operation of the propylene refrigerant compressors, and the control system which maintains constant pressures in the refrigerant flash drums. The propylene refrigeration control system was included as an integral part of the propylene refrigeration system model. The control system was designed to maintain constant pressures throughout the propylene refrigeration system by control of the pressures in the propylene flash drums (process modules SEP60, Nos. 1, 2 and 3 in Fig. 5.13). The pressure in the refrigerant surge drum (process module SUR60, No. 4 in Fig. 5.13) is determined by the temperature of the cooling water in the refrigerant condenser. Three control modules (CONT61, CONT62, CONT63 in Fig. 5.13) were used to adjust the vapour let down flows (stream nos. 11, 18 and 25 in Fig. 5.13) to maintain constant pressures in the flash drums.

A fairly detailed model of the propylene compressors, involving the interlinking of the compressor stages was required to describe adequately the performance of the propylene refrigeration system. The model comprised of three compression stage process modules (process modules COMP01 No. 5, COMP02 No. 6 and COMP03 No. 7 in Fig. 5.13). The design compressor characteristics for each stage (see Fig. 5.3), relating the compressor speed to the inlet volumetric flow and to the stage pressure ratio, were regression fitted and used in each of the compression stage modules. The compressor speed was calculated in the 1st compression stage process module COMP01 and then used in the 2nd and 3rd compression stage process modules (COMP02, COMP03) for calculating the refrigerant flows to and from the compression stages. Compression energies were calculated from heat balances across each compression stage. Dual compressor operation was simulated by doubling the capacity of one of the compressors and was equivalent to assuming that both compressors had the same characteristics and were balanced with equal loads. This representation was suitable for the initial modelling of the Cold End.

The propylene refrigeration model contained 'lumped' representations of the process refrigerant exchangers (process modules HEX61 Nos. 11, 15 and 17 in Fig. 5.13), at each of the three propylene refrigerant temperature levels. The function of these process modules was to use the process refrigerant duties, as calculated by the cracked gas compression and fractionation models to calculate the amount of propylene vapourised in the refrigerant exchangers. However, the ethylene tower reboiler exchanger (process module HEX61, No. 14 in Fig. 5.13), which is the only process exchanger involved in the condensation of refrigerant, was represented separately, since its heat duty had to be supplied by the condensation of the 2nd stage discharge flow (stream no. 6 in Fig. 5.13) and the overheads vapour flow from the 3rd stage separator (stream no. 17 in Fig. 5.13).

The calculation order of the process modules in the propylene refrigeration model can be followed by reference to Fig. 5.13 and the module linking program in Appendix 7. Convergence to a model solution was achieved by the three control modules CONT61, CONT62 and CONT63.

ii) Ethylene Refrigeration Model

Advantage was taken of the linear properties of the ethylene refrigeration system in formulating a simple linear model to determine the effect of the ethylene refrigeration system upon the propylene refrigeration system (propylene refrigerant is used to desuperheat and condense ethylene refrigerant). The model assumed that the fractional changes from design in the ethylene refrigerant compression energy and condensing duty were the same as the fractional change in the ethylene refrigerant duty required by the process. Also, as ethylene refrigerant is used solely in the demethaniser overhead system and in cooling ethylene liquid product, it was assumed in the model that the ethylene refrigerant duty required by the process varied linearly with the flow of ethane and lighter components in the demethaniser feed stream (stream no. 83 in Fig. 5.12) and with the ethylene liquid product flow to storage (stream no. 92 in Fig. 5.11). These assumptions were supported by the behaviour of the ethylene refrigeration system during plant operation.

Hence, the linear equation used to calculate the fractional change in ethylene refrigerant condensing duty and compression energy from their design values was of the form:-

$$\Delta C = a.F_1 + b.F_2 \qquad - \quad (5.6)$$

where ΔC is the fractional change

F_1 = flow of ethane and lighter components in the cracked gas to the demethaniser

F_2 = flow of liquid ethylene product

a,b = constants determined from design operating conditions

5.5.5.7 Cold End Model

The Cold End model was a combination of the local sub-system models described in the previous sections and possessed all the features of these models. Its structure, shown in Fig. 5.17, reflects the arrangement of the Cold End sub-systems shown in Fig. 5.5. The Cold End model first used the cracked gas compression model and the fractionation model, in that order, to calculate the cracked gas compression energy requirement and the process refrigerant heat duties. These duties were then used by the refrigeration model to provide measures of refrigeration compression energy.

5.5.6 Verification of Models

Verification of a model is part of the iterative nature of model building. By comparing the model results against a reference set of data, checks on the validity of the model can be made, and any necessary improvement in the model representations can be introduced.

The size and complexity of the Cold End sub-systems required that each sub-system model be verified individually before being merged to form the Cold End model. The Cold End models were verified against a reference set of design data, since comprehensive and accurate sets of plant data for such an exercise were not readily available. However, effective use was made of certain plant data to account for discrepancies between the model results and the reference data.

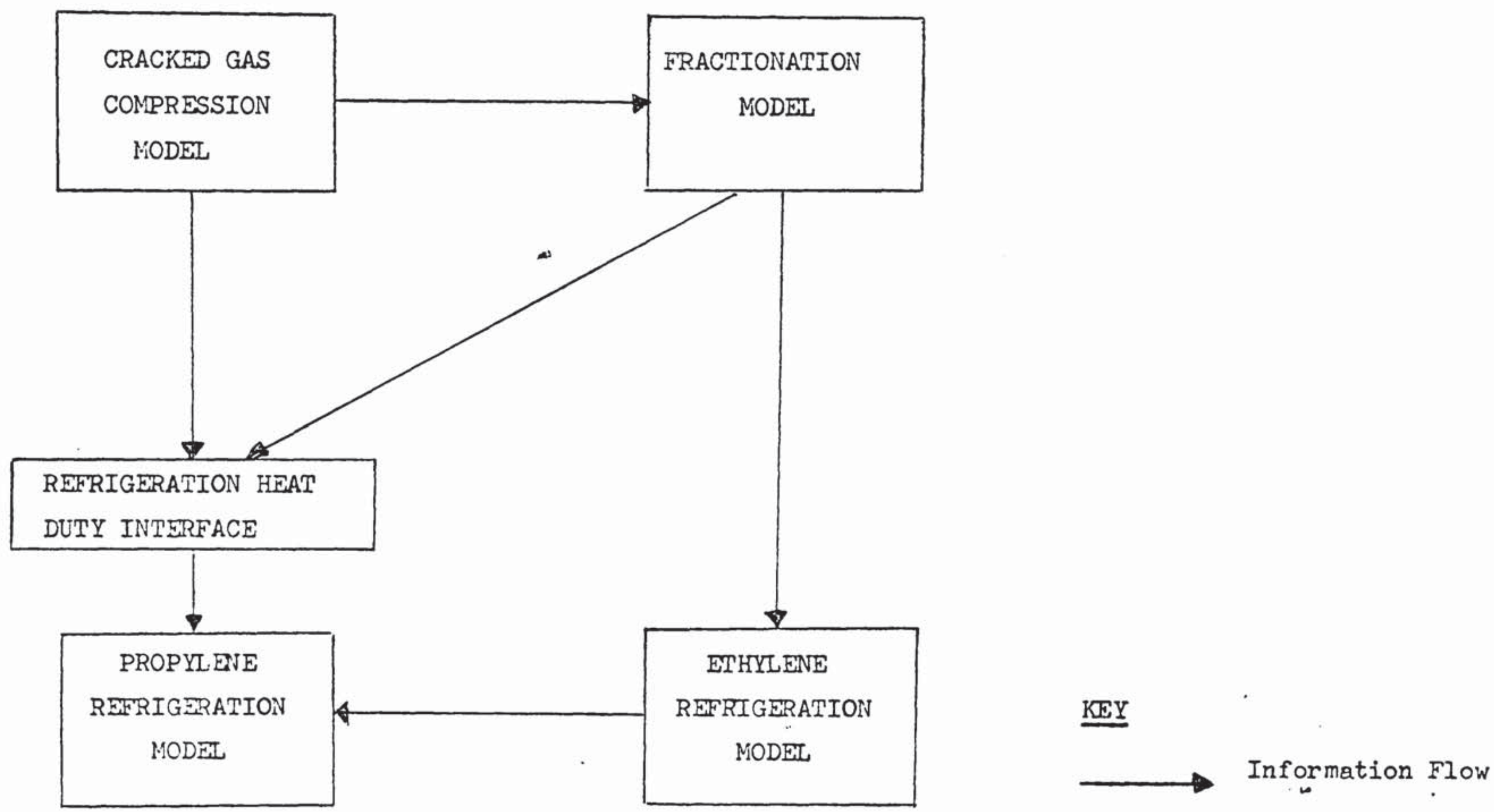


FIG.5.17 COLD END MODEL STRUCTURE SHOWING FLOWS OF INFORMATION BETWEEN SUB-SYSTEM MODELS.

The scope of the Cold End models is summarised in Fig. 5.18. Although the number of output data calculated by the models may appear to be particularly large compared with the number of input data (e.g. the fractionation model calculates 23 unknown streams, each with 26 parameters per stream, using 1 stream and 31 process operating data as input data) it should be appreciated that a significant number of the calculated streams in the cracked gas compression and fractionation models have the same stream parameter values. For instance, the 20 stream parameters that define the composition of a stream will be the same for the inlet and outlet streams of all heat exchanger and valve process modules. The fractionation model has 10 equipment items that use these process modules. Of the total number of output data calculated by the models, the key output data used to check the validity of the models made up about 30% of the total. The particular output data of interest are defined in the following sections which also discuss the verification of each of the Cold End models.

5.5.6.1 Cracked Gas Compression Model

In verifying the cracked gas compression model, the main model results examined were the stream parameter values of the vapour and liquid streams leaving the condensate stripper and each of the interstage separator drums (i.e. 12 streams). The vapour/liquid separations in the interstage drums determine the flow rate, composition and temperature of the streams fed to each compression stage. Between the interstage separator drums, the stream compositions and flows do not change significantly.

The cracked gas compression model initially produced results in which the temperatures of the vapour streams leaving the interstage separator drums were significantly lower (10 to 15^{O}F) than design

FIG. 5.18 SCOPE OF COLD END MODELS

MODEL	No. of Streams	No. of Parameters per Stream †	No. of Equipment Items									No. of Control Modules	No. of Convergence Modules	Model Input Data	
			Compression Stages	Separators	Junctions	Splitters	Valves	Heat Exchangers	Distillation Towers	Miscellaneous ‡	Total			No. of Streams	No. of Process Operating Data
Cracked Gas Compression	45	26	4	5	6	2	2	5	1	1	26	-	2	12	35
Fractionation	24	26	-	1	1	2	2	8	3	2	19	1	1	1	36
Refrigeration	25	6	3	3	1	3	-	6	-	1	17	3	-	-	18
Cold End	94	26/6	7	8	8	7	4	18	4	4	60	4	3	12	78

† See Appendix B for definition of stream parameters

‡ Includes trivial modules of caustic scrubber, cold box etc.

temperatures. The molar flow rates of the vapour streams leaving the interstage drums differed from design flows by between 3 and 6 per cent. It had been assumed in the modelling of the interstage separator drums (i.e. process modules SEP50 Nos. 23, 27, 32, 35 and 41 in Fig. 5.11) that all streams entering each interstage drum were thoroughly mixed and achieved an overall state of thermodynamic equilibrium, and hence uniform temperature throughout the drum.

Calculation checks on design data revealed that the separation of vapour and liquid streams in an interstage separator drum had been calculated by considering that all vapour streams entering the drum were mixed separately from the liquid streams. The vapour streams were assumed to achieve a state of thermodynamic equilibrium. Liquid streams were treated in a similar fashion. Examination of the geometry of the separator drums supported this model. The short residence time of the vapour streams in the drums and the positioning of the pipework where streams enter and leave the drums do not allow significant mixing of the liquid and vapour phases in the drums. This model representation produced temperature gradients across the drums of the order of 10°F.

Plant data confirmed that such temperature gradients occurred in practice. In light of this evidence, the representation of the interstage drums in the compression model was modified. This example demonstrates how selective plant data were used to decide which model representation was the more realistic.

The modified compression model produced separator drum overhead temperatures that were within 2°F of design. The molar flow rates of the vapour streams from the drums were within 3% of design. The minor discrepancies that still existed between the design data and the model results, were attributed to differences in physical property data. Differences between design and model vapour/liquid equilibrium data are discussed in Appendix 6.

5.5.6.2 Fractionation Model

The fractionation model was essentially concerned in calculating the heat duty requirements of 12 of the process refrigerant exchangers. As the model contained simple representations of process equipment based on design data, verification of the model results with design data was a check on the agreement between the model and design physical property data. The model produced refrigerant heat duties that were in close agreement with design values (within 4 per cent of design) and sufficiently accurate for the initial purpose of the modelling work.

5.5.6.3 Refrigeration Model

Significant differences between the propylene refrigeration model results and design data, as measured by the refrigerant flows to and from the compressor stages, were attributed to errors in the regression fitting of the propylene physical property data, and the fitting of the compression stage characteristics. The main source of error lay in the regression fitting of the specific volume data of superheated propylene as a function of temperature and pressure. It proved necessary to fit the specific volume data over 3 ranges of temperature and pressure in order to bring the compressor flows within 5 per cent of design values. The remaining error was mainly due to the fitting of the compressor stage characteristic curves.

A cursory comparison of selective plant data with design data, suggested that the propylene compressor design characteristics, as supplied by the compressor manufacturer, and used in the model, differed significantly from the true operating characteristics of the compressors.

Before the model can be used to reflect actual plant operation, it will be necessary to determine the true operating characteristics of the compressors. It was decided that there was little to be gained in the more accurate fitting of the compressor characteristics, until the true operating characteristics are established.

The separate verification of the implicit ethylene refrigeration model using design data was considered unnecessary since the simple linear model had been derived from design data.

5.5.6.4 Cold End Model

The Cold End Model, when verified using design data, produced results that were consistent with the results obtained from the verification of the individual sub-system models.

5.5.7 Review of Section 5.5

This section has described how the application of the systems engineering approach to modelling has enabled a steady state model of the Cold End to be formulated. The model, which was formulated with a view to examining the interactions that exist between and within the Cold End sub-systems and in relating the effect of such interactions on the performance of the cracked gas and refrigerant compressors, used simple model representations whenever possible. It was shown how the analysis and understanding of the refrigeration energy transfer between the process and fractionation streams greatly facilitated the modelling of the fractionation and refrigeration systems. Also, plant operating experience supported by an appreciation of the nature of the ethylene refrigerant duties required by the process, enabled a simple linear model of the ethylene refrigeration system to be defined. In the context of the Cold End modelling work, model verification was used to provide a measure of confidence in the models and to confirm that they were adequate for the initial purpose for which they were intended.

5.6 SIMULATION OF COLD END SYSTEMS

Once a model of the overall system has been built it must be converted from a passive device into an active device and be used to simulate the behaviour of the system. The objective of the Cold End simulation work was to explore and understand the interactions that exist between and within the Cold End sub-systems, and to relate the effect of such interactions on Cold End System performance.

It was realised that the size and complexity of the Cold End sub-systems justified, in some cases, an examination of the sub-systems as systems in their own right. The modular development of the Cold End sub-system models permitted the models to be used for simulating the separate behaviour of the sub-systems. The cracked gas compression system was the most suitable of the Cold End sub-systems to be examined in this way, since its material and energy interactions with the other sub-systems are not so involved. It was fully appreciated that the simulation of individual sub-systems would provide measures of sub-system performance which may not necessarily reflect the overall performance of the Cold End. It was also realised that due to the nature and accuracy of the Cold End models, model results would be more meaningful on a relative rather than an absolute basis, and could be used to examine changes about design conditions.

Therefore, before demonstrating how the Cold End model was used to simulate the behaviour of the Cold End, some of the sensitivity runs which were carried out on the sub-system models, are described.

5.6.1 Sub-System Simulation

5.6.1.1 Cracked Gas Compression System

The cracked gas compression model was used to examine the behaviour of the cracked gas compression system when subjected to changes in operating variables.

A 2^3 factorial set of computer runs was carried out on the cracked gas compression model to examine the performance of the compression system to changes in aftercooler exit temperatures.

Using design operating conditions as input data and simulating the operation of one compressor train, the 1st, 2nd and 3rd stage aftercooler temperatures were set in turn at $10^{\circ}F$ below design values. The model results are summarised in Fig. 5.19, which shows for run 1 the values of the performance variables under design conditions and for runs 2 to 8 the changes in the performance variables about the design values. The main performance variables examined for each compression stage were:-

i) inlet temperature

ii) molar flow rate

iii) molecular weight

iv) and compression energy as calculated from a compression stage heat balance.

The results suggest that the combined effect of changes in aftercooler temperatures on the performance variables is approximately linear over the temperature range considered. For instance, the effect of reducing both the 1st and 2nd stage aftercooler temperatures by $10^{\circ}F$ (Run 5) is approximately equal to the sum of the effects produced by separately reducing the 1st stage aftercooler temperature (Run 2) and the 2nd stage aftercooler temperature (Run 3).

Decreasing the outlet temperature from an aftercooler reduced the molar flow rate, temperature and molecular weight of the stream to the

FIG. 5.19 SUMMARY OF COMPRESSION MODEL SENSITIVITY RESULTS

RUN NO.	AFTERCOOLER TEMPERATURES (Deg F)			COMPRESSOR RECYCLE (Per Cent Recycled)		PERFORMANCE VARIABLES															
						COMPRESSOR FLOWS (Molar Flow Units)				COMPRESSOR FLOW MOLE WEIGHTS (lb/lb mol)				COMPRESSOR INLET TEMPERATURES (Deg F)				COMPRESSOR HEAT BALANCES (Energy Units)			
						COMPRESSOR STAGE															
	Stage 1	Stage 2	Stage 3	Low Pressure	High Pressure	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4
1	REFERENCE DATA					5.442	5.380	5.284	5.903	30.11	28.94	27.70	26.64	100.3	97.4	97.5	89.1	10.774	10.192	9.678	9.666
						CHANGES WITH RESPECT TO RUN 1															
2	-10	0	0	0	0	0	-0.033	-0.002	+0.003	0	-0.33	-0.03	+0.02	0	-9.5	0	-0.3	0	-0.415	-0.010	+0.002
3	0	-10	0			0	-0.002	-0.045	+0.001	0	-0.01	-0.34	+0.01	0	0	-9.5	-0.3	0	-0.008	-0.418	-0.002
4	0	0	-10			0	+0.006	+0.014	-0.123	0	+0.02	0.00	-0.33	0	0	0	-8.1	0	+0.021	+0.017	-0.506
5	-10	-10	0			0	-0.035	-0.043	+0.007	0	-0.32	-0.33	+0.02	0	-9.5	-9.5	-0.1	0	-0.430	-0.423	-0.004
6	0	-10	-10			0	+0.004	-0.032	-0.113	0	0.00	-0.32	-0.31	0	0	-9.5	-8.3	0	+0.013	-0.316	-0.523
7	-10	0	-10			0	-0.027	+0.012	-0.119	0	-0.31	-0.01	-0.33	0	-9.4	0	-8.3	0	-0.394	+0.025	-0.533
8	-10	-10	-10			0	-0.030	-0.051	-0.109	0	-0.31	-0.30	-0.30	0	-9.4	-9.6	-8.5	0	-0.409	-0.400	-0.514

next compression stage. These reductions were due to heavier components being removed from the cracked gas. The reductions in molar flow rate were of the order of 0.5% for the 2nd and 3rd stages and 2.0% for the 4th stage.

The larger change in the 4th stage flow was due to the increased removal of the heavier components from the cracked gas in the 3rd stage separator having a two-fold effect, i.e.

a) decreasing the overheads flow from the 3rd stage separator

b) decreasing the amount of light components removed with the heavier components in the 4th stage separator. Consequently, the overheads recycle flow from the condensate stripper to the 4th compression stage was reduced.

The results indicate that a decrease in an aftercooler temperature of 10°F reduced the compression energy loading of the next compression stage by between 3.8% and 5.5%, without significantly affecting the other compression stages. This is not strictly correct, since the representation of the compression stages in the cracked gas compression model did not take account of the inter-dependence of the compression stages, as was described in Section 5.5.5.3. The compression stage representation used in the model required that the interstage pressure between the two inter-dependent stages be fixed and supplied as model input data. In practice, a change in compression energy is shared between the two inter-dependent compression stages, and is accompanied by an adjustment of the interstage pressure. A compression stage representation, which includes the compressor stage characteristics, would be able to take account of this effect. Nevertheless, the results provide a meaningful estimate of the total compression energy change for the inter-dependent stages, even though the slight change in the interstage pressure has a marginal effect on the vapour/liquid separations in the interstage drums.

The model also showed that the removal of heavy components from the 1st stage cracked gas separator (i.e. stream 75 in Fig. 5.11) is more sensitive to changes in the 3rd stage aftercooler temperature than to changes in the other aftercooler temperatures. A decrease in the second stage aftercooler temperature had little effect on the liquid flow from the 1st stage cracked gas separator.

Conclusions

Although the cracked gas compression model was used successfully to investigate the distribution of flows throughout the compression system, and provided measures of changes to cracked gas compression energies, it was felt that more detailed and realistic representations of the compressor stages should be included in the model before more thorough investigations are undertaken.

5.6.1.2 Propylene Refrigeration System

The propylene refrigeration model was used first to simulate the propylene refrigeration system operating under design conditions, and then used to examine the effect on system behaviour of discrete changes in:-

i) refrigerant duties at each of the three refrigerant temperature levels.

ii) pressure in the

a) propylene suction drum, D-35

b) propylene 1st stage flash drum, D-36

c) propylene 2nd stage flash drum, D-37.

These changes were regarded as sufficient to provide an initial estimation of the behaviour and sensitivity of the propylene refrigeration system.

The model assumed throughout the simulation tests that the refrigerant compressors had identical characteristics and were equally loaded.

The performance variables examined were:-

i) compressor speed.

ii) compression energy - total and contribution of each of the stages.

iii) refrigerant aftercooler and condenser heat duty.

iv) temperatures of refrigerant drums D-35, D-36 and D-37 which correspond, respectively, to low, intermediate and high temperature refrigerant.

v) propylene refrigerant vapour let-down flows between refrigerant drums, as defined by streams 11, 18 and 25 in Fig. 5.13.

A summary of the results is given in Fig. 5.20.

i) <u>Changes in refrigerant duties (Runs 2 to 4, Fig. 5.20)</u>

The results show that an increase of 1 Energy Unit in process refrigerant duties at the low and high temperature levels (runs 2 and 4 respectively) produced approximately the same increases in compression energy and condenser heat duties. Although intuitively one would expect an increase in duty of low temperature refrigerant to produce a greater increase in compression energy than for high temperature refrigerant, the model results are a consequence of the refrigeration control system used to maintain constant pressures in the flash drums and the nature of the compressor characteristics. In run 4 it can be seen that the inlet temperature to the 1st stage suction (i.e. the temperature in drum D-35) has increased by $5^{\circ}F$, thus increasing the

FIG: 5.20 SUMMARY OF RESULTS - PROPYLENE REFRIGERATION MODEL

Run No.	Description of Run	Compressor Speed (Per Cent Design)	Compression Energy (Energy Units)				Condenser and Aftercooler Heat Duty (Energy Units)	Refrigerant Drum Temperatures (°F)			Vapour let-down flows between Refrigerant drums (Flow Units)		
			Stage 1	Stage 2	Stage 3	Total		D-35	D-36	D-37	D-39 to D-37	D-37 to D-36	D-36 to D-35
1	Reference Conditions	99.55	5.78	20.02	17.02	42.82	103.25	-36.1	-5.8	44.7	0	121.8	0
2	Reference + 1 Energy Unit low temp refrigerant	100.53	6.10	21.12	18.18	45.40	110.85	-36.1	-5.8	44.7	4.6	136.8	0
3	Reference - 1 Energy Unit inter temp refrigerant	99.55	5.78	20.02	17.02	42.82	98.21	-36.1	-5.8	44.7	42.6	121.8	0
4	Reference + 1 Energy Unit high temp refrigerant	100.60	6.82	21.52	18.44	46.78	112.07	-31.6	-5.8	44.7	0	167.0	27.4
5	D-35 Pressure Reference - 2 psi	103.8	6.20	24.38	21.98	53.56	113.26	-38.1	-5.8	44.7	202.4	331.0	0
6	D-36 Pressure Reference - 2 psi	99.6	6.82	19.66	17.48	43.94	104.28	-30.8	-7	44.7	0	46.2	52.0
7	D-37 Pressure Reference - 2 psi	100.7	6.86	21.54	17.84	46.04	106.72	-31.5	-5.8	44.0	0	196.0	30.8

compressor speed and the polytropic head of the 1st compression stage. The increase in temperature is due to 'hot' propylene vapour being let down in pressure, by the control system, between the refrigerant drums D-37, D-36 and D-35 (i.e. streams 18 and 25 in Fig. 5.13). It is interesting to note that a decrease in refrigerant duty at the intermediate temperature level (Run 3) produced no change in compression energy, but produced a decrease in condensing duty equal to the decrease in refrigerant duty. This effect was due to the control system allowing propylene vapour to be let down in pressure between drums D-39 and D-37 (i.e. flow 11 in Fig. 5.13).

An attempt was made to relate the behaviour of the propylene refrigeration system, as predicted by the model, to actual plant operation, but it became apparent that equal discrete changes in refrigerant duty at each temperature level do not occur in practice. A process change would affect the refrigerant duties at more than one temperature level. This situation emphasises the need to simulate the combined behaviour of the cracked gas compression, fractionation and refrigeration systems, as is demonstrated in section 5.6.2.

ii) Changes in refrigerant drum pressures (Runs 5 to 7, Fig. 5.20)

Runs 5 to 7 show that decreasing the pressure in an interstage drum lowers the corresponding refrigerant temperature level and increases the total compression energy requirement. A 2 psi decrease in the pressure of drum D-35, (Run 5), had the greatest effect on compressor performance since, as the 1st compressor stage operates at low absolute pressures, a change in suction pressure significantly affects the pressure ratio and polytropic head of the stage. This results in an appreciable increase in compressor speed which consequently affects the 2nd and 3rd stage compression energies. A decrease in pressure in D-36, (Run 6) had marginal effect on the overall compression energy since although it increased the 2nd stage pressure ratio, it reduced the pressure ratio of the 1st stage which was the most sensitive and dominant stage. A larger increase in compression energy resulted from a 2 psi decrease in pressure in D-37, (Run 7) which increased the 3rd stage pressure ratio but left the 1st and 2nd stage pressure ratios unchanged.

iii) Conclusions

The simulation tests using the model provided a valuable insight into the operation of the propylene refrigeration system, and demonstrated how the behaviour of the refrigeration system is very dependent on the performance of the refrigerant compressors and control system. The tests also revealed the disadvantages of not examining the combined behaviour of interacting systems.

5.6.2 System Simulation

Three examples are given to demonstrate how the Cold End model was used to simulate the combined behaviour of the cracked gas compression, refrigeration and fractionation systems when subjected to changes in operating parameters.

The operating parameters selected were:-

i) reflux ratio of T-10, ethylene tower (Process module DIST51, No. 58 in Fig. 5.12).

ii) reflux ratio of T-9, deethaniser (Process module DIST51, No. 60 in Fig. 5.12).

iii) exit temperature of E-22, cracked gas compression after-cooler (Process module HEX50, No. 40 in Fig. 5.11).

These operating parameters were selected since they have a major influence on plant operation. Model simulations were performed with the reflux ratio operating parameters adjusted to ±5% and ±10% either side of design values. The exit temperature of E-22, was set at 5°F and 10°F above and below its design value. All other operating parameters were kept at design values.

The performance variables examined were:-

i) propylene refrigeration compression energy (Fig. 5.21).

ii) propylene compressor speed, (Fig. 5.22).

iii) ethylene refrigeration compression energy (Fig. 5.23).

iv) cracked gas compression energy (Fig. 5.24).

v) propylene refrigerant vapour let down flows between the refrigerant drums, as defined by streams 11, 18 and 25 in Fig. 5.13 (Figs. 5.25 to 5.27).

vi) propylene refrigerant duties at each temperature level (Figs. 5.28 to 5.30).

vii) propylene refrigeration condensing duty (Fig. 5.31).

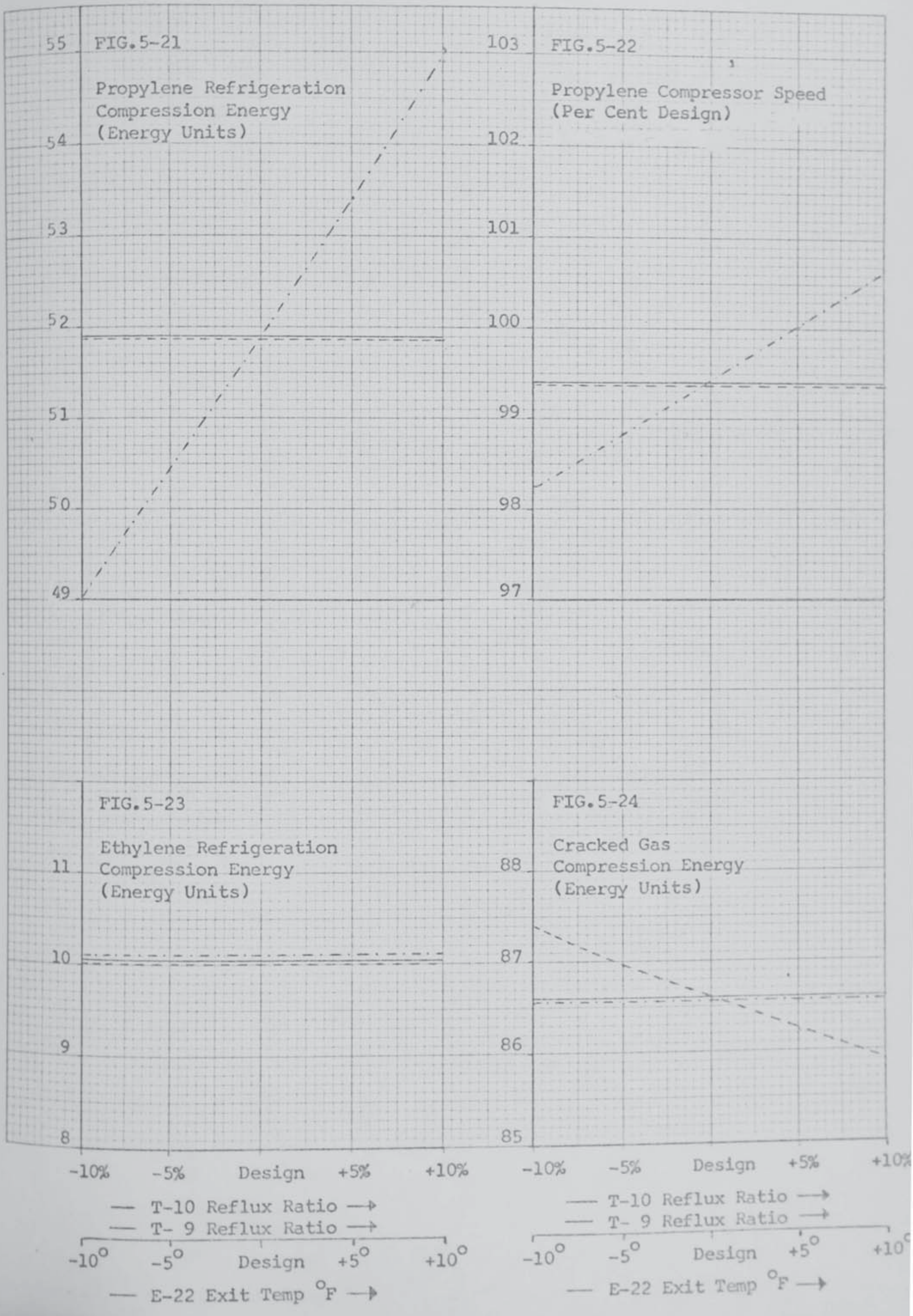
The behaviour of these performance variables, which is shown graphically in Figs. 5.21 to 5.31, is discussed for each of the selected operating parameters.

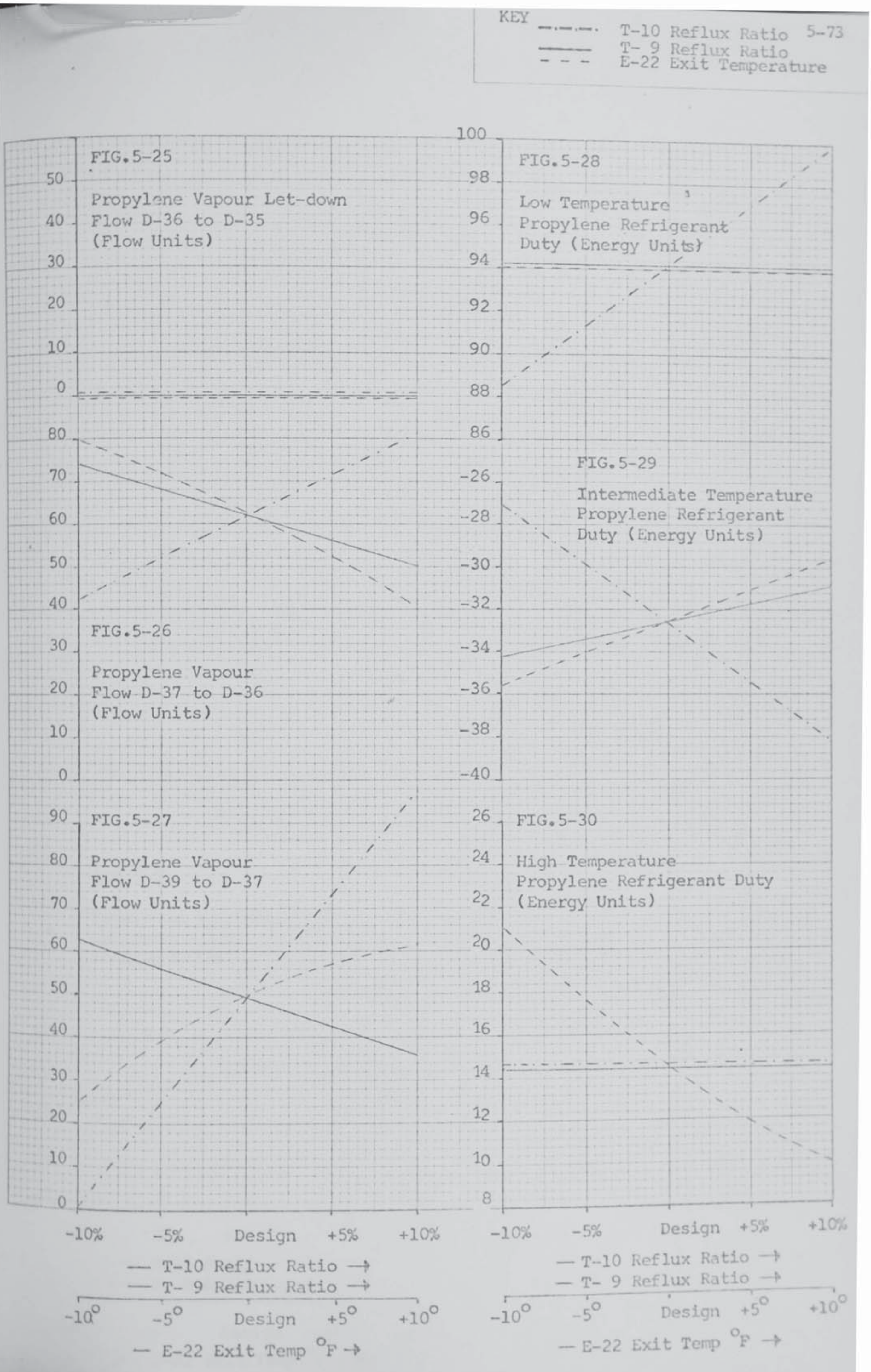
5.6.2.1 T-10 Reflux Ratio

It can be seen from Fig. 5.21 that an increase in T-10 reflux ratio produced an increase in the propylene refrigeration compression energy. The propylene compressor speed (Fig. 5.22), which is a directly observable plant measurement, reflects the changes in the propylene refrigeration compression energy. No changes occurred in either the ethylene refrigeration or cracked gas compression energies (Figs. 5.23 and 5.24).

A 10% increase in the T-10 reflux ratio produced an increase of approx. 6 energy units in propylene low temperature refrigeration duty (Fig. 5.28) and a decrease of approx. 6 energy units in intermediate

KEY
- · — · — · — T-10 Reflux Ratio
- ———— T- 9 Reflux Ratio
- - - - E-22 Exit Temperature




KEY
T-10 Reflux Ratio
T- 9 Reflux Ratio
E-22 Exit Temperature
FIG.5-25
Propylene Vapour Let-down
Flow D-36 to D-35
(Flow Units)
50
40
30
20
10
0
FIG.5-26
Propylene Vapour
Flow D-37 to D-36
(Flow Units)
80
70
60
50
40
30
20
10
0
FIG.5-27
Propylene Vapour
Flow D-39 to D-37
(Flow Units)
90
80
70
60
50
40
30
20
10
0
-10%
-5%
Design
+5%
+10%
— T-10 Reflux Ratio →
— T- 9 Reflux Ratio →
-10°
-5°
Design
+5°
+10°
— E-22 Exit Temp °F →
FIG.5-28
Low Temperature
Propylene Refrigerant
Duty (Energy Units)
100
98
96
94
92
90
88
86
FIG.5-29
Intermediate Temperature
Propylene Refrigerant
Duty (Energy Units)
-26
-28
-30
-32
-34
-36
-38
-40
FIG.5-30
High Temperature
Propylene Refrigerant Duty
(Energy Units)
26
24
22
20
18
16
14
12
10
8
-10%
-5%
Design
+5%
+10%
— T-10 Reflux Ratio →
— T- 9 Reflux Ratio →
-10°
-5°
Design
+5°
+10°
— E-22 Exit Temp °F →

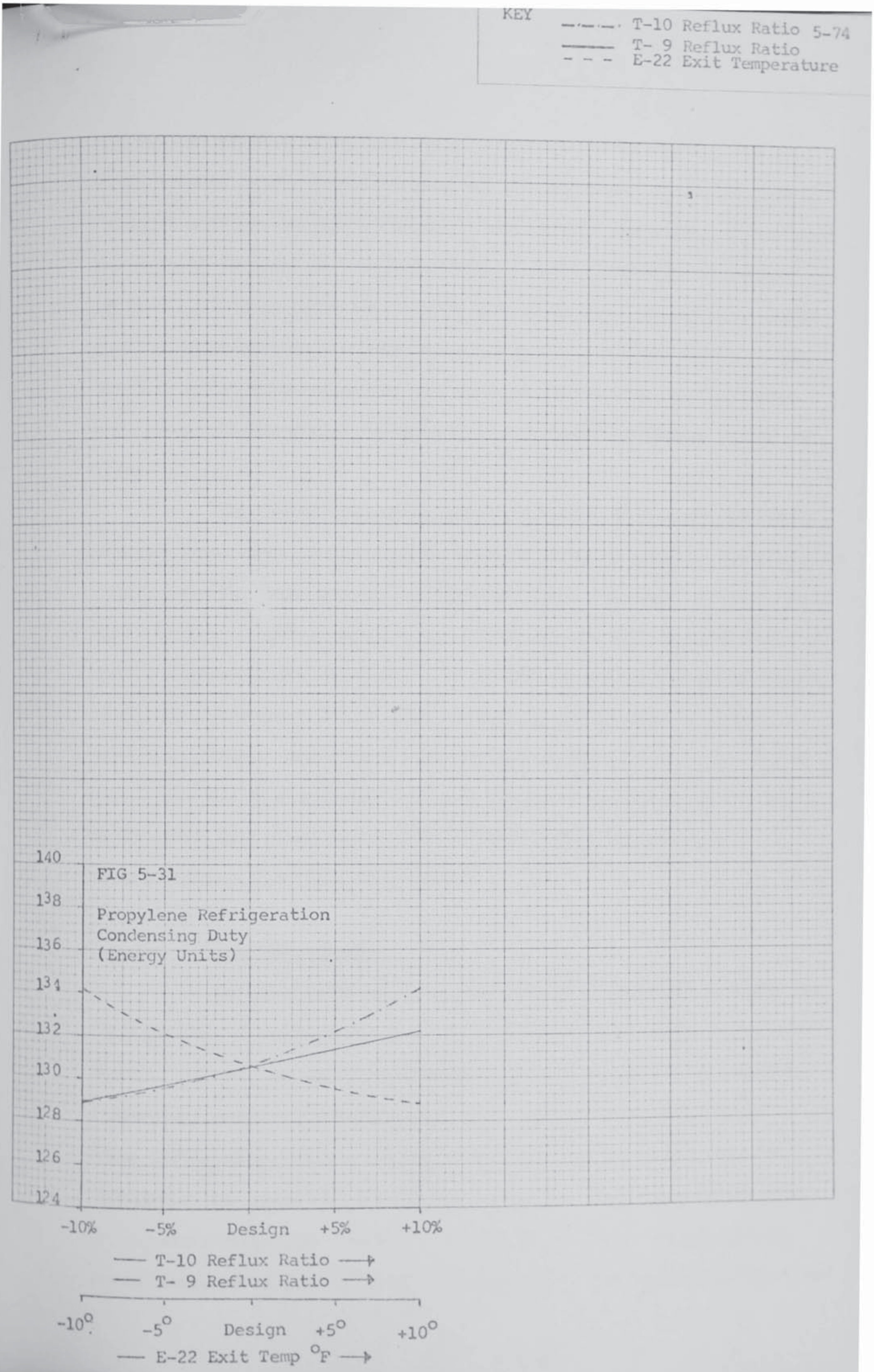


FIG 5-31

Propylene Refrigeration
Condensing Duty
(Energy Units)

temperature refrigeration duty (Fig. 5.29). (Low temperature refrigerant is used in the T-10 condenser and intermediate temperature refrigerant is used in the T-10 reboiler). These refrigerant heat duty changes produced an increase in propylene refrigeration compression energy of approx. 3.5 energy units (Fig. 5.21) and an increase in propylene refrigeration condensing duty of approx. 3.5 energy units (Fig. 5.31). The increase in compression energy was equal to the increase in condensing duty since the net effect of changes in propylene refrigerant duties was zero.

The changes in refrigerant heat duties at the low and intermediate temperature levels were accompanied by an increase in the propylene vapour let-down flows between refrigerant drums D-39, D-37 and D-36 (Figs. 5.26 and 27). The propylene vapour flow between D-36 and D-35 (Fig. 5.25) remained fixed at zero. It is worth commenting that the three vapour let down flows (Figs. 5.25, 26 and 27) should theoretically, be zero under design conditions. The non-zero design flows in Figs. 5.26 and 27 are due to differences in model results from design data. These differences were discussed in Section 5.5.6, which described the verification of the Cold End models.

5.6.2.2 T-9 Reflux Ratio

Adjustments to the T-9 reflux ratio did not affect either the refrigeration or cracked gas compression energy requirements (Figs. 5.21 to 24). A 10% increase in T-9 reflux ratio increased the intermediate temperature propylene refrigerant duty by approx. 1.5 energy units (Fig. 5.29), (intermediate temperature refrigerant is used in the T-9 condenser), but produced no change in the low or high temperature refrigerant duties (Fig. 5.28 and 30). The propylene refrigeration control system compensated for this change by decreasing the vapour let-down flows between drums D-39, D-37 and D-36 (Fig. 5.26 and 27). No change occurred in the propylene refrigeration compression energy (Fig. 5.21) but the propylene refrigeration condensing duty was increased by approx. 1.5 energy units (Fig. 5.31) (i.e. by an amount equal to the change in intermediate temperature propylene refrigerant duty).

5.6.2.3 E-22 Exit Temperature

The E-22 exit temperature can be adjusted by changing the level of refrigerant in the E-22 heat exchanger.

A 10^{o}F increase in E-22 exit temperature produced a decrease of approximately 0.7 energy units in cracked gas compression energy (Fig. 5.24) but produced no change in either the propylene or ethylene refrigeration compression energies (Figs. 5.21 and 23). The intermediate temperature propylene refrigerant duty was increased by approx. 2 energy units (Fig. 5.29) whilst the high temperature refrigerant duty decreased by approx. 4 energy units (Fig. 5.30). This produced a decrease of 2 energy units in propylene refrigeration condensing duty (Fig. 5.31).

The required refrigerant duties were satisfied by increasing the vapour let-down flow between D-39 and D-37 (Fig. 5.27) and decreasing the vapour let-down flow between D-37 and D-36 (Fig. 5.26). No change was required in propylene refrigeration compression energy.

5.6.2.4 Conclusions

These examples demonstrate the value of examining the combined performance of the Cold End sub-systems. Model simulation enabled the relative effects of changes in the operating parameters on Cold End system performance to be quantified. It can be concluded from these examples that:-

i) Operating parameters that produce changes in refrigerant duty will affect the propylene refrigeration condensing duty. All selected operating parameters had this effect. It was shown, for instance, that the propylene refrigeration condensing duty can be decreased by increasing the exit temperature of heat exchanger E-22.

ii) An operating parameter that produces a change in low temperature propylene refrigerant duty (e.g. T-10 reflux ratio) will change the propylene refrigeration compression energy. Since the ethylene refrigeration condenser also uses low temperature propylene refrigerant it follows that a change in ethylene refrigeration duty will affect the propylene refrigeration compression energy.

iii) A change in high or intermediate temperatures propylene refrigerant duties need not necessarily affect the propylene refrigeration compression energy. It was shown that an adjustment to T-9 reflux ratio did not affect the propylene refrigeration compression energy since the required changes in refrigerant duty were 'taken up' by adjustment of the vapour let-down flows between the refrigerant drums. The vapour let-down flow between drums D-36 and D-35 (Fig. 5.25), however, remained fixed at zero for each of the selected operating parameters indicating that low temperature refrigerant was the dominant refrigerant temperature level.

iv) None of the selected operating parameters produced changes in the ethylene refrigeration compression energy, since the separation of ethane and lighter components in the de-methaniser, T-8, overheads system, which is the main user of ethylene refrigerant, was unaffected by the changes produced by the operating parameters.

5.7 CONCLUSIONS

The conclusions to be drawn from this study of the Cold End are:-

i) The study has shown how necessary it is to apply systems engineering to the analysis, modelling and simulation of a large scale industrial process system.

The more complex the system, the greater the need to apply systems engineering, and to examine the system as a series of interlinking sub-systems. Some comments on systems engineering as applied to the Cold End are discussed briefly.

a) Systems engineering ensures that the system being examined has an objective and a performance criterion. The objective of this study was to explore and understand the interactions that exist between and within the Cold End sub-systems, and to relate the effect of such interactions on Cold End system performance. An emphasis was placed upon the energy interactions between the process and refrigeration sub-systems. The performance of the cracked gas and refrigerant compressors was used initially as a measure of both system and sub-system performance.

b) Model building in systems engineering requires that one should start with whatever knowledge is available, and build on this in whatever way, time, resources, and the accuracy needed by the model, dictate. Such a policy was adopted throughout the Cold End modelling work, which used a consistent, parsimonious approach in the development of the models. A substantial amount of modelling effort was required to establish a consistent physical property base, since physical property data that adequately reflected plant operation were fundamental to the Cold End modelling work.

It was not expedient during the first year of Ethylene Plant operation to embark on any plant experimentation or large scale data collection exercises. As the objective of the Ethylene Plant during this period was reliable operation, there existed, as far as the Baglan Bay Factory was concerned, neither the incentive nor, the resources to undertake such exercises. Although plant data were not used as a reference set in the verification of the Cold End models, selective plant data were used to discriminate between rival models. This was typified by the modelling of the cracked gas compression interstage drums.

c) The size and complexity of the Cold End was such that the Cold End sub-systems, in addition to the Cold End System, were considered worthy of examination as systems in their own right. It is safe to examine a sub-system in this way provided interactions with the other sub-systems are accounted for. For instance, it would be pointless spending considerable effort in increasing the capacity of the cracked gas compression system, which is known to be throughput limiting, only to discover that the extra capacity cannot be accommodated by the refrigeration system.

ii) <u>The study provided an insight into the interactions and basic principles of operation of the Cold End sub-systems</u>

The simulation of the Cold End system and sub-system behaviour using the Cold End models revealed the magnitude and extent of system interactions. For instance, sensitivity tests on the cracked gas compression sub-system model enabled the relative effects of changes in aftercooler temperatures on cracked gas compressor performance to be assessed.

iii) <u>The Cold End model has provided a basis upon which future modelling work can be built</u>

Future work on the development of the Cold End model has three courses - the model can be developed for:-

a) On-line supervisory control of the Cold End

The original motivation behind the development of a Cold End model was to enable supervisory control of the Ethylene Plant to be effected. A considerable amount of additional time and effort are required to produce a steady state model that simulates, for different modes of plant operation, the behaviour of the Cold End to sufficient accuracy for plant supervisory control. It must be established whether the Cold End of the No. 2 Ethylene Plant has sufficient flexibility in its design and control system to benefit from the availability of such a model. Plant experimentation must be used to establish whether the development of the model can be justified. The results of these experiments can be used for any improvement of plant performance and to provide data for future model building. Plant data are required to identify limiting items of equipment, and to reflect the operating characteristics of equipment into the Cold End model.

Possible areas for improvement of Cold End operation are:-

1) the development of operating strategies for the parallel cracked gas compressor trains.
2) the allocation of pressure levels for refrigerant.
3) the recovery of refrigeration energy from product and intermediate streams.

Before the existing Cold End model can be put to further effective use it is essential to establish more accurate models of the cracked gas and refrigerant compressors.

b) Off-line studies of Cold End operation (e.g. as a plant 'debottlenecking' aid)

A steady state model, that reflects the operation of the Cold End of the No. 2 Ethylene Plant, can be used, off-line, to examine the flexibility of plant operation as governed by the operating characteristics of plant equipment. This model could be used in plant 'debottlenecking' exercises and in studies involving minor process modifications to the plant.

c) Design of new Ethylene Plants

The requirements of a design model are different from a control model. A control model is normally required to be accurate over a small operating range, whilst a design model is often less accurate, but must be capable of covering a wider range of conditions.

As a design aid, the Cold End model could be used for estimating the energy duties of major process and refrigerant equipment, upon which detailed design calculations can be based. Its modular structure permits alternative Cold End configurations to be examined.

CHAPTER 6

GENERAL CONCLUSIONS

CHAPTER 6 - GENERAL CONCLUSIONS

The project has demonstrated how the application of systems engineering principles and techniques can contribute effectively to the successful operation of the No. 2 Ethylene Plant. As a joint University/ Industry venture, the project enabled both sides to benefit from an exchange of ideas and approach. It clearly demonstrated how any undertaking of this kind is strongly influenced by the priorities of the industrial environment. The commissioning of the No. 2 Ethylene Plant was the dominant factor in determining the timing and scope of the project activities. This made the adoption of the disciplined approach of systems engineering essential to the success of the project, and required that project objectives be re-appraised, at intervals, throughout the work.

The human element played an important role in the project, particularly in the development and application of the plant computer system and of data reconciliation. Particular attention was paid to enlisting and then sustaining the co-operation and interest of personnel associated with the systems that were being analysed and developed. For instance, the training of personnel to use and appreciate the plant computer system was regarded of fundamental importance.

It was realised that no matter how potentially useful a technique may be, if it is not used properly its benefit is lost. With this in mind, simple and reliable techniques capable of producing limited but definite improvement were preferred to complicated unreliable techniques of potentially greater value. This philosophy was borne out in the way the Ethylene Plant Computer System was specified and applied, and also in the selection and application of the robust and well proven technique of linear programming for data reconciliation.

The project demonstrated how a plant computer system through its display, logging, alarming and calculation facilities, improved the operability of the No. 2 Ethylene Plant. The systematic preparation of the computer system and the establishment of a good working relationship with the No. 2 Ethylene Plant personnel, were the main factors in ensuring that the computer system was used effectively. During Ethylene Plant commissioning, the outstanding virtue of the computer system was its flexibility in being able to provide invaluable assistance in overcoming unexpected problems.

Automatic data reconciliation provided a means of consistently rationalising data from a large scale industrial mass flow measuring system, and provided No. 2 Ethylene and Factory Management with high quality consistent data upon which decisions could be made. An examination of the errors in industrial flow data revealed that it is the gross systematic errors that dominate and provide the major data reconciliation problems. A linear data reconciliation error criterion was shown to be suitable for reconciling data containing such errors. This enabled the versatile technique of linear programming to be used for data reconciliation. Data reconciliation, and the plant computer system, which was mainly responsible for the acquisition of the raw unreconciled data, proved to be incentives for maintaining high standards of flow instrumentation.

It was demonstrated how the analysis, modelling and simulation of a large scale industrial process system (i.e. the Cold End of the No. 2 Ethylene Plant) benefited from the systems engineering approach. In particular, systems engineering was used successfully to decide where modelling effort should best be directed and how the models should be developed. The Cold End was divided into its component sub-systems and those sub-systems which had the greatest effect on system performance were modelled and simulated. A modular and parsimonious approach characterised the modelling of the Cold End. The study provided an insight into the interactions and basic principles of operation of the Cold End sub-systems and established a foundation upon which future Cold End modelling and simulation work can be based.

APPENDICES

APPENDIX 1

C2 HYDROGENATION COMPUTER CONTROL SCHEME

i) SUMMARY

The Plant Computer provided facilities for improved control of the C2 hydrogenation system of the No. 2 Ethylene Plant. The computer performed on-line logical and arithmetic calculations on plant data and the resulting answers, which were displayed and logged by the computer, were used by process operators to re-set the C2 hydrogenation control panel analogue controllers. The computer facilities can be described as a simple form of open-loop computer supervisory control.

ii) PROCESS DESCRIPTION AND ANALOGUE CONTROL SCHEME

The short residence time and high temperature cracking of the naphtha feedstock can result in unacceptable acetylene concentrations in the ethane/ethylene mixture from the de-ethaniser column. It is essential that the acetylene concentration in the ethylene product be reduced to a very low level in order that ethylene product user plants can operate efficiently.

The C2 Hydrogenation System removes acetylene by adding a measured amount of high purity hydrogen to the ethane/ethylene stream and passing the mixture over a palladium based catalyst to hydrogenate acetylene to ethylene and ethane. The following reactions take place:-

1) $H_2 + C_2H_2 \rightarrow C_2H_4$ (Hydrogen + acetylene $\rightarrow$ ethylene)

2) $2H_2 + C_2H_2 \rightarrow C_2H_6$ (Hydrogen + acetylene $\rightarrow$ ethane)

A schematic of the C2 hydrogenation system showing the analogue flow ratio control system is shown in Fig. A1-1.

The hydrogenation is accomplished by using a series of reactors. The high purity hydrogen required for hydrogenation is injected, under flow ratio control, into the ethane/ethylene stream fed to each of the reactors. The bulk of the hydrogenation is performed in the first reactor (H-D-104) where the acetylene concentration is reduced to less than 1 per cent. The subsequent reactors further reduce the acetylene content to the required few ppm.

It is important that the correct amount of hydrogen is injected into the ethane/ethylene system. Too little hydrogen will result in an intolerable amount of acetylene in the ethylene product, while too much hydrogen will result in the undesirable hydrogenation of the more valuable ethylene product to ethane. Although it is always expedient to operate with a slight excess of the theoretical hydrogen required, a large excess of hydrogen will represent inefficient operation.

The analogue control system controls the amount of hydrogen injected into the process by ratioing the hydrogen flows to the ethylene/ethane flow. However, the control system is unable to take account of the fluctuating acetylene concentration in the ethane/ethylene stream from the de-ethaniser, fluctuating hydrogen purity, or the state of the catalyst used in the hydrogenation reactors.

iii) COMPUTER CONTROL SCHEME

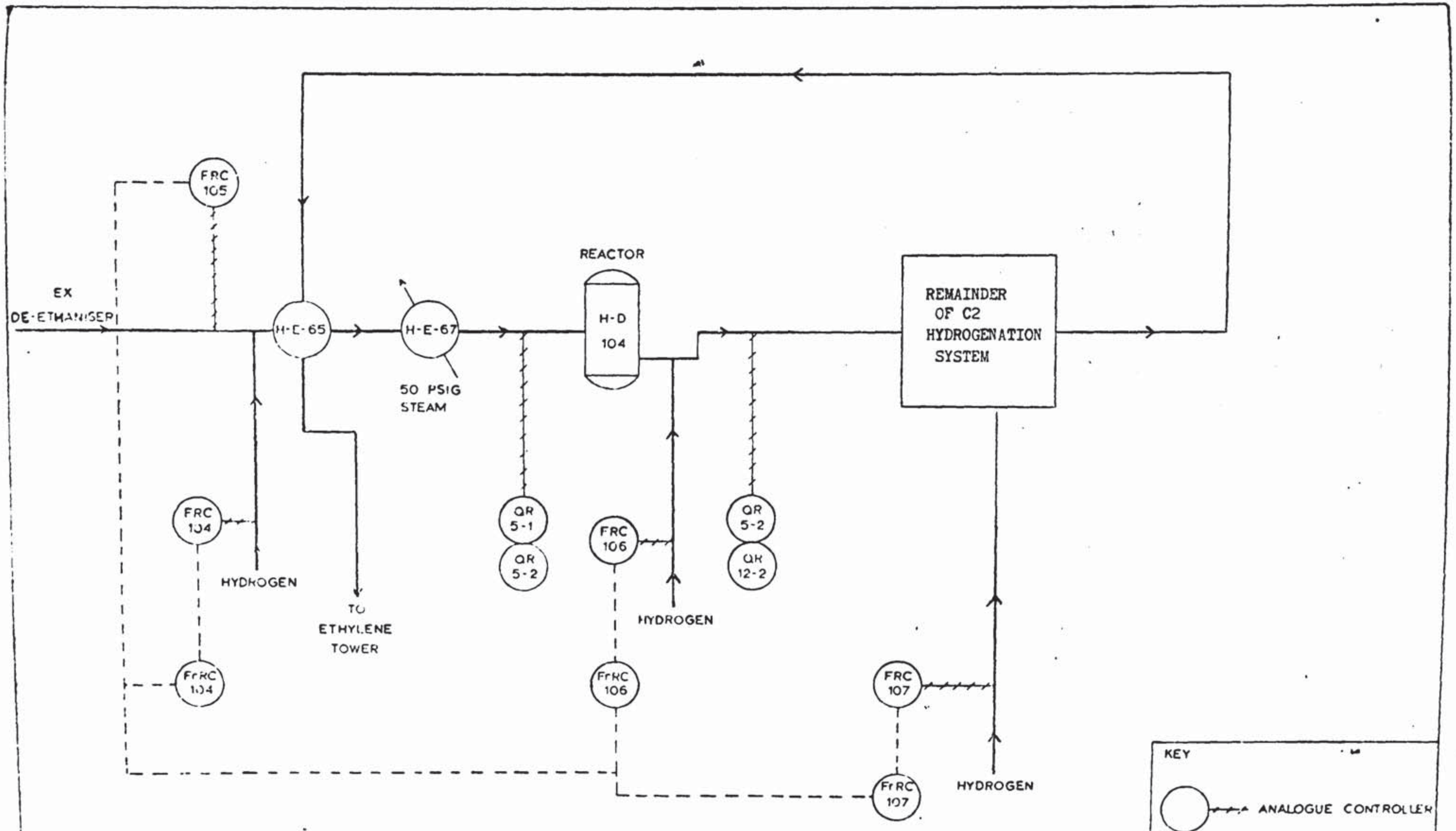
Improved control of the C2 hydrogenation system was achieved using the computer control scheme shown in Fig. A1-2, which is a simple form of computer supervisory control. Fig. A1-3 is a schematic of the C2 hydrogenation system showing the computer loops. The computer loops, which are summarised in Fig. A1-4, can be sub-divided into two types - those that display basic plant data and those that perform calculations and display derived data. Full details of the computer loops are found in (33).

A computer loop EX401 (see Fig. A1-3) was defined which used inputs from the hydrogenation system flow meters and on-line analysers to calculate how much hydrogen is theoretically required to hydrogenate the acetylene in the ethane/ethylene stream. The process operator was required to manually update the computer with values of the concentration of the high purity hydrogen (computer loop EX402) and the required hydrogen/acetylene ratio (computer loop EX400). This ratio required periodic updating to take account of the delay in the activity of the reactor catalyst. The hydrogen concentration was used to correct the density of the hydrogen flows.

A computer loop EF415 summed the three hydrogen injection flows to the hydrogenation system and compared the total with the theoretical amount of hydrogen required. Computer alarm limits were placed on this difference to ensure that the excess hydrogen flow lay between upper and lower limits. Whenever the difference exceeded these limits the computer alarm was activated and the process operator manually adjusted the control panel flow ratio controllers until the excess hydrogen flow was back within limits. Computer loops EX403 and EX404 measured the hydrogen/acetylene ratios at the inlet and outlet of the isothermal reactor H-D-104. A computer trend log (Fig. A1-5) containing six hydrogenation system loops was displayed and updated every five minutes on the control room visual display unit. The log enabled the process operator to continually monitor the state of the C2 hydrogenation system.

iv) CONCLUSIONS

This computer scheme has demonstrated to plant management how the computer can be used to improve control of the plant. It has enabled process operators to appreciate the concepts of computer supervisory control and is an important precursor to future closed-loop computer supervisory control applications.



C2 HYDROGENATION SYSTEM SHOWING
ANALOGUE FLOW RATIO CONTROL SYSTEM (FIG A1-1)

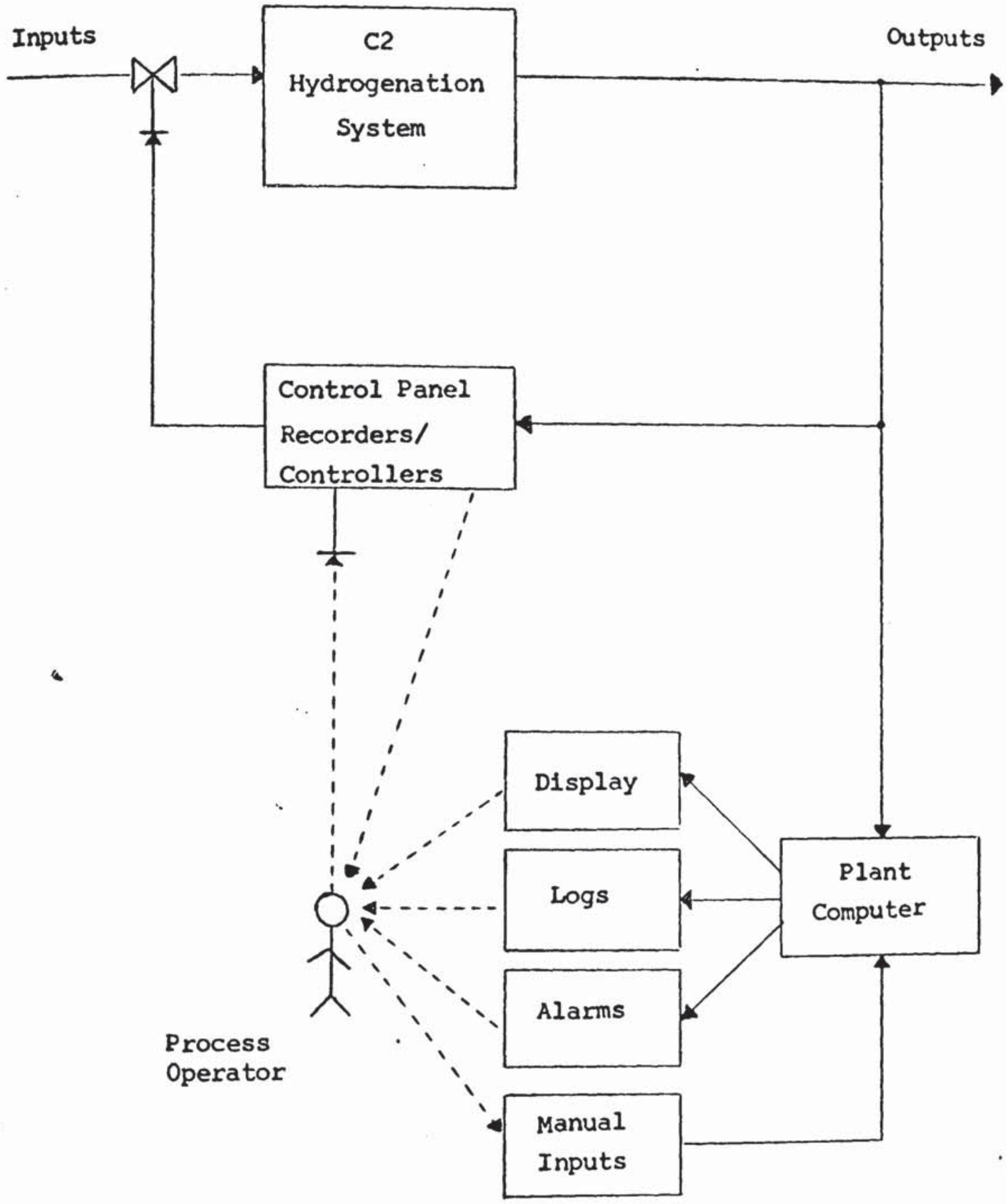
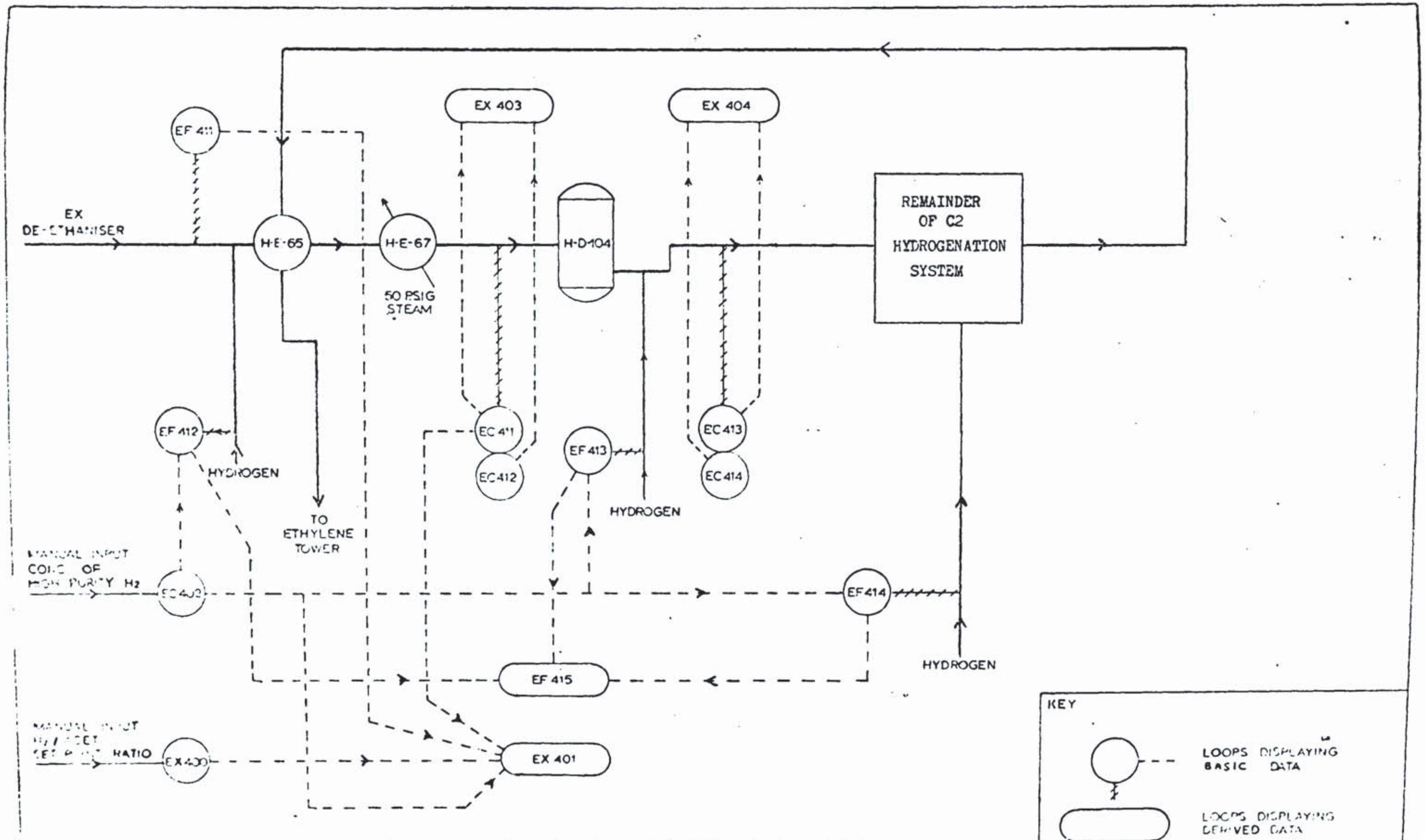


FIG. A1-2 C2 HYDROGENATION COMPUTER CONTROL SCHEME



C2 HYDROGENATION SYSTEM SHOWING COMPUTER LOOPS (FIG A1-3)

Fig. A1-4 Summary of C2 Hydrogenation System Computer Loops

Computer Loop	Description	Comments
EC402	High purity hydrogen concentration - Manual Input	Used by Process Operator to manually update and display the molar concentration of high purity hydrogen
EC411	Acetylene concentration ex H-E-67	Used to display input from on-line acetylene analyser H-QR-5-1
EC412	Hydrogen concentration ex H-E-67	Used to display input from on-line hydrogen analyser H-QR-12-1
EC413	Acetylene concentration ex H-D-104	Used to display input from on-line acetylene analyser H-QR-5-2
EC414	Hydrogen concentration ex H-D-104	Used to display input from on-line hydrogen analyser H-QR-12-2
EF412	High purity hydrogen flow to 1st Reactor	Used to display hydrogen flow as metered by H-FRC-104. Density corrected using input from loop EC402.
EF413	High purity hydrogen flow to 2nd Reactor	Used to display hydrogen flow as metered by H-FRC-106. Density corrected using input from loop EC402.
EF414	High purity hydrogen flow to 3rd Reactor	Used to display hydrogen flow as metered by H-FRC-107. Density corrected using input from loop EC402.
EF415	Total measured flow of high purity hydrogen to C2 hydrogenation system	EF415 = EF412 + EF413 + EF414
EX400	(Hydrogen/Acetylene) Set Point Ratio - Manual input	Used by Process Operator to manually update and display required (hydrogen/acetylene) molar set point ratio.
EX401	Total theoretical flow of high purity hydrogen required by C2 hydrogenation system	EX401 = (Acet. flow to D104) x $\frac{H_2}{Acet}$ molar set point = fn (EF411, EC411, EX400, EC402)
EX402	(Hydrogen/Acetylene) ratio - overall	EX402 = $\frac{\text{(Total pure hydrogen flow)}}{\text{(Acet. flow to D104)}}$ = fn(EF415, EC402, EF411, EC411)
EX403	(Hydrogen/Acetylene) ratio inlet to H-D-104	EX403 = $\frac{EC412}{EC411}$
EX404	(Hydrogen/Acetylene) ratio inlet to H-D-106	EX404 = $\frac{EC414}{EC413}$

13.30 HRS 30/09/84 LOG 03

TIME	E X400	E X401 KLBS/HR	E X402	E F415 KLBS/HR	E F411 KLBS/HR	E C411 %	
13.00	2.000	.2825	2.181	0.306	116.2	1.303	03
13.05	2.000	.2823	2.186	0.307	116.1	1.303	03
13.10	2.000	.2828	2.184	0.307	116.3	1.303	03
13.15	2.000	.2821	2.192	0.307	116.0	1.303	03
13.20	2.000	.2817	2.194	0.307	115.8	1.303	03
13.25	2.000	.2820	2.183	0.306	116.0	1.303	03
13.30	2.000	.2813	2.189	0.306	115.7	1.303	03
13.35	2.000	.2814	2.181	0.304	115.7	1.303	03
13.40	2.000	.2812	2.180	0.305	115.7	1.303	03
13.45	2.000	.2819	2.188	0.307	116.0	1.303	03
13.50	2.000	.2825	2.189	0.307	116.2	1.303	03
13.55	2.000	.2760	2.231	0.304	113.5	1.303	03

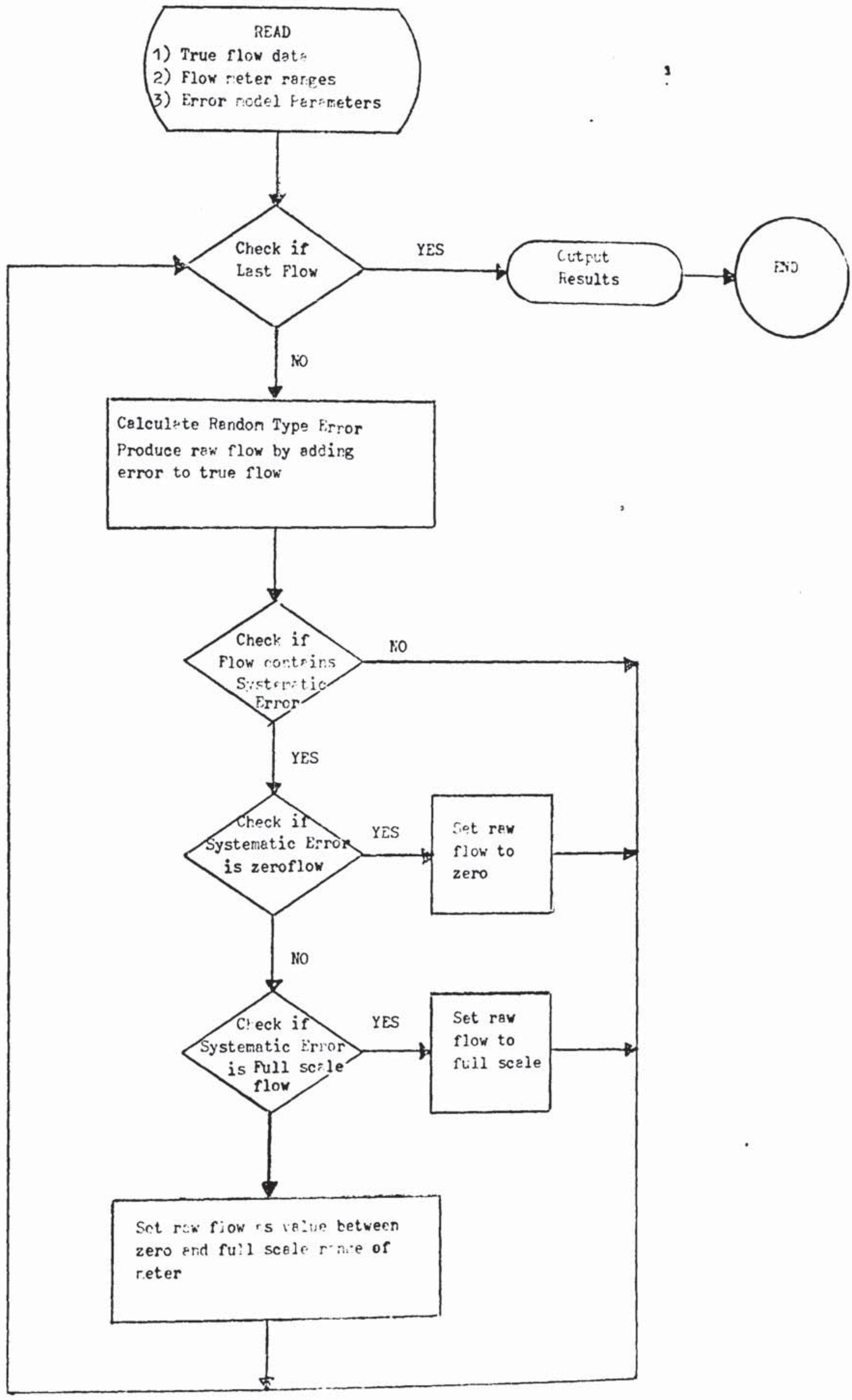
FIG. A1-5 C2 HYDROGENATION COMPUTER TREND LOG

(False data have been used)

APPENDIX 2

MODEL OF ERRORS IN INDUSTRIAL FLOW DATA

FLOWCHART OF ERROR MODEL



```
      MASTER GENFLOWS
C     ************************
C     DHT  26/6/74
C
C     PROGRAM TO GENERATE SET OF APPARENT FLOW DATA AND REPEAT DATA
C     CONTROL PARAMETERS
C
      DIMENSION      FRANGE(30),FTRUE(30),FACT(30)
      READ(1,030)NDSET,NSETS,WEIGHT
C-----READ START NUMBER FOR RANDOM NO GENERATOR
      READ(1,030)NR
C-----READ NO OF METERS,SYSTEMATIC ERROR PROBS AND MEAN PER CENT TOLERANCE
      READ(1,900)   KMETERS,PSYS,PZERO,PFR,TM
C
C-----READ METER FLOW RANGES
      READ(1,910)    (FRANGE(J),J=1,KMETERS)
C
C-----READ TRUE METER FLOWS
      READ(1,910)    (FTRUE(J),J=1, KMETERS)
C-----GENERATE SETS OF APPARENT DATA
      WRITE(3,950)NDSET,PSYS,PZERO,PFR,TM,NR
      WRITE(3,955)(I,I=1,KMETERS)
      K=0
      WRITE(3,960) K,(FTRUE(J),J=1,KMETERS)
      DO 50 K=1,NSETS
      DO 100 I=1,KMETERS
      CALL INHERR(L,FRANGE(L),TM,FTRUE(L),FACT(L),NR)
      CALL SYSERR(L,FRANGE(L),PSYS,PZERO,PFR,FACT(L),NR)
  100 CONTINUE
      WRITE(2,800)  K,KMETERS,(L,FACT(L),L=1,KMETERS)
      WRITE(3,960) K,(FACT(L),I=1,KMETERS)
      WRITE(2,825)WEIGHT
   50 CONTINUE
      WRITE(2,850)
      WRITE(3,860)NR
      STOP
  030 FORMAT(2I5,10X,A4)
  900 FORMAT(I5,5X,4F10.4)
  910 FORMAT(8F10.2)
  800 FORMAT(4HLINE/3H  1/5HRUN  ,I3/5HFLOWS/I3,(/6(I3,1X,F7.2,1X)))
  825 FORMAT(6HWEIGHT/A6/5HPRINT/7HMODULUS/2HGO)
  850 FORMAT(4H*** )
  860 FORMAT(1H1,//29H LAST RANDOM NUMBER GENERATED,I5)
  955 FORMAT(/// 4X,6HRUN NO,50X,8HMETER NO,/5X,6(1H-),50X,8(1H-)//10X,
     113(3X,I2,3X),/10X,99(1H-)/)
  950 FORMAT(1H1,/,50X,12HDATA SET NO ,I3///30X,40HPROBABILITY OF GROSS
     1SYSTEMATIC ERROR = ,F5.2/30X,40HPROBABILITY OF ZERO FLOW
     2    = ,F5.2/30X,40HPROBABILITY OF FULL SCALE FLOW         = ,F5.2/
     330X,40HPER CENT MEAN TOLERANCE OF METER SET  = ,F5.2/30X,40HSTART
     4RANDOM NO USED                          = ,I5)
  960 FORMAT(6X,I2,2X,13(1X,F6.2,1X))
      END
```

END OF SEGMENT, LENGTH   266, NAME GENFLOWS

```
      SUBROUTINE INHERR(NM,RM,TM,FT,FA,NR)
C     ****************************************
C     DHT  26/6/74
C
C     ROUTINE TO CALCULATE FLOW ERROR DUE TO INHERENT SYSTEMATIC
C     AND RANDOM ERRORS IN INSTRUMENTS
C
C     ARGUMENT LIST : NM = METER NUMBER
C                     RM = METER FLOW RANGE
C                     TM = PER CENT MEAN TOLERANCE OF METER SET
C                     FT = TRUE FLOW
C                     FA = APPARENT FLOW
C                     NR = RANDOM NO   (0-40000)
      STDX=0.5*TM
      EX=0
      CALL NORMAL(EX,STDX,X)
      FA=FT+RM*X/100.0
      IF(FA.LT.0.0.AND.FT.GE.0.0)FA=0.0
      RETURN
      END

END OF SEGMENT, LENGTH    95, NAME  INHERR
```

```
      SUBROUTINE SYSERR(NM,RM,PSYS,PZERO,PFR,FA,NR)
C     ************************************************
C     DHT  26/6/74
C
C     ROUTINE TO DETERMINE WHETHER METER CONTAINS GROSS SYSTEMATIC
C     ERROR AND TO DETERMINE VALUE OF ERROR
C
C     ARGUMENT LIST  NM    = METER NUMBER
C                    RM    = METER FLOW RANGE
C                    PSYS  = PROBABILITY OF GROSS METER ERROR OCCURING
C                    PZERO = PROBABILITY FLOW IS ZERO IF ERROR EXISTS
C                    PFR   = PROBABILITY FLOW IS FULL SCALE IF ERROR EXISTS
C                    FA    = APPARENT FLOW IF GROSS SYSTEMATIC ERROR EXISTS
C                    NR    = RANDOM NO   0-40000
C-----CHECK IF METER CONTAINS GROSS SYSTEMATIC ERROR
      IF(RND(NR).GT.PSYS)RETURN
C
C-----CHECK TYPE OF SYSTEMATIC ERROR
      RAND=RND(NR)
      FA=0.0
      IF(RAND.LE.PZERO)RETURN
      FA=RM
      PSUM=PZERO+PFR
      IF(RAND.GT.PZERO.AND.RAND.LE.PSUM)RETURN
      FA=RND(NR)*RM
      RETURN
      END

END OF SEGMENT, LENGTH   125, NAME  SYSERR
```

```
      SUBROUTINE NORMAL(EX,STDX,X,NR)
C     ******************************
C     DMT 26/6/74
C
C     ROUTINE TO GENERATE NORMAL VARIATES
C
C     ARGUMENT LIST : EX = MEAN OF DISTRIBUTION
C                     STDX= STANDARD DEVIATION OF DISTRIBUTION
C                     X  =  NORMAL SAMPLED VARIATE
C                     NR =  RANDOM NUMBER (0-40000)
      SUM=0.0
      DO 10 K=1,12
   10 SUM=SUM+RND(NR)
      X=STDX*(SUM-6.0)+EX
      RETURN
      END

 END OF SEGMENT, LENGTH    68, NAME  NORMAL
```

```
      FUNCTION RND(NR)
C     ************************
C
C     DMT  26/6/74
C
C     ROUTINE TO GENERATE PSEUDO-RANDOM NUMBERS BETWEEN 0 AND 1
C
      NN=NR*201 + 37
      NM=(NN/40000)*40000
      NR=NN-NM
      RND=FLOAT(NR)/40000
      RETURN
      END

 END OF SEGMENT, LENGTH    51, NAME  RND
```

APPENDIX 3

EVALUATION OF DATA RECONCILIATION ERROR CRITERIA

RAW DATA SETS 1 TO 3

TYPICAL SET OF RECONCILED RESULTS (DATA SET 1, RUN 1)

DATA SET NO 1

PROBABILITY OF GROSS SYSTEMATIC ERROR = 0.00
PROBABILITY OF ZERO FLOW = 0.00
PROBABILITY OF FULL SCALE FLOW = 0.00
PER CENT MEAN TOLERANCE OF METER SET = 3.00
START RANDOM NO USED = 31494

RUN NO	METER NO 1	2	3	4	5	6	7	8	9	10	11	12	13
0	104.00	0.40	82.00	8.60	13.00	13.00	38.00	44.00	-2.00	26.00	58.00	0.00	14.00
1	102.15	0.40	82.56	7.91	13.87	13.32	38.05	42.82	-2.28	25.27	59.20	0.00	13.72
2	106.89	0.40	83.13	9.03	13.11	13.25	38.62	43.38	-2.08	25.97	57.54	0.00	14.98
3	106.04	0.39	79.64	8.50	12.69	12.77	37.38	43.84	-1.93	25.43	57.42	0.00	14.69
4	103.23	0.41	81.85	8.50	13.00	13.39	39.55	41.96	-1.83	26.03	57.18	0.00	14.34
5	102.09	0.38	83.90	9.01	12.90	12.86	37.29	42.25	-1.78	25.99	56.79	1.11	14.68
6	104.44	0.42	83.85	8.96	13.51	13.04	37.58	44.69	-2.37	25.30	61.31	1.58	12.71
7	103.00	0.39	81.68	8.34	12.08	13.19	38.67	43.67	-2.41	25.17	57.30	0.00	15.18
8	105.06	0.39	81.32	8.79	13.01	12.19	37.08	44.81	-1.90	25.58	59.87	0.00	13.09
9	105.15	0.40	82.74	8.67	12.57	12.66	38.03	42.48	-2.04	26.55	60.63	0.80	16.19
10	103.29	0.42	84.01	8.81	13.07	13.10	37.17	43.44	-1.02	26.87	56.22	0.10	13.97
11	104.90	0.40	83.18	8.38	13.54	12.76	37.98	43.18	-1.85	25.94	58.39	0.22	13.20
12	104.56	0.41	84.14	8.20	12.85	13.52	36.98	42.83	-2.13	26.16	57.06	0.26	12.37
13	105.89	0.41	79.09	8.54	12.89	12.74	38.52	44.65	-0.66	25.14	58.96	0.00	14.48
14	107.07	0.40	83.64	8.85	12.51	13.06	38.25	44.12	-2.24	25.26	57.37	0.14	13.53
15	106.30	0.40	86.08	8.34	13.24	12.60	37.05	44.63	-2.67	25.94	57.32	0.00	14.77
16	105.37	0.39	82.51	8.34	12.81	12.48	37.51	42.79	-1.94	25.97	53.78	1.51	15.20
17	102.49	0.39	86.74	8.59	13.10	13.46	39.64	40.87	-2.46	25.36	58.50	0.00	14.81
18	106.72	0.41	86.76	8.55	13.36	13.29	38.22	43.36	-2.43	25.89	58.05	0.00	14.37
19	105.36	0.40	84.53	8.49	12.84	13.08	36.74	43.51	-1.85	26.38	55.79	0.37	13.87
20	102.04	0.40	80.34	8.41	12.66	12.85	37.79	43.57	-3.11	26.82	61.79	0.00	13.31

DATA SET NO 2

PROBABILITY OF GROSS SYSTEMATIC ERROR = 0.10
PROBABILITY OF ZERO FLOW = 0.20
PROBABILITY OF FULL SCALE FLOW = 0.10
PER CENT MEAN TOLERANCE OF METER SET = 0.00
START RANDOM NO USED = 31494

METER NO

RUN NO	1	2	3	4	5	6	7	8	9	10	11	12	13
0	104.00	0.40	82.00	8.60	13.00	13.00	38.00	44.00	-2.00	26.00	58.00	0.00	14.00
1	104.00	0.40	82.00	8.60	13.00	13.00	38.00	44.00	-2.00	26.00	58.00	0.00	14.00
2	104.00	0.40	82.00	8.60	13.00	13.00	38.00	44.00	-2.00	26.00	58.00	0.00	14.00
3	104.00	0.40	82.00	8.60	13.00	8.62	38.00	44.00	-2.00	26.00	58.00	0.00	14.00
4	15.61	0.40	82.00	17.25	13.00	13.00	38.00	44.00	-2.00	36.24	58.00	0.00	38.03
5	104.00	0.40	82.00	8.60	13.00	13.00	38.00	44.00	-2.00	26.00	58.00	0.00	14.00
6	104.00	0.04	82.00	8.60	13.00	13.00	38.00	44.00	-2.00	26.00	58.00	59.00	14.00
7	66.58	0.40	82.00	8.60	13.00	13.00	38.00	44.00	13.38	26.00	58.00	0.00	24.25
8	104.00	0.40	47.40	8.60	13.00	13.00	38.00	44.00	-2.00	26.00	58.00	0.00	14.00
9	104.00	0.40	82.00	8.60	13.00	13.00	38.00	44.00	-2.00	26.00	58.00	0.00	14.00
10	104.00	0.40	82.00	8.60	13.00	13.00	38.00	44.00	-2.00	26.00	58.00	1.11	14.00
11	104.00	0.40	82.00	8.60	13.00	13.00	38.00	44.00	-2.00	26.00	58.00	0.00	14.00
12	44.72	0.40	82.00	8.60	13.00	13.00	38.00	44.00	-2.00	26.00	58.00	0.00	14.00
13	104.00	0.18	82.00	8.60	13.00	13.00	38.00	44.00	-2.00	26.00	58.00	0.00	14.00
14	0.00	0.40	82.00	8.60	13.00	13.00	38.00	31.48	-2.00	26.00	58.00	0.00	48.06
15	104.00	0.40	82.00	0.00	13.00	13.00	38.00	44.00	-2.00	26.00	58.00	0.00	14.00
16	0.00	0.40	82.00	8.60	2.46	13.00	38.00	44.00	-2.00	26.00	58.00	0.00	14.00
17	104.00	0.40	82.00	8.60	13.00	13.00	38.00	44.00	-2.00	23.00	58.00	0.00	14.00
18	104.00	0.40	82.00	8.60	13.00	13.00	56.62	44.00	-2.00	26.00	0.00	0.00	14.00
19	79.91	0.40	14.84	8.60	13.00	13.00	38.00	58.54	-2.00	26.00	58.00	0.00	14.00
20	104.00	0.40	82.00	8.60	13.00	13.00	38.00	44.00	-2.00	39.85	58.00	0.00	14.00

DATA SET NO 3

PROBABILITY OF GROSS SYSTEMATIC ERROR = 0.20
PROBABILITY OF ZERO FLOW = 0.20
PROBABILITY OF FULL SCALE FLOW = 0.10
PER CENT MEAN TOLERANCE OF METER SET = 3.00
START RANDOM NO USED = 31494

RUN NO	METER NO 1	2	3	4	5	6	7	8	9	10	11	12	13
0	104.00	0.40	82.00	8.60	13.00	13.00	38.00	44.00	-2.00	26.00	58.00	0.00	14.00
1	102.15	0.40	82.56	7.91	13.87	13.32	38.05	42.82	-2.28	25.27	38.01	0.00	13.72
2	106.89	0.40	83.13	9.03	13.11	13.25	38.62	43.38	0.00	36.13	57.54	0.00	14.98
3	106.04	0.21	79.64	8.50	12.69	12.77	37.38	43.84	-1.93	5.16	57.42	0.00	47.93
4	103.23	0.41	81.85	8.50	13.00	22.65	3.70	41.96	-1.83	26.03	41.92	0.00	14.34
5	102.09	0.38	83.90	9.01	12.90	12.86	37.29	42.25	2.45	25.99	56.79	1.11	14.68
6	104.44	0.42	83.85	8.06	0.00	13.04	37.58	41.27	-2.37	25.30	61.31	1.58	12.71
7	103.00	0.39	43.48	8.34	12.08	13.19	28.13	43.67	-2.41	14.59	57.30	0.00	15.18
8	87.75	0.39	81.32	8.79	13.91	12.19	37.08	44.81	-1.90	25.58	59.87	0.00	13.09
9	105.15	0.35	82.74	8.47	10.87	12.66	38.03	42.48	-2.04	26.55	60.63	0.80	0.94
10	103.29	0.42	84.01	8.81	13.07	13.10	37.17	43.44	-1.02	21.60	56.22	0.10	18.48
11	104.90	0.40	83.18	12.06	13.54	12.76	37.98	43.18	-1.85	25.94	58.39	17.96	50.00
12	104.56	0.41	84.14	8.20	12.85	13.52	36.98	42.83	0.00	37.73	57.06	0.26	12.37
13	105.89	0.25	79.09	8.44	12.89	12.74	55.75	44.65	-0.66	25.14	0.00	0.00	14.48
14	90.20	0.40	31.09	0.00	12.51	13.06	38.25	7.99	-2.24	25.26	57.37	0.14	13.53
15	106.30	0.40	86.08	8.34	13.24	12.60	21.14	44.63	-2.67	25.94	64.41	0.00	14.77
16	61.07	0.39	82.51	8.34	12.81	24.40	37.51	42.79	-1.94	0.00	4.88	1.51	15.20
17	102.49	0.07	80.74	8.59	2.34	13.46	39.64	40.87	-2.46	25.36	58.50	0.00	14.31
18	106.72	0.41	80.76	8.55	13.36	13.29	38.22	43.36	39.85	25.89	58.05	0.00	0.00
19	105.36	0.40	84.53	1.74	12.84	13.08	36.74	43.51	-1.85	26.38	52.06	0.37	13.87
20	102.04	0.40	0.00	14.73	12.46	12.85	37.79	43.57	-3.11	26.82	0.00	55.07	13.31

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COMPUTER PROGRAM 'MASS' -- MASS BALANCE CORRECTION BY SPARSE MATRIX METHODS DGP/TR 1968

TEST SYSTEM CONFIGURATION DATA FOR USE WITH PROGRAM LTAKMOD
D M THOMAS
PCS

NO. UNITS IN OVERALL BALANCE 5
MAX. NO. FLOWS PER UNIT 5
TOTAL NO. FLOWS INVOLVED 13

UNIT	DISCREPANCY	NO. FLOWS	CONFIGURATION
UNIT 1	0.0	5	1 -2 -3 -4 -5
UNIT 2	0.0	3	3 -7 -8
UNIT 3	0.0	4	7 -9 -10 -13
UNIT 4	0.0	4	8 13 -11 -12
UNIT 5	0.0	2	5 -6

A-20

LEAST SQUARES SOLUTION

FLOW NO.	WEIGHTING FACTOR.	ACTUAL VALUE.	RECONCILED VALUE	CHANGE	% CHANGE	TRUE VALUE	FLOW RANGE
1	0.10	102.15	97.44	4.71	4.61	104.00	121.00
2	0.00	0.40	0.42	-0.02	4.61	0.40	0.60
3	0.08	82.56	74.85	7.71	9.34	82.00	130.00
4	0.01	7.91	8.27	-0.36	4.61	8.60	18.00
5	0.01	13.87	13.90	-0.03	0.23	13.00	25.00
6	0.01	13.32	13.90	-0.58	4.37	13.00	25.00
7	0.04	38.05	38.02	0.03	0.07	38.00	58.00
8	0.04	42.82	36.83	5.99	14.00	44.00	75.00
9	-0.00	-2.28	-2.60	0.32	0.00	-2.00	40.00
10	0.03	25.27	28.81	-3.54	14.02	26.00	40.00
11	0.04	38.01	48.63	-10.62	27.95	58.00	112.00
12	0.00	0.00	0.00	-0.00	0.00	0.00	59.00
13	0.01	13.72	11.81	1.91	13.93	14.00	50.00

PERFORMANCE CRITERIA

AVM(ACT-TRU)	AVM(REC-TRU)	AVM(ACT-REC)	AVS(ACT-TRU)	AVS(REC-TRU)	AVS(ACT-REC)
2.0615	2.9251	2.7567	31.2889	19.0898	19.0172

PAVM(ACT-TRU)	PAVM(REC-TRU)	PAVM(ACT-REC)	PAVS(ACT-TRU)	PAVS(REC-TRU)	PAVS(ACT-REC)
2.5497	4.1465	3.7220	27.3956	25.4466	24.3765

MODULUS MINIMISATION

FLOW NO.	WEIGHTING FACTOR.	ACTUAL VALUE.	RECONCILED VALUE	CHANGE	% CHANGE	TRUE VALUE	FLOW RANGE
1	0.00	102.15	102.16	-0.01	0.01	104.00	121.00
2	0.00	0.40	0.40	0.00	0.02	0.40	0.60
3	0.20	82.56	80.09	2.47	2.99	82.00	130.00
4	0.00	7.91	7.91	0.00	0.00	8.60	18.00
5	0.00	13.87	13.76	0.11	0.77	13.00	25.00
6	0.01	13.32	13.76	-0.44	3.33	13.00	25.00
7	0.00	38.05	38.01	0.04	0.11	38.00	58.00
8	0.03	42.82	42.08	0.74	1.72	44.00	75.00
9	0.00	-2.28	-2.28	-0.00	0.00	-2.00	40.00
10	0.03	25.27	26.57	-1.30	5.13	26.00	40.00
11	0.68	38.01	55.80	-17.79	46.81	58.00	112.00
12	0.00	0.00	0.00	-0.00	0.00	0.00	59.00
13	0.00	13.72	13.72	-0.00	0.00	14.00	50.00

PERFORMANCE CRITERIA

AVM(ACT-TRU)	AVM(REC-TRU)	AVM(ACT-REC)	AVS(ACT-TRU)	AVS(REC-TRU)	AVS(ACT-REC)
2.0615	0.8625	1.7418	31.2889	1.3575	23.0094

PAVM(ACT-TRU)	PAVM(REC-TRU)	PAVM(ACT-REC)	PAVS(ACT-TRU)	PAVS(REC-TRU)	PAVS(ACT-REC)
2.5497	1.5475	1.8498	27.3956	3.9223	20.8306

APPENDIX 4

FORMULATION OF DATA RECONCILIATION MODEL USING LINEAR PROGRAMMING TECHNIQUE

i) INTRODUCTION

The general formulation of a linear programming model is as follows:

Minimise the linear objective function $\sum_{i=1}^{n} c_i \quad x_i$

Subject to linear constraints

$$\sum_{i=1}^{n} a_{ji} \quad x_i \quad \begin{matrix} \leqslant \\ = \\ \geqslant \end{matrix} \quad b_j \qquad j = 1,2 \text{ ---} m$$

$$x_i \quad \geqslant \quad o \qquad i = 1,2 \text{ ---} n$$

where

x_i are the activities

c_i are the coefficients or weights of the objective function

a_{ji} represent the matrix of coefficients of the left-hand sides of the constraints

b_j are the right-hand side of the constraints

n is the number of activities

m is the number of constraints

The formulation of a data reconciliation model using the linear programming technique can be illustrated by considering the simple single balance process in Fig. A4-1.

The process consists of two feed streams (streams 1 and 2) which chemically react to produce a product (stream 3) and by-product (stream 4). The process also has a non metered material loss (stream 5).

ii) DEFINITION OF PLANT MATERIAL BALANCE

If F_i^*, i = 1 to 4 are the measured raw flows of streams 1 to 4, then a material balances gives

$$F_1^* + F_2^* - F_3^* - F_4^* - F_5^* = \Delta \qquad - (1)$$

where

F_5^* is an estimated measure of the loss flow (set as zero if unknown).

Δ is the material balance error.

If Fi, i = 1 to 5 are defined as the reconciled set of flows which satisfy the material balance, then

$$F_1 + F_2 - F_3 - F_4 - F_5 = 0 \qquad - (2)$$

Subtracting eqn (2) from eqn (1)

$$(F_1 - F_1^*) + (F_2 - F_2^*) - (F_3 - F_3^*) - (F_4 - F_4^*) - (F_5 - F_5^*) = -\Delta$$

or $f_1 + f_2 - f_3 - f_4 - f_5 = -\Delta$ - (3)

where $f_i = (F_i - F_i^*)$, i = 1 to 5 are the flow changes made in the measured raw flows to produced reconciled flows.

Eqn (3) is defined as the material balance equality constraint.

iii) DEFINITION OF PLANT LOSS

An unaccountable plant loss can be expressed in one of three ways as:-

a) a constant loss

i.e. $f_5 = 0$ - (4)

Eqn (4) states that there must be no change in the loss flow.

b) a fixed percentage of some other flow or flows, e.g. the loss in Fig. A4-1 could be specified as 3% of stream 1.

$$0.03\ F_1 - F_5 = 0 \qquad - (5)$$

Defining eqn (5) in term of flow change variables

$$0.03\ (f_1 + F_1^*) - (f_5 + F_5^*) = 0$$

$$0.03\ f_1 - f_5 = K1 \qquad - (6)$$

where

$K1 = F_5^* - 0.03\ F_1^*$

c) a variable loss, where the loss might depend upon plant operation. Upper and lower limits may be assigned e.g. the loss in Fig. A4-1 could be specified as lying between 1% and 3% of the flow of stream 1. This representation gives rise to the following two inequality constraints.

$$0.01\ f_1 - f_5 \geqslant K2 \qquad - (7)$$

$$0.03\ f_1 - f_5 \leqslant K3 \qquad - (8)$$

where

$K2 = F_5^* - 0.01\ F_1^*$

$K3 = F_5^* - 0.03\ F_1^*$ are both functions of the measured flows.

The loss representation shown in Fig. A4-2 is expressed as a fixed percentage of stream 1 as defined by eqn (6). The LP technique also permits loss flows to be constrained between upper and lower absolute bounds.

iv) DEFINITION OF PLANT PERFORMANCE CONSTRAINTS

Inequality constraints can arise from the need to put limits on plant efficiencies and yields, e.g. the yield of product in stream 3 must lie between 60% and 80% of the raw material stream 1. This constraint would be of the form:-

$$0.6 \leq \frac{F_3}{F_1} \leq 0.8 \qquad - (9)$$

Eqn (9) can be defined in terms of flow changes

$$0.6\ f_1 - f_3 \leq K4 \qquad - (10)$$

$$0.8\ f_1 - f_3 \geq K5 \qquad - (11)$$

where

$K4 = F_3^{*} - 0.6\ F_1^{*}$

$K5 = F_3^{*} - 0.8\ F_1^{*}$ are both functions of the measured flows.

v) RE-DEFINITION OF FLOW CHANGE VARIABLES

The linear programming technique requires that all activities must remain positive. As the flow change activities defined above can be either positive or negative it is necessary to re-define each flow change as the difference between a positive flow activity and a negative flow activity.

i.e. $f_i = f_i^{+} - f_i^{-}$

where $f_i^{+} \geq 0$

$f_i^{-} \geq 0$ for $i = 1$ to 5

All equations defined in terms of flow changes must be re-defined in terms of these positive and negative flow activities.

e.g. Eqn (3) becomes

$$(f_1^+ - f_1^-) + (f_2^+ - f_2^-) - (f_3^+ - f_2^-) - (f_4^+ - f_4^-) - (f_5^+ - f_5^-) = -\Delta$$

vi) BOUNDING OF FLOWS

By setting absolute bounds on negative flow activities (i.e. f_i^- activities) equal to the corresponding raw flow measurements, positive flows can be prevented from going negative.

e.g. upper bound on f_1^- would be set at $F_1^\bullet$.

vii) OBJECTIVE FUNCTION

The data reconciliation error criterion minimises a weighted sum of the moduli of the changes to the flows.

$$\text{Minimise} \quad \sum_{i=1}^{5} W_i \ (f_i^+ + f_i^-)$$

where W_i are the weights.

The data reconciliation LP matrix for the system in Fig. A4-1 with the loss expressed as a fixed percentage of the flow of stream 1 is shown in Fig. A4-2. The set of reconciled flows can be formed by adding the reconciled flow changes to the measured raw flows.

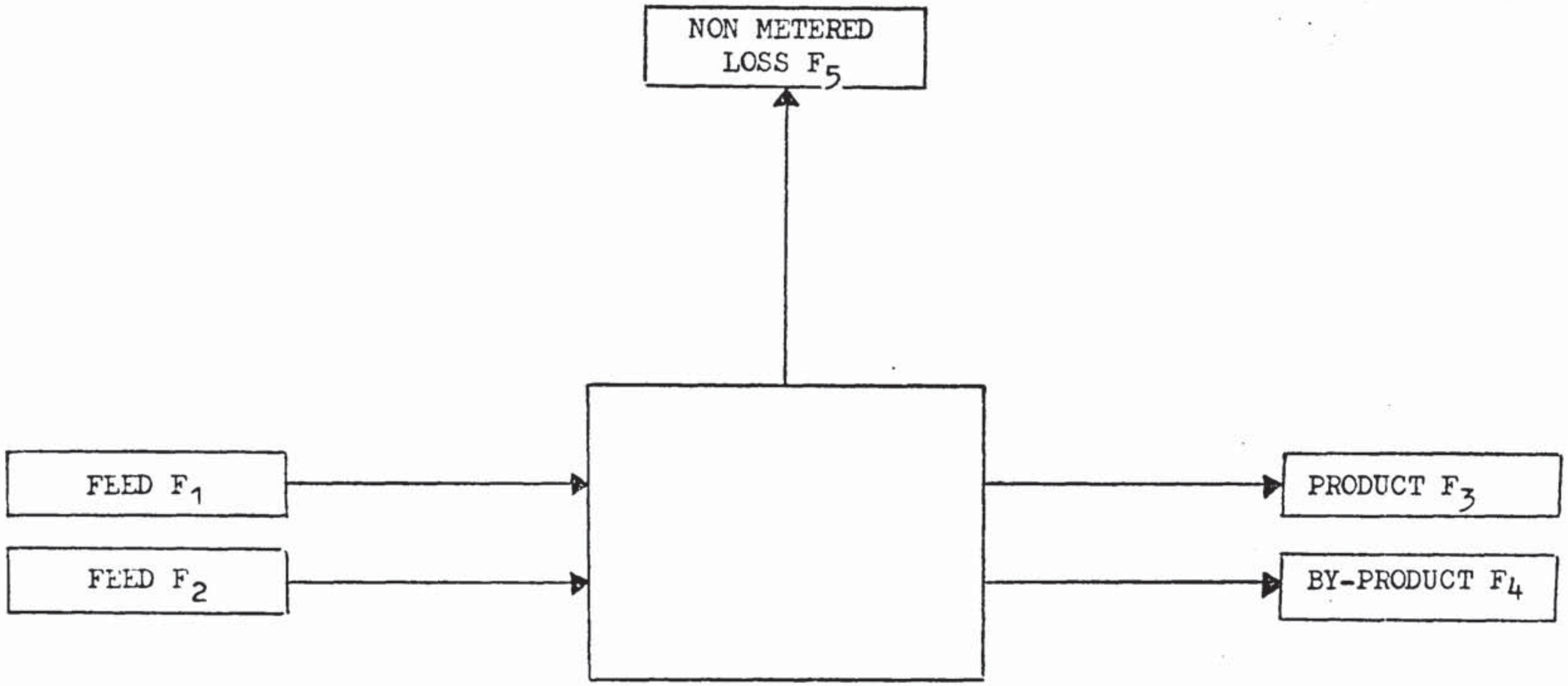

FIG. A4-1 SIMPLE SINGLE BALANCE PROCESS

EQUATION NUMBERS	CONSTRAINT DESCRIPTIONS	FLOW ACTIVITIES											RHS
		f_1^+	f_1^-	f_2^+	f_2^-	f_3^+	f_3^-	f_4^+	f_4^-	f_5^+	f_5^-		
3	Material Balance	+1	-1	+1	-1	-1	1	-1	+1	-1	+1	$=$	$-\Delta$
6	Loss	+0.03	-0.03							-1	+1	$=$	K1
10	Efficiency	+0.6	-0.6			-1	1					$\leq$	K4
11		+0.8	-0.8			-1	1					$\geq$	K5
	OBJECTIVE	W_1	W_1	W_2	W_2	W_3	W_3	W_4	W_4	W_5	W_5		

FIG.A4-2 LP MATRIX FOR SYSTEM SHOWN IN FIG.A4-1

APPENDIX 5

NO. 2 ETHYLENE DATA RECONCILIATION REPORTS

NO 2 ETHYLENE PLANT MASS BALANCE SUMMARY

		RAW VALUE (TONNES)	RECONCILED VALUE (TONNES)	RECONCILED VALUE % OF NAPHTHA FLOW
INPUTS	NAPHTHA FEED ETHANE TO FURNACES FUEL OIL EX GTU WASH OIL EX GTU VENTS EX GTU VENT EX —	(Actual Data has been Deleted)		
	TOTAL	3615.20	3698.87	106.46
OUTPUTS	ETHANE TO FURNACES LOW PURITY HYDROGEN PRODUCT ETHYLENE VAPOUR PRODUCT ETHYLENE LIQUID PRODUCT C3 PRODUCT (EXCL C3 EX PHH) C4 PRODUCT GASOLINE PRODUCT FUEL OIL PRODUCT RESIDUE GAS TO FG ETHYLENE TO FG ETHANE TO FG NET C3S EX ETHYLENE TO FG C4'S TO FG OTHERS FLARE (INCL ETHYLENE TO FLARE) LOSS	(Actual Data has been Deleted)		
	TOTAL	3615.20	3698.86	106.46
OTHERS **	ETHYLENE TO REFRIG LOW PURITY HYDROGEN TO GTU HIGH PURITY HYDROGEN PRODUCT LOW PURITY HYDROGEN TO FG HIGH PURITY HYDROGEN TO FG HYDROGENATED C2S TO FG CRACKED GAS EX DEHYDRATORS TO FG C3S EX T14 TO REFRIGERATION LIQUID ETHANE ETHYLENE TO SURGE DRUMS C3S TO SURGE DRUMS	(Actual Data has been Deleted)		
		9.255	68.20	

NO 2 ETHYLENE PLANT PROCESS MASS BALANCE

INPUTS

	RAW VALUE (TONNES)	RECONCILED VALUE (TONNES)
NAPHTHA FEED	(Actual Data has been Deleted)	
ETHANE TO FURNACES		
VENT EX ——		
C3 MAKE UP EX ——		
WASH OIL EX GTU TO H-C-1A&B		
WASH OIL EX GTU TO H-T-3		
STAB O/H EX GTU		
HP VENT EX GTU		
RE-RUN TOWER BOTS EX GTU		
TOTAL	3622.09	3705.76

OUTPUTS

	RAW VALUE (TONNES)	RECONCILED VALUE (TONNES)
ETHANE TO FURNACES	(Actual Data has been Deleted)	
LOW PURITY HYDROGEN TO GTU		
LOW PURITY HYDROGEN PRODUCT		
HIGH PURITY HYDROGEN PRODUCT		
ETHYLENE VAPOUR PRODUCT		
ETHYLENE LIQUID PRODUCT		
C3 LIQUID PRODUCT		
C4 LIQUID PRODUCT		
RAW GASOLINE PRODUCT		
FUEL OIL PRODUCT		
LOW PURITY HYDROGEN TO FG		
HIGH PURITY HYDROGEN TO FG		
RESIDUE GAS TO FG		
ETHYLENE TO FG		
ETHANE TO FG		
HYDROGENATED C2S TO FG		
CRACKED GAS EX DEHYDRATORS TO FG		
C3S EX MAP TOWER TO FG		
C3S EX DEPROPANISER TO FG		
C3S EX ETH2 TO C3 VAPORISER(FG)		
C3S EX —— TO C3 VAPORISER(FG)		
C4S EX DEBUTANISER TO FG		
C4S EX SEC-DEPROPANISER TO FG		
ETHYLENE TO REFRIGERATION		
ETHYLENE TO FLARE		
C3S EX T14 TO REFRIGERATION		
C3S EX PHH TO REFRIGERATION		
LIQUID ETHANE		
ETHYLENE TO SURGE DRUMS		
C3S TO SURGE DRUMS		
FLARE(EXCL ETHYLENE TO FLARE)		
LOSS		
TOTAL	3622.09	3705.75

NO. 2 ETHYLENE PLANT - AVERAGE NAPHTHA FURNACE YIELD PATTERN:

NAPHTHA SG (60/60) : —

NAPHTHA FURNACE OPERATION

AVERAGE COIL EXIT TEMPERATURE : — (F)
AVERAGE FURNACE FEED RATE : — K,LBS/HR
: — % DESIGN

ETHANE FURNACE OPERATION

AVERAGE COIL EXIT TEMPERATURE : — (F)
AVERAGE FURNACE FEED RATE : — K,LBS/HR
— % DESIGN

COMPONENT	EX.FURNACE YIELDS (WT.% H/C FEED) NAPHTHA CRACKING	EX.FURNACE YIELDS (WT.% H/C FEED) ETHANE CRACKING	EX.PLANT YIELDS (WT.% H/C FEED)	PRODUCT SEPARATION RECOVERY FACTORS (%)
HYDROGEN				
METHANE				
ETHANE				
ETHYLENE				
TOTAL C3,S				
C4.S				
BUTADIENE				
GASOLINE				
FUEL OIL				
	100.00	100.00		

(Actual Data has been Deleted)

NOTES

1. CALCULATIONS ARE LOSS FREE, PLANT MATERIAL LOSSES ARE ACCOUNTED FOR IN THE CALCULATION

2. RECOVERY FACTORS ESSENTIALLY CONVERT FURNACE PRODUCT MAKER INTO BATTERY LIMIT PRODUCTS

3. EXTERNAL FEEDS ARE SUBTRACTED OUT OF THE CALCULATIONS

NO 2 ETHYLENE COMPLEX FUEL GAS BALANCE

INPUTS

		RAW VALUE (TONNES)	RECONCILED VALUE (TONNES)
EX SITE	IMPORT EX BPRL	(Actual Data has been Deleted)	
	HYDROGEN EX CHLORINE		
	C3'S EX IPA		
	C3'S EX PMH		
	C4 RAFFINATE		
	RAW C4'S		
EX NO 2 ETHYLENE	LOW PURITY HYDROGEN		
	HIGH PURITY HYDROGEN		
	RESIDUE GAS		
	ETHYLENE		
	ETHANE		
	HYDROGENATED C2'S		
	CRACKED GAS EX DEHYDRATORS		
	C3'S EX MAP TOWER		
	C3'S EX DEPROPANISER		
	C3'S EX ETH2 TO C3 VAPORISER		
	C4'S EX DEBUTANISER		
	C4'S EX SEC-DEPROPANISER		
EX NO 2 GTU	HP VENT EX GTU		
	STABILISER VENT EX GTU		
EX NO 2 BUTADIENE	C4'S EX POST FRACTIONATOR		
	C4'S EX WASTE GAS ABSORBER		
	C4 RAFFINATE		
	TOTAL	702.76	932.06

OUTPUTS

	RAW VALUE (TONNES)	RECONCILED VALUE (TONNES)
FG TO CRACKING FURNACES	(Actual Data has been Deleted)	
FG TO FACTORY RING MAIN		
FG TO POWER STATION BOILERS		
FG TO FURNACES H-F-2&3		
C4S TO GASOLINE PRODUCT		
LOSS + HOT RELIEF		
TOTAL	702.76	932.06

ETHYLENE GROUP
INSTRUMENT REPORT SECTION 1 - READINGS NOT AVAILABLE PAGE 1

CODE	METER	DESCRIPTION
H2EF200	H-FR-34	FUEL OIL (F.O) PRODUCT
H2EF435	H-FRS-242	ETHANE RECYCLE TO FURNACES-TURBINE METER
H2EF704	H-FR-613	C4'S RAFFINATE OR LPG IMPORT
H2EF713	H-FR-618	EXCESS FG TO BOILER
H2GF000	J-FRS-1	RAW GASOLINE FEED INLET J-TK-1
H2GF008	J-FRS-16	GASOLINE PRODUCT

ETHYLENE GROUP
INSTRUMENT REPORT SECTION 2 - READINGS CHANGED >5% PAGE 1

CODE	METER	DESCRIPTION	RAW VALUE	NOMINAL ACCURACY	%CHANGE
H2EF060	H-FRC16-1/4A	TOTAL ETHANE FEED TO FURNACE H-F-6A		%	-36.959
H2EF065	H-FRC16-1/4B	TOTAL ETHANE FEED TO FURNACE H-F-6B	(Actual Data	%	-36.959
H2EF710	H-FRC-614	C4 RAFFINATE/LPG TO H-D-10	has been	%	-100.000
H2EF3?0	H-FRC-131	H-T-11 (DEPROPANISER) BTMS	Deleted)	%	10.475
H2EF538	H-FI-151	MAP TOWER O/H		%	11.495
H2EF204	H-FR-54	DISTILLATE EX H T-18 (DIST.STRIPPER)		%	-7.562
H2EF510	H-FR-135	RAW GASOLINE EX H-T-12 (DEBUTANISER)		%	-7.589
H2EF701	H-FR-612	FUEL GAS TO FACTORY RING MAIN		%	5.620

APPENDIX 6

PHYSICAL PROPERTY DATA

The BP Sunbury computer program STAGE 1 (28) was used as a source of vapour/liquid equilibrium (K-value) and enthalpy data in the cracked gas compression and fractionation models. The program was selected on the basis of its availability and suitability for hydrogen-methane-hydrocarbon type systems. A computer algorithm was used which is based on well-known methods for calculating flash equilibria. The thermodynamic principles and correlations involved are described by Shelton (29).

The Grayson and Streed (30) extension of the Chao and Seader (31) correlations predicted ν_i^o, the fugacity of the substance in the pure liquid state. The activity coefficient of a component in liquid solution, γ_i was calculated from Hildebrand's regular solution theory, and Θ_i the fugacity coefficient of a component in the vapour mixture was obtained by solving the Redlich-Kwong two constant equation of state.

These three thermodynamic properties ν_i^o, γ_i and Θ_i were used to predict vapour liquid equilibrium values K_i from the equation.

$$K_i = \frac{\nu_i^o \, \gamma_i}{\Theta_i} \qquad - \quad (1)$$

The program also calculated vapour and liquid enthalpies for the stream components which are consistent with the vapour/liquid equilibrium values. Details of the enthalpy calculation are given in (29).

The K-values and enthalpies generated by the program were curve fitted as functions of temperature and pressure. The equation fitted for K-values is based on the Antoine relationship for vapour pressure:-

$$\text{Log } K = a + \frac{b}{T} + c.T + d.\text{ Log } P \qquad - (2)$$

The equation for enthalpies is:-

$$H = a + \frac{b}{T} + c.T + d.P \qquad - (3)$$

where

K is the vapour/liquid equilibrium value

H is the enthalpy (BTU/lb)

T is the temperature (^{O}R)

P is the pressure (psig)

a, b, c, d are regression curve fitting constants

The regression constants were held as data in the physical property data array of the model and used with the associated regression equations to generate enthalpy and K-value data.

As the compression and fractionation systems cover a wide spectrum of operating conditions it was necessary to define two temperature and pressure ranges over which the STAGE 1 (28) physical property data would be regression fitted. The first range 60 to 250^{O}F and 15 to 550 psia served the compression system; and the second range -60 to 160^{O}F and 200 to 530 psia served the fractionation system.

An exercise (34) to evaluate and compare the K-value data used in the cracked gas compression system model with design K-value data revealed that:-

i) At low pressures (i.e. 35-90 psig) the mole percentage vapourisation of the cracked gas compression hydrocarbon and streams, as calculated using STAGE 1 K-value data, agreed (to within 1%) with the values predicted using design data. The differences increased (up to 8%) at higher pressures (i.e. 220-530 psig).

To validate the accuracy of the K-value data a comparison must be made with plant derived data. This, however, was not possible within the time scale of the project.

ii) The regression fitting of the K-value data introduced errors of between 2 and 3% in the mole percentage vapourisation of the cracked gas compression hydrocarbon streams. (i.e. the K-values generated using the STAGE 1 regression equations gave percentage vapourisations that were within 3% of those calculated using K-values generated directly by STAGE 1.)

This was regarded as acceptable for the initial Cold End modelling work.

Dowling and Todd (32) have recently reviewed the relative merits of the popular Chao-Seader, Grayson-Streed and A.P.I. correlations for predicting hydrocarbon vapour-liquid equilibrium ratios. They used as a basis for their study 48 different mixtures and attempted to define areas of maximum reliability for each correlation. They concluded that for both methane and hydrogen systems (which predominate in the Cold End systems) the Chao-Seader correlation appeared to be the most reliable. For systems containing hydrogen and high boiling petroleum fractions, the Grayson-Streed model is marginally best. However, for both types of systems, the A.P.I. correlation was unacceptable.

APPENDIX 7

COLD END MODEL SPECIMEN PROGRAM LISTINGS

```
                  MASTER COLD END MODEL
      C           ***************************
      C           MODULE LINKING PROGRAM---COLD END MODEL
      C           DMT
      C           11/6/74
      C
      C           GENERAL MODULES REQUIRED : DATIN,DATOUT,DIAGUT
      C
      C
      C           STREAM PARAMETERS  (PROCESS)
      C           *****************
      C             1. FLAG
      C             2. STATE CODE
      C             3. TEMPERATURE             (DEG.F)
      C             4. PRESSURE                (PSIG)
      C             5. TOTAL HEAT              (MBTU/H)
      C             6. TOTAL FLOWRATE          (KLBS/HR)
      C             7. HYDROGEN
      C             8. METHANE
      C             9. ETHYLENE
      C            10. ETHANE
      C            11. PROPYLENE
      C            12. PROPANE
      C            13. BUTADIENE
      C            14. BUTENE
      C            15. N-BUTANE
      C            16. N-PENTANE
      C            17. BENZENE
      C            18. N-HEXANE
      C            19. TOLUENE
      C            20. N-HEPTANE
      C            21. O-XYLENE
      C            22. ETHYL BENZENE
      C            23. N-C8
      C            24. N-C9
      C            25. N-C10
      C            26. N-C11
      C
      C
      C           STREAM PARAMETERS (REFRIGERATION)
      C           *********************************
      C             1. STATE CODE
      C             2. TEMPERATURE (DEG.F)
      C             3. PRESSURE    (PSIG)
      C             4. HEAT FLOW   (MBTU/H)
      C             5. MASS FLOW   (KLB/H)
      C             6. VOL  FLOW   (KCFM)
      C
      COMBLOCK
      C
      C
      C----------------------
      C
      C           BP CHEM SIMULATION SYSTEM COMMON DECK
      C
            COMMON /SSDIM1/ MAXSTM,MAXCMP,MXASTM,MXXCMP,MAXPM,MAXMS
            COMMON /SSDIM2/ MAXCTM,MAXCVM,MAXUTL,NPMUT
            COMMON /STREM1/ STRM(105,26),MLIST(30,2),MTITLE(20),MSTNAM(20)
            COMMON /PRDIM1/ NUMSTM,NUMCMP,NEXSTM,NEXCMP,NUMPM
            COMMON /PRDIM2/ NUMCTM,NUMCVM,NUTIL
            COMMON /EXTND1/ EXTRM(1,1),NXLIST(1,1)
            COMMON /EQUIP/ PMPAR(250),KEMINI(60,4),KALC(80)
            COMMON /PRIC/ KPM(1,1),NUMNME(40,2)
```

```
            COMMON /CONT/ KONT(15,7),KCTINT(15,2),CTPAR(100),LECTM(15)
            COMMON /CONV1/ KONV(5,4),COSTH1(10,30),CMPAR(20),KCVINC(5,2)
            COMMON /CONV2/ TOL(30),LPCVM(5)
            COMMON /UTIL1/ UARRAY(1,1),UUI(1,1),UTREF(1,1)
            COMMON /COST/ OPCOST(1),CFLOW(1,1)
            COMMON /PPDA/ COEFF(20,20),XCOEFF(1,1),NPPSET
            COMMON /FLAG1/ IDIAG,ISOL,IABORT,ICONV,ICOUNT,INCV,IREPT,IUNIT
            COMMON /SCPAD/ ISP(1),SP(1,1)
            COMMON /GEN4/ LP1,LP2,NCP1,NCP2,NCR1,NCR2,NPR1,NPR2,NPP1,NPP2
            COMMON /GEN1/  LOOP,NCYCLE(20),NPAGE
            COMMON/CNTFLGS/ICONV1,ICONV2,ICONV3
C
C----------------------
C
COMEND
C
      WRITE(LP1,100)
C
      IREPT=0
    1 CONTINUE
      CALL DATIN
C
C
C-----COMPRESSION SYSTEM MODULE LINKING STATEMENTS
C     ************************************************
      NPPSET=1
    2 CONTINUE
      CALL SPL50(28,33,-42,-41)
      CALL JUNC50(20,30,64,65,42,0,-31)
      CALL COMP50(21,31,-32)
      CALL HEX50(22,32,-33)
      CALL JUNC50(29,41,60,0,0,0,-43)
      CALL COMP50(30,43,-44)
      CALL HEX50(31,44,-45)
      CALL SEP50(32,45,70,0,0,0,-46,-47)
      CALL VLVE50(45,47,-48)
      CALL CAU50(33,46,-49)
    3 CONTINUE
      CALL SEP50(35,50,0,0,0,0,-51,-52)
      CALL JUNC50(36,51,72,0,0,0,-53)
      CALL COMP50(37,53,-54)
      CALL JUNC50(38,54,73,0,0,0,-55)
      CALL HEX50(39,55,-56)
      CALL HEX50(40,56,-57)
      CALL SEP50(41,57,0,0,0,0,-58,-59)
      CALL SPL50(42,58,-61,60)
      CALL DIST51(43,59,-62,-63)
      CALL JUNC50(34,49,62,71,74,0,-50)
      CALL CONV01(1,50)
      LOOP=1
      NCYCLE(LOOP)=NCYCLE(LOOP)+1
      IF(ICONV.EQ.0.AND.ICOUNT.EQ.0)GO TO 3
      CALL DIAGUT
C
      CALL VLVE50(44,39,-40)
      CALL SEP50(23,33,40,66,0,0,-34,-75)
      CALL JUNC50(24,34,67,0,0,0,-35)
      CALL COMP50(25,35,-36)
      CALL HEX50(26,36,-37)
      CALL SEP50(27,68,61,37,48,52,-38,-39)
      CALL CONV01(2,38)
      LOOP=2
      NCYCLE(LOOP)=NCYCLE(LOOP)+1
      IF(ICONV.EQ.0.AND.ICOUNT.EQ.0)GO TO 2
      CALL DIAGUT
C
```

```
C-----FRACTIONATION SYSTEM MODULE LINKING STATEMENTS
C     ***********************************************
      NPPSET=2
C
C-----USE CBX50 MODULE TO SET ESTIMATE OF STREAM 83
      CALL CBX50(55,60,-83)
   10 CONTINUE
      CALL SPL50(50,60,-76,-77)
      CALL HEX50(51,77,-78)
      CALL CBX50(55,70,-82)
   12 CONTINUE
      CALL DIST51(57,83,-84,-85)
      CALL DIST51(58,85,-86,-87)
      CALL C2H50(59,86,-88)
      CALL DIST51(60,88,-90,-89)




   14 CALL PRECOOL(67,60,93,97,-83,-94,-98)



      CALL CONT51(4,83,3,53,2)
      LOOP=3
      NCYCLE(LOOP)=NCYCLE(LOOP)+1
      IF(ICONV.EQ.0.AND.ICOUNT.EQ.0)GO TO 14
      CALL CONV01(3,83)
      LOOP=4
      NCYCLE(LOOP)=NCYCLE(LOOP)+1
      IF(ICONV.EQ.0.AND.ICOUNT.EQ.0)GO TO 12
C
      CALL HEX50(63,94,-95)
      CALL HEX50(64,95,-96)
      CALL HEX50(66,98,-99)
      CALL DIAGUT
C
      CALL FRLINK(83,92,66,64,40,60,63,58,51,53,11,14,15,17)
C
C     PROPYLENE REFRIGERATION SYSTEM MODULE LINKING STATEMENTS
C     ***********************************************************
   20 CONTINUE
      IFLAG=0
      CALL PRESET
      CALL HEX60(17,23,-24)
   90 CALL SPLT60(16,22,-3,-25)
      CALL SEP60(1,24,25,0,-1,-26)
      CALL COMP01(5,1,-2)
      CALL COMP02(6,2,3,-5)
      IF(IFLAG.EQ.0)GO TO 40
      CALL CONT64(3,3,16)
      IF(ICOUNT.EQ.1)GO TO 50
      IF(ICONV3.EQ.1)GO TO 90
      IF(ICONV3.EQ.0)GO TO 50
   40 IFLAG=1
   50 CONTINUE
      CALL COMP03(7,5,-6,-8)
      CALL HEX61(8,8,-9)
   60 CONTINUE
      CALL SPLT60(9,9,-10,-11)
      CALL HEX62(10,10,-12)
      CALL SUR60(4,12,-13)
      CALL HEX61(11,13,-14)
      CALL SEP60( 3,14,11,0,-15,-16)
   70 CONTINUE
      CALL SPLT60(12,15,-17,-18)
```

```
                 CALL JUNC60(13,17,6,0,-19)
                 CALL CONT62(1,19,14,9,12)
                 IF(ICOUNT.EQ.1)GO TO 80
                 IF(ICONV1.EQ.0)GO TO 80
                 IF(ICONV1.EQ.1)GO TO 70
                 IF(ICONV1.EQ.2)GO TO 60
              80 CONTINUE
                 CALL DIAGUT
                 CALL HEX61(14,19,-20)
                 CALL HEX61(15,16,-21)
                 CALL SEP60( 2,21,20,18,-22,-23)
                 CALL SPLT60(16,22,-3,-25)
                 CALL CONT63(2,24,9,16)
                 IF(ICOUNT.EQ.1)GO TO 95
                 IF(ICONV2.EQ.1)GO TO 60
                 IF(ICONV2.EQ.2)GO TO 90
                 IF(ICONV2.EQ.0)GO TO 95
      C
              95 CONTINUE
                 CALL DIAGUT
                 IF(ISOL.EQ.1)GO TO 900
                 ISOL=1
                 GO TO 20
             900 CONTINUE
                  CALL DATOUT
                 GO TO 1
                 STOP
             100 FORMAT(///15X,25HBP CHEM SIMULATION SYSTEM//
               1          15X,14HCOLD END MODEL)
                 END

END OF SEGMENT, LENGTH   792, NAME  COLDENDMODEL
```

```
      SUBROUTINE COMP50(NMOD,NIN,NOUT)
C     **********************************
C     TRIVIAL MODULE OF COMPRESSOR STAGE
C
C     DMT  25/1/74
C
C     OPERATING PARAMETERS : 1 POLYTROPIC STAGE FACTOR
C                            2 DISCHARGE PRESSURE (PSIG)
C     SUBPROGRAMS REFERENCED;ENTH  LSTPAR
COMBLOCK
C
C
C---------------------
C
C      BP CHEM SIMULATION SYSTEM COMMON DECK
C
       COMMON /SSDIM1/ MAXSTM,MAXCMP,MXXSTM,MXXCMP,MAXPM,MAXMS
       COMMON /SSDIM2/ MAXCTM,MAXCVM,MAXUTL,NPHUT
       COMMON /STREM1/ STRM(105,26),NLIST(30,2),MTITLE(20),MSTMNO(20)
       COMMON /PRDIM1/ NUMSTM,NUMCMP,NEXSTM,NEXCMP,NUMPM
       COMMON /PRDIM2/ NUMCTM,NUMCVM,NUTIL
       COMMON /EXTND1/ EXSTRM(1,1),NXLIST(1,1)
       COMMON /EQUIP/ PMPAR(250),KPMIND(66,2),KALC(80)
       COMMON /PROC/ KPM(1,1),MODNME(66,2)
       COMMON /CONT/ KONT(15,7),KCTIND(15,2),CTPAR(100),LPCTM(15)
       COMMON /CONV1/ KONV(5,4),CVSTRM(10,30),CMPAR(20),XCVIND(5,2)
       COMMON /CONV2/ TOL(30),LPCVM(5)
       COMMON /UTIL1/ UARRAY(1,1),KUIA(1,1),UTDEF(1,1)
       COMMON /COST/ OPCOST(1),CFLOW(1,1)
       COMMON /PPDA/ COEFF(26,26),XCOEFF(1,1),NPPSET
       COMMON /FLAG1/ IDIAG,ISOL,IABORT,ICONV,ICOUNT,INCV,IREPT,IUNIT
       COMMON /SCPAD/ ISP(1),SP(1,1)
       COMMON /GEN4/ LP1,LP2,NCP1,NCP2,NCR1,NCR2,NPR1,NPR2,NPP1,NPP2
       COMMON /GEN1/  LOOP,NCYCLE(20),NPAGE
       COMMON/CNTFLGS/ICONV1,ICONV2,ICONV3
C
C---------------------
C
COMEND
C
      DIMENSION NAM(2)
C
      DATA NAM(1),NAM(2)/ 4HCOMP,2H50/
C10
      IF(IDIAG.GT.0)WRITE(LP1,200)NAM,NMOD
C
C20
      IF((ISOL.EQ.1).OR.(IABORT.LT.0))RETURN
      IF(STRM(NIN,6).LT.0.01)RETURN
C
      NIN=IABS(NIN)
      NOUT=IABS(NOUT)
C
C-----OPERATING PARAMETERS
      K1=KPMIND(NMOD,1)
      POLFAC=PMPAR(K1)
      PRES=PMPAR(K1+1)
C
C-----TRANSFER STREAM PARAMETERS FROM INPUT TO OUTPUT
      DO 100 N=1,NUMCMP
  100 STRM(NOUT,N)=STRM(NIN,N)
C
C-----SET OUTPUT PRESSURE AND TEMPERATURE
```

```
            PABSO=PRES+14.7
            PABSI=STRM(NIN,4)+14.7
            TABSI=STRM(NIN,3)+460.0
            TABSO=TABSI*(PABSO/PABSI)**POLFAC
            STRM(NOUT,3)=TABSO-460.0
      STRM(NOUT,4)=PRES
C
C-----CALCULATE DISCHARGE ENTHALPY
      STRM(NOUT,5)=ENTH(NOUT)
C
C-----DIAGNOSTIC ROUTINE
      IF(IDIAG.NE.2)GO TO 150
      MSTMNO(1)=NIN
      MSTMNO(2)=-NOUT
      CALL LSTPAR(NAM,NMOD,2)
  150 CONTINUE
      RETURN
  200 FORMAT(1H /1X,A4,A2,I5)
       END

END OF SEGMENT, LENGTH   174, NAME  COMP50
```

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