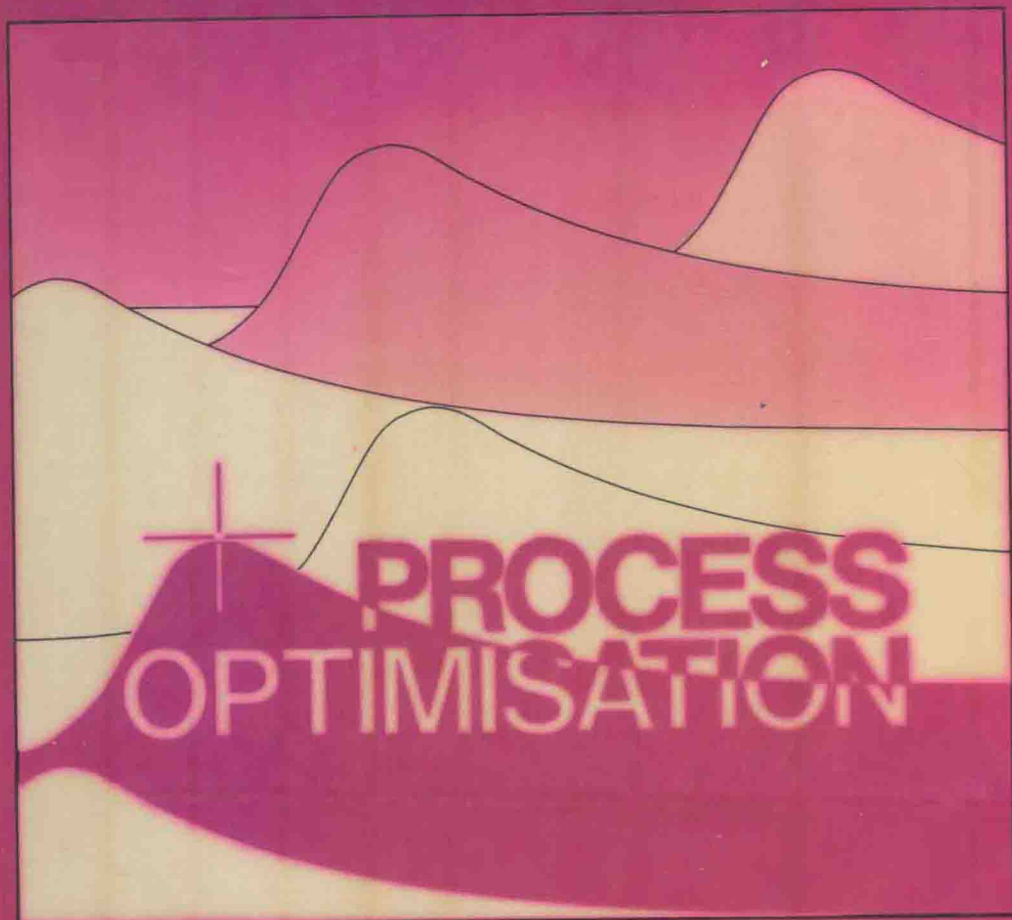


European Federation of Chemical Engineering
Europäische Föderation für Chemie-Ingenieur-Wesen
Fédération Européenne du Génie Chimique

EFCE Publication Series No. 61



The Institution of
Chemical Engineers

Pergamon
Press



Process Optimisation

A three-day Symposium organised by the Midlands Branch of The Institution of Chemical Engineers and held at the University of Nottingham, 7-9 April 1987.

Organising Committee

J.K. Walters (Chairman)

University of Nottingham

P.K. Andow

Loughborough University of Technology

A.V. Bridgwater

University of Aston

N. Emery

University of Birmingham

J.B. Guy

The Boots Co. Ltd

W.E. Jones

University of Nottingham

U. Joshi

British Gypsum

J.S. Parkinson

Scartaulds Ltd

K.E. Porter

University of Aston

J.I.T. Stenhouse

Loughborough University of Technology

R.B. Wilcockson

Loughborough University of Technology

J.A. Wilson

University of Nottingham

A. Wint

University of Nottingham



**THE INSTITUTION OF CHEMICAL ENGINEERS
SYMPOSIUM SERIES No. 100**

ISBN 0 85295 205 8

All rights Reserved. No part of this publication may be reproduced, stored in a retrieval system or transmitted in any form or by any means: electronic, electrostatic, magnetic tape, mechanical, photocopying, recording or otherwise, without permission in writing from the copyright owner.

First edition 1987 – ISBN 0 85295 205 8

**MEMBERS OF THE INSTITUTION OF CHEMICAL ENGINEERS
(Worldwide) SHOULD ORDER DIRECT FROM THE INSTITUTION**

Geo. E Davis Building, 165–171 Railway Terrace, Rugby, Warks CV21 3HQ.

Australian orders to:

R M Wood, School of Chemical Engineering and Industrial Chemistry,
University of New South Wales, PO Box 1, Kensington, NSW, Australia 2033.

***Distributed throughout the world (excluding Australia) by Pergamon Press Ltd, except to
ICChemE members.***

U.K.	Pergamon Press Ltd., Headington Hill Hall Oxford OX3 0BW, England.
U.S.A.	Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, New York 10523, U.S.A.
CANADA	Pergamon Press Canada Ltd., Suite 104, 150 Consumers Road, Willowdale, Ontario M2J 1P9, Canada
FEDERAL REPUBLIC OF GERMANY	Pergamon Press GmbH, 6242 Kronberg-Taunus, Hammerweg 6, Federal Republic of Germany
JAPAN	Pergamon Press, 8th Floor, Matsuoka Central Building, 1–7–1 Nishishinjuku, Shinjuku-ku, Tokyo 160, Japan
BRAZIL	Pergamon Editora Ltda, Rua Eça de Queiroz, 346, CEP 04011, São Paulo, Brazil
PEOPLES REPUBLIC OF CHINA	Pergamon Press, Qianmca Hotel, Beijing, People's Republic of China

BRITISH LIBRARY CATALOGUING IN PUBLICATION DATA

Process optimisation: a three-day symposium organised by the Midlands Branch of the Institution of Chemical Engineers and held at the University of Nottingham, 7–9 April 1987. – (EFCE event; no. 350). – (The Institution of Chemical Engineers Symposium Series; no. 100).

1. Chemical processes

I. Institution of Chemical Engineers *Midlands Branch* II. Series III. Series

660.2'8 TP155.7

ISBN 0-08-034818-1 ISBN 0-85295-205-8 Institution of Chemical Engineers

LIBRARY OF CONGRESS CATALOGING IN PUBLICATION DATA

Process optimization.

(The Institution of Chemical Engineers symposium series; no. 100)

"EFCE event no. 350."

1. Chemical process control – Congresses.

I. Walters, J. K. II. Institution of Chemical Engineers (Great Britain). Midlands Branch.

III. Series: Symposium series (Institution of Chemical Engineers (Great Britain)); no. 100.

TP155.75.P764 1987 660.2'81 87-14790 ISBN 0-08-034818-1

Dedication

To the memory of Dr. J.C. Mecklenburgh

Foreword

The initiative for this Symposium on Process Optimisation came from Dr. J.C. Mecklenburgh, a Senior Lecturer at the University of Nottingham, who was Chairman of the Organising Committee from its inception until his sudden death in November 1986.

John Mecklenburgh was a scholarly man, an acknowledged authority on Plant Layout and Safety and a man very active in all aspects of the Institution's affairs. His death represents a great loss to the profession of Chemical Engineering.

The Symposium splits logically into three parts and follows the development of Process Plant from conception to operation. On the first day Project Selection is discussed, with financial implications, resource availability and energy matters being emphasised. This is followed by a day devoted to Process Design where detailed optimisation possibilities are considered including safety and hazard assessment. On the third day Plant Operation is discussed with condition monitoring, revamp and computing and control systems all considered for optimisation.

Improvement is always possible at all stages of a project and we have in this Symposium presentations on the latest ideas for Process Optimisation.

J.K. Walters

Contents

Project Selection

1. Optimisation of gas separation schemes for the ENSOL process.
D.G. Arundale (*Humphreys & Glasgow*) 1
2. Product and process selection: Aspects of expert systems
in design
S.A. Gregory 17
3. Formulation of the large-scale NLP problem for optimisation
of reactor-separator processes.
P. Floquet, L. Pibouleau and S. Domenech (*ENSIGC, France*) 31
4. Process intensification: fluid bed heat transfer.
A. Murphy, R. Sibbet and C. Ramshaw (*ICI plc, New Science
Group*) 41
5. Modern project investment appraisal: return to simplicity.
C.L. Hicks (*BP Chemicals Ltd*) 53
6. Total process plant analysis by process integration.
I.C. Kemp (*Energy & Process Integration Service*) 67
7. Synthesis of distillation sequences: a comparison of
enumerative and AI methods.
J.C. Conners, V. Vadhvana (*BP Research*), R.J. Best, N.S. Dhallu
and W.R. Johns (*Polytechnic of the South Bank*) 79
8. Expert systems for production separator design.
D.R. Dick and M. Zelouf (*BP International Ltd*) 95
9. Optimisation of acid gas emission control strategies in the UK
power generation industry.
W.S. Kyte and J.R.P. Cooper (*CEGB*) 109

Process Design

10. Optimal cost design of a cyclohexanol plant.
R. Scott (*University of Edinburgh*) 117
11. Optimisation of batch plant design.
J.S. Grist (*John Brown Constructors Ltd*) 129
12. Hazards assessment at initial layout stage.
R.J. Aldridge (*Isopipe Ltd*) and J.C. Mecklenburgh (*University
of Nottingham*) 141
13. Optimisation and safety.
T.A. Kletz (*University of Technology, Loughborough*) 153
14. Dynamic model based optimisation in the design of a batch
process involving simultaneous reaction and distillation.
J.A. Wilson (*University of Nottingham*) 163

Detailed Design

- | | |
|---|-----|
| 15. Integrated controlled random search: application to a wastewater treatment plant model.
J.R. Banga and J.J.C. Long (<i>Universidad de Santiago de Compostela, Spain</i>) | 183 |
| 16. Explosion venting of weakly flammable mixtures: implications for existing plant modifications.
D.G. Robson (<i>BP Chemicals Ltd</i>) | 193 |
| 17. An optimal overdesign strategy for fouling.
E. Kotjabasakis and B. Linnhoff (<i>UMIST</i>) | 211 |
| *18. Re-vamp of high pressure distillation columns using random packings.
K. Robinson (<i>Norton Chemical Process Products</i>) | 339 |

Plant Operation

Part I: Case Studies

- | | |
|---|-----|
| 19. Condition based maintenance – the optimum route to enhanced plant availability.
P.C. Baguley (<i>PA Management Consultants</i>) | 237 |
| 20. Statistical process control in the plantations industry.
A.F. Shafii (<i>Harrisons Malaysian Plantations Bhd, Malaysia</i>) | 251 |
| 21. Maximising waste utilisation in palm oil mills.
N.M. Sulaiman (<i>University of Malaya</i>) and A.F. Shafii (<i>Harrisons Malaysian Plantations Bhd, Malaysia</i>) | 265 |
| *22. Optimisation of phosphate grinding.
Y. Vincent (<i>FMA, Nancy, France</i>) and S.B. Smoult (<i>PEC-Engineering, Cergy-Pointoise, France</i>) | 351 |

Part II

- | | |
|---|-----|
| 23. Computer control of an olefine plant using an on-line optimiser.
P.C. Prichard (<i>ICI plc, Chemicals and Polymers Group</i>) | 277 |
| 24. On-line optimization of fluidized catalytic crackers.
S. Wright, P. Lawrence and Z. Friedman (<i>KBC Process Automation Ltd</i>) | 285 |
| 25. Strategies for desalination optimisation.
J.R. Flower and J. Pardoe (<i>University of Leeds</i>) | 299 |
| 26. Optimal unit selection in a combined heat and power station
D. Foster (<i>ICI plc</i>) | 311 |
| 27. Process optimisation – design and operation: a practical experience.
D.H. Lott, M.L. Preston and D. Foster (<i>ICI plc</i>) | 327 |
| Index | 367 |

* These papers are printed out of page sequence.

OPTIMISATION OF GAS SEPARATION SCHEMES FOR THE ENSOL PROCESS

D.G. Arundale*

SYNOPSIS

This paper describes the application to the ENSOL (natural gas to ethanol) process of a method of evaluating alternative flowschemes.

The method was developed as a flexible, computer based model capable of generating material and energy balances together with capital cost estimates. Flowschemes are outlined for production and separation of synthesis gas by the steam reforming, partial oxidation and methanol decomposition routes.

INTRODUCTION

In 1984 BASF, Monsanto and H&G jointly announced the ENSOL process route as a new, efficient and economical method of converting natural gas (or other hydrocarbons) into pure bulk ethanol. In view of the range of distinct processes linked by the ENSOL concept there is considerable scope for integration and optimisation. This paper describes the method developed for screening and evaluating the options available when designing for specific feedstock, site and market requirements.

THE ENSOL PROCESS

It will be sufficient in this paper to offer only a brief description of the essential ENSOL process. Technological, economic and market factors have been discussed in greater detail in various publications - see references 1 and 2, for instance.

The process chemistry and flowscheme are illustrated by Figures 1 and 2, from which it is clear that a series of more or less separate plants are involved. Initially a gaseous feedstock is converted into synthesis gas using H&G's own process technology and this syngas is then separated into three streams:

- Stream (1) : Hydrogen
- Stream (2) : Carbon Monoxide
- Stream (3) : Methanol synthesis gas

* Humphreys & Glasgow Ltd.

Stream (3) passes as make up to the Methanol Loop to produce part or all of the methanol which joins with stream (2) as feed to the Acetic Acid plant. This plant applies Monsanto's well established carbonylation technology.

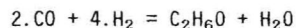
The key innovation is vapour phase hydrogenation of the acetic acid with stream (1) to give ethanol at very high yield. This reaction is well known but has only become feasible on a commercial scale now that BASF have developed and proved the catalyst.

Ethanol has excellent properties as a gasoline additive and a blending octane number as high or higher than other oxygenates such as MTBE, GTBA and methanol used for this purpose. As well as ethanol's position as a major motor fuel in Brazil, blends containing up to 10% of fermentation ethanol are already marketed in the USA and to a lesser extent in Western Europe. However, special circumstances or subsidies have been needed for economic viability. The new process, particularly when based on remotely located sources of natural or associated gas which would otherwise be flared, opens up the prospect of large scale use of ethanol. Moreover, there is not the restriction on feedstock availability that applies to more complex chemicals based on C_2 , C_3 and C_4 hydrocarbons.

PROCESS OPTIONS

The part of the ENSOL process for which H&G have primary responsibility is the front end i.e. gas generation, gas separation and methanol synthesis. The essential products are feed materials at defined battery limit conditions for the acetic acid/ethanol end of the plant. This oversimplification is shown on Figure 3 for the balanced case (although methanol import or export cases are equally possible).

The "ideal" ENSOL material balance can be represented as:



i.e. the Gas Generator output must have a minimum H_2/CO ratio of 2. In practice CO_2 is also present (and is a vital component) and leads to some loss of hydrogen so that actual ratios are in the range 2.2-2.5. Ratios outside this indicate downgrading of CO or H_2 from product to fuel value.

Problems in Gas Separation are mainly caused by the presence of inert components - CH_4 , N_2 and Argon. CO_2 is, of course, a useful part of the methanol make up gas. The most difficult operation is reduction of inerts in the CO stream to less than 5% and preferably 2%. Therefore the strategy is to build up a Loop make-up-gas which has both an acceptable stoichiometry and contains most of the inerts. The presence of the Methanol Loop confers a great advantage on the ENSOL process because of its incidental ability to act as an inerts purge.

A wide choice of options is available for both gas generation and gas separation:

Gas Generation Processes

Steam Reforming
 Steam Reforming with CO₂ recycle
 Partial Oxidation
 Partial Oxidation with part purge recycle
 Steam Reforming followed by Partial Oxidation
 CO Shift (if needed for H₂/CO ratio adjustment)
 Methanol Decomposition

Gas Separation Processes

CO₂ Removal
 Cryogenic Separation
 PSA (Pressure Swing Adsorption by molecular sieves)
 Prism (Monsanto's proprietary membrane separator)
 CO Extraction (e.g. Cosorb)
 Methanol Synthesis

Choice of processes for these front end operations will be influenced not only by the factors mentioned above but also by project variables, e.g. feedstock composition or requirements for integration with other site facilities.

PROCESS FLOWSCHEMES

The methods developed to evaluate four flowschemes based upon the above processes will now be explained and some results presented.

Steam Reforming

The syngas produced by a steam reformer contains an excess of H₂ (typically H₂/CO about 3) but most or all of the surplus is readily used for furnace firing. Figure 4 shows the standard arrangement where CO₂ is removed from the syngas and compressed into the Loop, after which the balance of the gas is treated cryogenically.

Figure 4 also shows the alternative scheme where the CO₂ is recycled to the reformer feed. This reduces the H₂ excess and, as demonstrated later, is likely to give a better overall performance.

Partial Oxidation

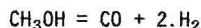
The partial oxidation process gives rise to a syngas with H₂/CO ratio less than 2 but by means of the CO Shift reaction this can be raised sufficiently to prevent excessive carbon rejection to the fuel by-product stream.

The scheme shown in Figure 5 takes advantage of the high reaction pressure to purify the CO through two stages of Prism membrane separation. The Methanol Loop and PSA parts of the scheme are similar to those in steam reforming. In some circumstances it may be worth recycling part of the Loop purge to recover hydrogen. References 3 and 4 give information about the principles of PSA and Prism operation.

Methanol Decomposition

Syngas separation would be a much simpler operation if the inert components were not there. To some extent ENSOL already achieves this effect by use of the Methanol Loop and an interesting possibility is to carry this to its logical conclusion by passing all the syngas into the Loop.

A speculative scheme is shown in Figure 6. The conventional large, high efficiency methanol synthesis plant produces enough methanol both for direct ENSOL feed and for the $H_2/CO=2$ product of decomposition:



Although this idea represents a novel application, decomposition itself is an established catalytic process carried out at moderate conditions. Reactor products include unreacted methanol and trace by-products as well as CO and H_2 . Methanol and most of the by products are washed from the gas and recycled to the synthesis plant. The resultant syngas contains 1-3% inerts and is relatively easy to separate by a PSA/Prism arrangement into CO and H_2 streams.

METHOD OF EVALUATION

It was apparent from the outset of this work that, faced with so many schemes and options, we needed to develop a systematic and reproducible method of evaluating process alternatives in relation to feedstock consumption, energy balance and capital cost. The method had to be flexible enough for process optimisation over the range of basic raw material and design constraints likely to be encountered.

The approach taken was to reduce the essential balances to modular subroutines with easily adjustable parameters. These modules were incorporated into a computer program which also contained the data correlations and procedures for calculations such as equilibrium conditions, energy and power consumptions.

Process and Energy Balances

Referring to the general scheme of Figure 3, these calculations fall into three parts:

(1) Gas generation

Thermodynamic calculations define the synthesis gas composition together with (by overall energy balance) waste heat in the form of high pressure steam.

(2) Gas separation

The syngas is split into CO, H_2 , and a make up gas (MUG) which is converted to methanol. A waste gas is also produced for use as fuel.

(3) Energy System

The electrical or mechanical power requirements of gas generation, separation and compression are met by a boiler/turbo-alternator system utilising all the HP steam and fuel gases, plus additional feed gas as necessary.

Figures 4 to 6 present specific examples of this general scheme for steam reforming, partial oxidation and methanol decomposition cases. Each block represents a modular set of calculation subroutines. Changes in pressure level are indicated by compressors, the power consumption of which is estimated from stream flow and pressure. The Reforming and Partial Oxidation modules carry out conventional K_s and K_r equilibrium and heat balance calculations. Most of the other modules are simple stream splitters into 2 or 3 products, the partition factors being treated as program parameters to be reset as specific design or vendor information becomes available.

Primarily to show module structure, factors typical of those which have been used for the Cryoseparation and Prism cases are given on Figure 7.

Capital Cost Estimate

Gross feedstock consumptions derived from material and energy balances cannot be compared in isolation - it is essential to have some indication of the capital cost impact. The method has therefore been developed to generate approximate costs for the various units and services defined on the flowschemes (e.g. Figures 4 - 6).

At this level of evaluation the requirement is more to highlight broad differences between schemes rather than to produce detailed estimates. A number of in-house estimates for comparable plants have been used to derive unit rates for total installed cost at the 2000 MTD Ethanol scale. These rates are then adjusted by the cost/capacity exponent method for the relatively small differences between 2000 MTD cases. However for services, where the range can be greater, slightly more complex functions are used.

This series of 2000 MTD based factors is given as Figure 8. They are satisfactory when used to compare variations between the ENSOL schemes but will not necessarily be suitable for use in different contexts.

RESULTS AND COMMENTS

The theme of this paper is development of a methodology applicable to most sets of project requirements in order to make a "broad brush" optimisation and selection between alternative ENSOL flowschemes. The intention is not to arrive at a single conclusion, but to present series of results which identify significant variables and demonstrate typical quantities for schemes of the type under discussion. The basic assumptions are as follows:

Feedstock composition	CH ₄	89.4% (mol)
	C ₂ H ₆	10.0%
	N ₂	0.6%
Product streams	H ₂	4135 kg.mol/h
	CO	2080 kg.mol/h
	Methanol	1846 kg.mol/h
Ethanol equivalent	2000 MID	

In addition to total feedstock consumption and capital cost the most important performance index for any scheme is the purity of the CO product stream - because of its impact upon the economics of the (extremely expensive) downstream acetic acid plant.

Steam Reforming Schemes

Effect of reforming conditions:-

Reformer pressure (bara)	12	20	25
temperature (C)	900	870	850
CO Product purity (mol%)	96.7	95.2	93.8
Process feedstock (MMkcal/h)	959	1055	1147
Total Plant Feed (MMkcal/h)	1142	1138	1151
Total Installed Cost (£million)	139.7	141.4	146.7

Effect of CO₂ Recycle:-

Reformer pressure (bara)	12	20	25
temperature (C)	900	870	850
CO Product purity (mol%)	97.3	96.6	96.0
Process feedstock (MMkcal/h)	933	986	1035
Total Plant Feed (MMkcal/h)	1126	1115	1119
Total Installed Cost (£million)	132.3	130.8	133.8

Effect of methanol loop efficiency:-

Carbon conversion (%)	94	85	75
Loop Pressure (bara)	80	70	60
CO Product purity (mol%)	96.6	96.5	96.4
Process feedstock (MMkcal/h)	986	1041	1118
Total Plant Feed (MMkcal/h)	1115	1119	1128
Total Installed Cost (£million)	130.8	129.8	129.1

Partial Oxidation Schemes

Effect of methanol loop efficiency:-

Carbon conversion (%)	94	85	75
Loop Pressure (bara)	80	70	60
CO Product purity (mol%)	96.4	96.9	97.4
Process feedstock (MMkcal/h)	1046	1049	1074
Total Plant Feed (MMkcal/h)	1095	1085	1080
Total Installed Cost (£million)	156.2	153.0	150.7

Flowsheet variations with 85%/70 bar Loop:-

Type of variation	Standard	Steam addition	Partial recycle
CO Product purity (mol%)	96.2	95.3	94.3
Process feedstock (MMkcal/h)	1103	1175	1127
Total Plant Feed (MMkcal/h)	1125	1175	1171
Total Installed Cost (£million)	166.1	173.9	175.1

CONCLUSIONS

At this stage in the development of ENSOL there is no virtue in rejecting any of the schemes. All of them have something in their favour, as may be seen from the following table:

Comparison of best case for each scheme

Scheme	Steam Reforming	Stm.Ref.+ CO ₂ Recycle	Partial Oxidation	Methanol Decomp'n
CO purity (mol%)	96.7	97.3	97.4	98.5
Feedstock (MMkcal/h)	959	933	1074	1122
Total Feed (MMkcal/h)	1142	1126	1080	1203
Cost (£million)	139.7	132.3	150.7	173

This evaluation shows that Steam Reforming, particularly with CO₂ recycle, is the process with the lowest capital cost. On the other hand Partial Oxidation gives the highest thermal efficiency. Methanol Decomposition has the potential to give the best level of CO product purity and hence to reduce the cost of the downstream acetic acid plant.

The particular market for which the ENSOL process is considered most suitable is the exploitation of surplus gas at remote locations i.e. low price feedstock and high cost of capital. In those circumstances the steam reforming schemes are clearly to be preferred and can give attractive investment returns (see Reference 1).

REFERENCES

1. C.L. Winter: Make Ethanol via Syngas.
Hydrocarbon Processing-April 1986. pp 71-73.
2. J. Griffiths & A. Horton:
Synthetic Ethanol - Gas to Liquid Assets.
Carbon One Chemical Technology: I.Chem.E.Symposium 1986.
3. J.A. Heck:
First U.S. Polybed PSA unit proves its reliability.
Oil & Gas Journal, February 1980.
4. D.J. Stookey, C.J. Patten & G.L. Malcolm:
Membranes separate Gases selectively.
Chemical Engineering Progress, November 1986

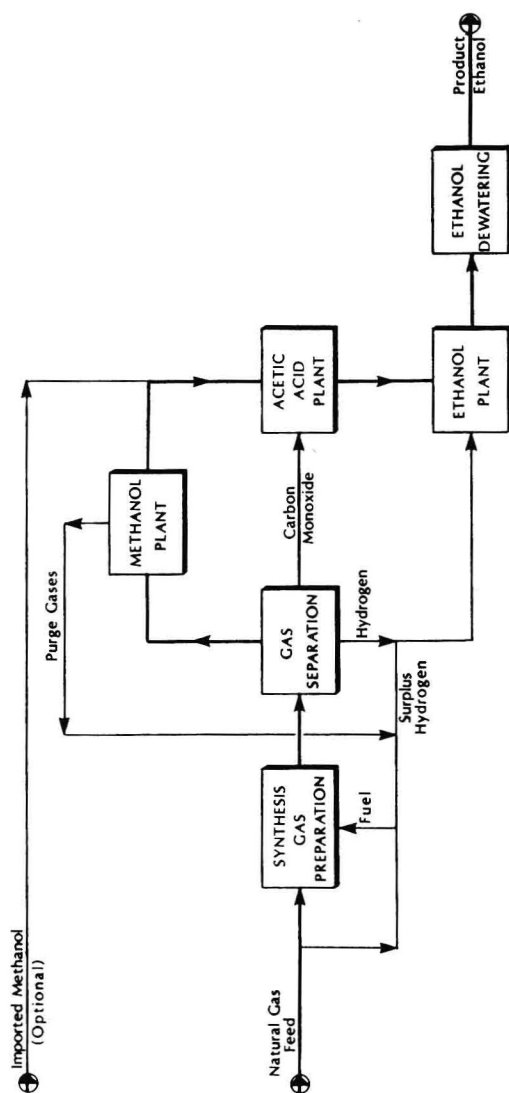


FIGURE 2
ETHANOL PLANT BLOCK FLOWSHEET
BASIC SCHEME