ChemShare News

2

1985

Announcing DesignMaster

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ChemShare news at a glance

Announcing DesignMASTER

A database system capable of handling nearly all process engineering activities in an integrated manner is available now. (See page 3)

Introducing DESIGN II/PC

Easy, interactive program creates DESIGN II input file quickly using your IBM PC. (See page 13)

DESIGN II

A library of crude oils is available in DESIGN II. (See page 15)

Depressuring analysis can be calculated for vessels exposed to external heat. (See page 21)

A general equilibrium reactor module allows calculation of any gas-phase reaction in your flowsheet. (See page 25)

Set flash conditions for regular FLAsh module. (See page 27)

PHAse MAP module calculations can now use several different thermodynamic options. (See page 28)

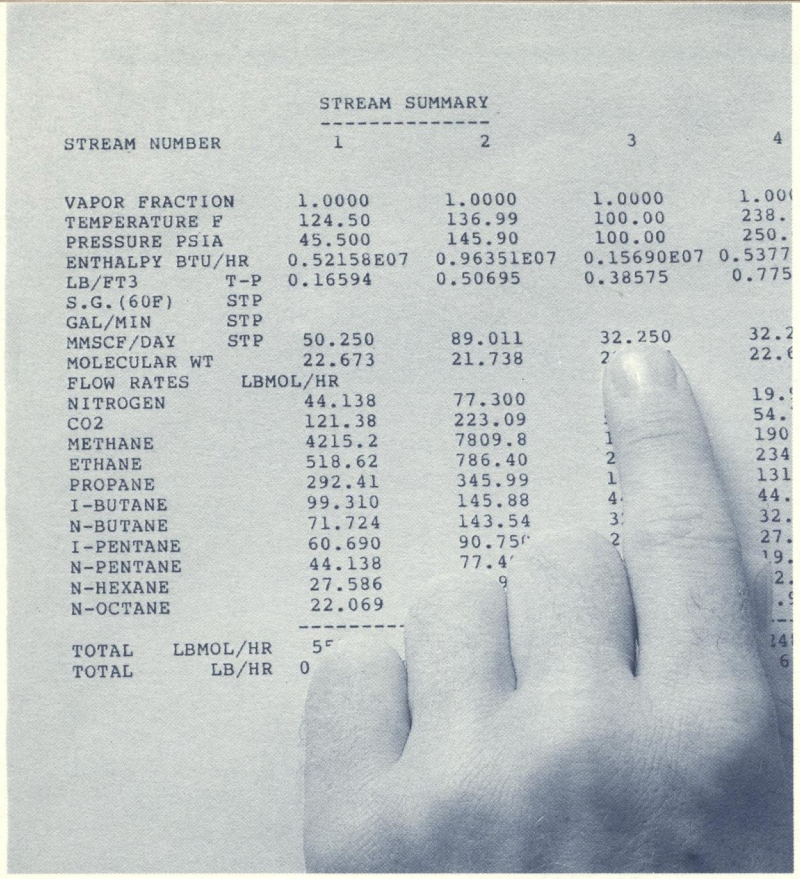
Thermodynamics

Lee-Kesler-Ploecker correlation has been added to DESIGN II (See page 28)

General

Learn how ADNOC improved process engineering productivity using a flowsheet simulator. (See page 37)

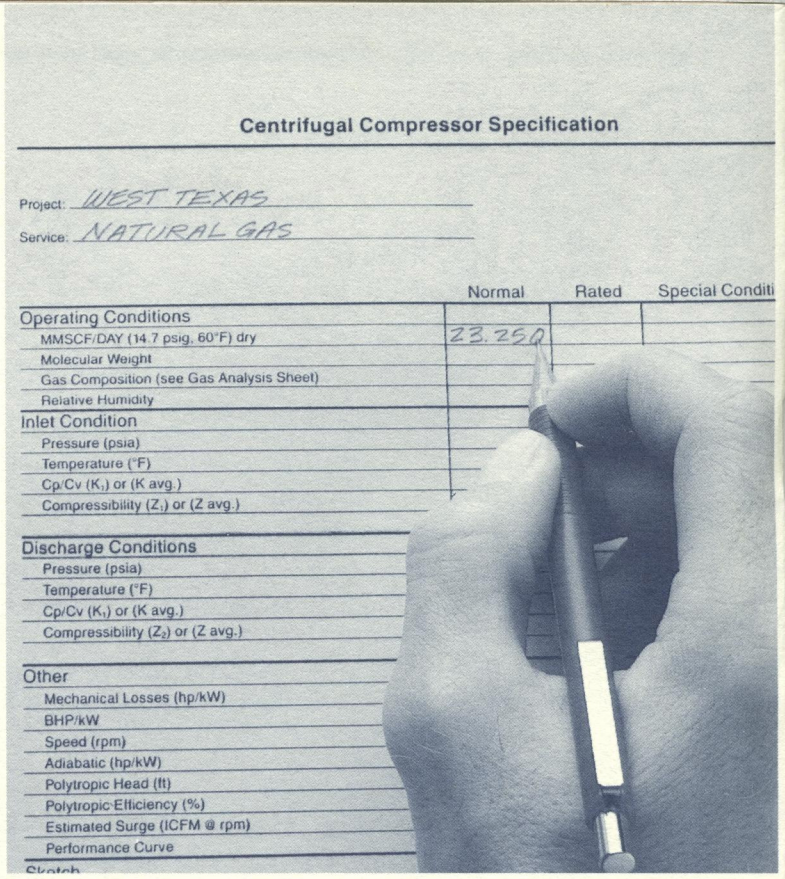
DESIGN II User's Guides are here! (See page 47)



STREAM SUMMARY

STREAM NUMBER		1	2	3	4
VAPOR FRACTION		1.0000	1.0000	1.0000	1.00
TEMPERATURE F		124.50	136.99	100.00	238.
PRESSURE PSIA		45.500	145.90	100.00	250.
ENTHALPY BTU/HR		0.52158E07	0.96351E07	0.15690E07	0.5377
LB/FT3	T-P	0.16594	0.50695	0.38575	0.775
S.G.(60F)	STP				
GAL/MIN	STP				
MMSCF/DAY	STP	50.250	89.011	32.250	32.2
MOLECULAR WT		22.673	21.738	2	22.6
FLOW RATES	LBMOL/HR				
NITROGEN		44.138	77.300		19.
CO2		121.38	223.09		54.
METHANE		4215.2	7809.8	1	190
ETHANE		518.62	786.40	2	234
PROPANE		292.41	345.99	1	131
I-BUTANE		99.310	145.88	4	44.
N-BUTANE		71.724	143.54	3	32.
I-PENTANE		60.690	90.75	2	27.
N-PENTANE		44.138	77.4		19.
N-HEXANE		27.586	9		2.
N-OCTANE		22.069			
TOTAL	LBMOL/HR	5			14
TOTAL	LB/HR	0			6

The left hand



Centrifugal Compressor Specification

Project: WEST TEXAS

Service: NATURAL GAS

	Normal	Rated	Special Conditi
Operating Conditions			
MMSCF/DAY (14.7 psig, 60°F) dry	23.25Q		
Molecular Weight			
Gas Composition (see Gas Analysis Sheet)			
Relative Humidity			
Inlet Condition			
Pressure (psia)			
Temperature (°F)			
Cp/Cv (K_1) or (K avg.)			
Compressibility (Z_1) or (Z avg.)			
Discharge Conditions			
Pressure (psia)			
Temperature (°F)			
Cp/Cv (K_1) or (K avg.)			
Compressibility (Z_2) or (Z avg.)			
Other			
Mechanical Losses (hp/kW)			
BHP/kW			
Speed (rpm)			
Adiabatic (hp/kW)			
Polytropic Head (ft)			
Polytropic Efficiency (%)			
Estimated Surge (ICFM @ rpm)			
Performance Curve			

The right hand

You are looking at a very innocent, very simple $207,900 mistake.

It seems so simple. Just read a stream flowrate off a computer printout and write it on a compressor specification sheet. But there it is: a transposed number, and someone — maybe you — is going to get a plant with a compressor too small to put product in the pipeline. Fixing the problem will add at least $207,900* to the cost of the plant.

But why? Why spend all that time and risk all those mistakes in transferring data? Why do it by hand? Because until now, that's been the only way. The last primitive link in the world of computer process design.

Introducing hands-off, error-free data transfer

Now, there's DesignMaster,℠ a design database that provides direct interfaces so all your computer programs can communicate with each other and with devices such as plotters and printers. Here are just a few of the advantages.

- DesignMaster can send output from any process simulator (even your own) directly and *error-free* to other programs for sizing columns, heat exchangers, vessels and pipelines.
- DesignMaster can print equipment specification sheets and equipment lists automatically and *error-free* in any format.
- DesignMaster can produce process flow diagrams quickly and *error-free*.
- DesignMaster will do all these things in any units you want — automatically — so there won't be any conversion errors, either.

And the DesignMaster database can be completely tailored to any company's design standards, so you don't have to change your systems in order to get the benefits of DesignMaster's automatic, error-free data transfer.

So far, we're talking just about preventing costly errors. We haven't even mentioned increased productivity, time savings, or better process designs, the other major benefits of DesignMaster. To find out more, or to arrange a free demonstration, call or write ChemShare today.

*Another 595 horsepower at $350 per horsepower is needed.

DesignMaster is a registered service mark of The ChemShare Corporation.

DesignMaster

by ChemShare®

The ChemShare Corporation
1900 Lummus Tower • Houston, Texas 77056
Phone: 713/627-8945 • TWX: 910-881-2793

ChemShare Process Systems Ltd.
Brook House Church Street • Wilmslow, Cheshire SK9 1AT England
Phone: 0625-532113 • Telex: 666905

Announcing DesignMASTER℠

ChemShare introduces the world's first advanced integrated process design system. DesignMASTER spearheads the "new generation" of design systems.

Where are we now?

Productivity gains for process engineers using currently available computer calculational aids have been most significant in the use of flowsheet simulators, such as DESIGN II, for calculation of energy and material balances. However, usage of these programs represents only 10-15% of the activities of the average process design engineers.

Where are we going?

In order to forecast how the next major step in process design productivity can be achieved, let's review the typical activities of a process engineer or process team. Simply stated, these are:

- evaluate and select the best thermophysical property data for the flowsheet and individual equipment calculations.
- calculate energy and material balances for a proposed base case design together with alternative load cases, such as start-up, shutdown, and emergency or hazard cases.
- produce drawings of process and utility flow diagrams with energy and material balances.
- calculate and specify equipment duties and modes of operation.
- produce detailed equipment designs for heat exchangers, separators, distillation towers, etc.
- advise upon control requirements and procedures.
- write down and deliver process design information for other engineering disciplines and/or equipment vendors.
- produce additional studies as a design project proceeds.

Such a list of activities makes it clear why computer software tools are important. It also highlights the leading role of process design in a total project. It also emphasizes the need to communicate data in a suitable form for team decision making.

The process design activities described above can be grouped into the following specific activities relating to process design:

- expert evaluation of **data** (e.g. thermophysical properties).
- calculation of **data** (e.g. heat and material balances).
- transfer of **data** (e.g. results of one calculation are input for other calculations).
- communication of **data** (e.g. equipment specification sheets).

The common denominator of process design activities is **data** and particularly its timely and accurate communication to the rest of the design team.

In the past, the focus for improving process productivity has been on increasing the speed and capability of calculations. This focus will of course continue with the increasing penetration of expert systems and process synthesis techniques. However, each program is a "stand-alone" package with its own oddities of input and output of data. Results of one calculation typically require manual transmission of data to be used as input for another calculation.

The focus for improving process productivity has changed. Most experts now firmly believe that the next major productivity increase will result from handling process **data** in much more efficient ways than in the past.

R. L. Motard, Professor of Chemical Engineering at Washington University (2), summarized this:

> "Computers will be more useful when today's program-centered approach to large-scale applications is replaced by a data-centered approach. In the past, the program and its developer dominated the application, and data had a secondary role. The solution is a data-centered approach to program development. After all, decision making depends on the information content of the data, and not on the

program. The business community discovered this long ago, and moved to database-management techniques. Now it is the engineering community's turn."

How much design data is involved?

During the design of a process plant, an enormous amount of data must be transferred manually, often to more than one location. R. L. Peters of Bechtel Petroleum, Inc. (1) provides some interesting insights into the structure of the data organization for process plants. While Peters refers to mega-projects of up to 1 million technical manhours, the general relationships are still valid for much smaller projects. For example, Table 1 illustrates just the number of data sheets (or specification sheets) required for a mega-project.

TABLE 1

Characteristics of Projects

	MEGAPROJECT		AVERAGE
Items	Number	Data Sheets	%
Major Equipment	550	550	27
Bid Summaries	550	300	15
Instrument/ Control	10,000	1,000	48
Pipelines	4,000	200	10
TOTAL	15,000	2,050	100

To appreciate the problems of data consistency and inefficiency, consider that a single item of process data typically appears on several different specification sheets. For example, the pressure of a stream in a pipeline to the inlet to a heat exchanger could appear in at least 4 specification sheets and 1 drawing:

- line schedule (stream P)
- pump specification sheet (discharge P)
- heat exchanger specification sheet (inlet P)
- instrument specification sheet (operating P)
- energy/material drawing (stream P)

As all project and process managers recognize, putting one process data value (such as stream pressure) in at least 4 specification sheet locations can

- be time consuming
- be error prone
- introduce inconsistencies

These concerns are magnified if a previously specified value is changed during the design and needs to be recommunicated to other members of the design team.

Bechtel (1) further identified 570,000 separate, individual data items that became 2 million input operations and 24 million access operations over the 3-year life of a project. Presented a different way, a single item of process data (e.g. stream pressure) appeared in an average of 3-4 specification sheets and was accessed an average of 42 times. Bechtel concluded that an engineering database system would reduce the number of manual entries to specification sheets by a factor of 10. In addition, integrating computer calculation programs with the project database would allow 30% of all required data to be entered directly onto the specification sheets without the need for manual intervention.

In the process design area, we estimate that computer programs can provide over 70% of all process data specifications. Therefore, integrating computer calculations with a data storage system, which can automatically generate specification sheets, would cut manual data entry by at least two thirds.

How do we handle this mass of data?

Within the chemical engineering field, and particularly the Engineering and Construction (E&C) firms, the emphasis is usually on the total project and hence the total project database. However, such centralized databases are likely to be very large databases. This leads to a costly development activity and long lead times before such large database systems can be implemented in a working design environment.

An alternative approach is to recognize that the total project is in fact a series of interconnected, mini-project tasks (e.g. process, mechanical, instruments, electrical, civil, steelwork, etc.). Each of these engineering groups is capable of working independently on its own tasks and, as a consequence, could easily use its own smaller satellite

database. This concept of smaller satellite databases connected together is shown in Figure 1. Such smaller satellite database systems have significant advantages over the total database, namely:

- reduced development time
- earlier implementation
- reduced computing requirements
- more local processing
- phased introduction
- isolated testing and verification

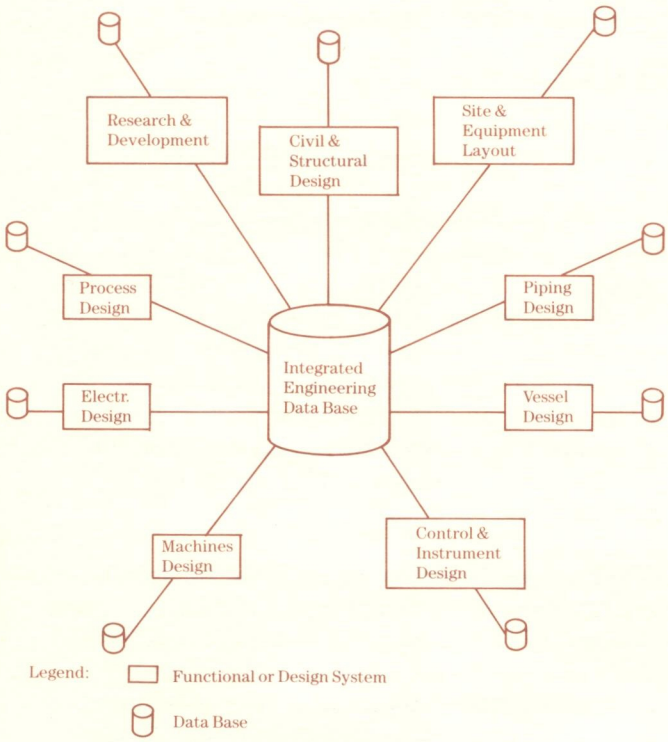


Figure 1. Satellite Data Base System

How is the data organized?

The process data for a major engineering project can be structured as shown in Figure 2. Usually a PROJECT (e.g. oil refinery) will be divided into a number of PLANTS (e.g. crude unit, off sites, LPG, etc.). Each plant may be organized into many flowsheets (MODELS) and calculated under a set of alternative CASES (DESIGNS and PERFORMANCES). At the lower levels of this data structure is the detailed data associated with items of equipment (UNITS) and streams (STREAMS). This data structure, which is inherent in process plant data, is the basis of the DesignMASTER integrated process design system.

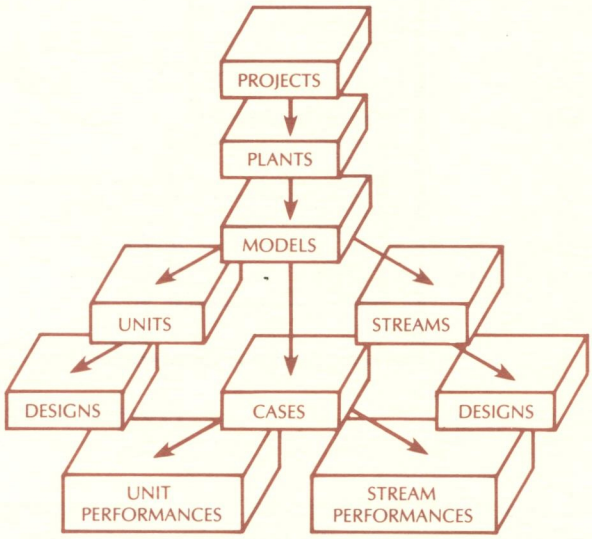


Figure 2. DesignMASTER Database Organization

At appropriate times, under the control of project management, data from one satellite database can be called to the central integrated database or communicated to others as needed. This concept of a central project database interacting with a series of satellite databases is the basis for the DesignMASTER system.

What is DesignMASTER?

DesignMASTER is a computerized database system capable of handling process engineering activities in an integrated manner. The DesignMASTER system coordinates the tasks of process flowsheeting, equipment design and specialized thermophysical programs with the automatic production of "spec" sheets, equipment lists and drawings. All the information is held (and therefore updated) in the computer's one common database. The system, marketed by ChemShare, is shown in Figure 3.

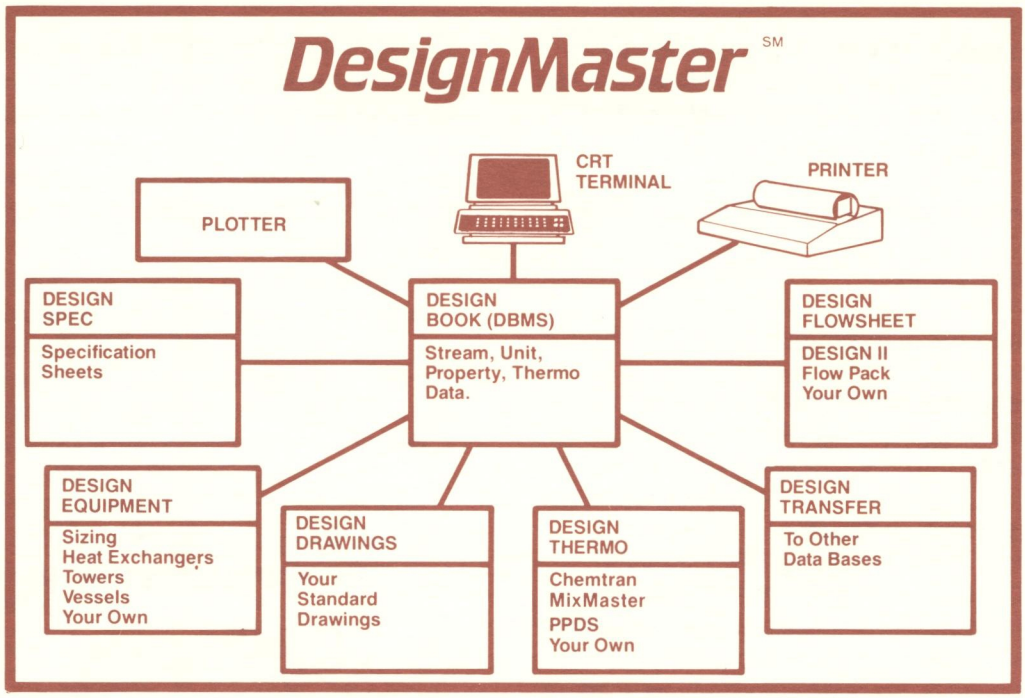


Figure 3. DesignMASTER System

DesignMASTER provides the process engineer and his manager with the following capabilities:

- Database storage of flowsheets, equipment data and stream data.
- Integration of all computerized calculations for process flowsheets and equipment design.
- Communication of process data to specification sheets, equipment lists, drawings and other databases.
- Management of process data by controlling access, monitoring changes and issue release.

DesignMASTER is provided as a standard package with interfaces to ChemShare's DESIGN II flowsheet simulator, separator sizing and line sizing programs. The key to DesignMASTER is the ability to easily interface **your own software** or other licensed programs you may currently use, such as HTRI, AIDEX, B-JAC, etc.

A major benefit that comes "free" with a database system is elimination of error in data transfer. Data consistency and availability also show dramatic increases.

What can DesignMASTER do?

The DesignMASTER system can be used on large or small projects. In the case of a single plant, design work normally starts with the process flow sketch and energy and material balances. At this initial stage, the DesignDRAWINGS graphics facility can be used to prepare a process flow diagram and to define the equipment items and their stream connections. This topography is then stored on the database and is independent of the simulation program.

The specifications required for the flowsheet energy and material balance calculation are assembled easily using DesignFLOWSHEET which contains an easy-to-use, interactive program for creating DESIGN II input files. Your in-house simulator can also be interfaced through DesignFLOWSHEET. A special output file is created during execution of DESIGN II which allows the results to be loaded directly onto the database.

Once the simulator or equipment design results are on the database, case studies for flowsheets and/or equipment items can be rapidly reviewed with the COMPARE feature. This generates a table of all differences between the cases and prints them in a concise, clear format. The COMPARE can be used globally or on selected process stream/equipment information, and is very effective for large flowsheets. See Figure 4a for a comparison of results when process flows and composition were modified slightly by the client for the flowsheet shown in Figure 4.

Component	Case Rev A Flow (lbmol/hr)	Case Rev B Flow (lbmol/hr)
METHANE	1000	1100
ETHANE	750	800
PROPANE	500	600
N-BUTANE	275	350
N-PENTANE	180	220
PCUT	100	120

(where PCUT is a petroleum fraction with API gravity of 37, mean average boiling point of 350, and molecular weight of 175).

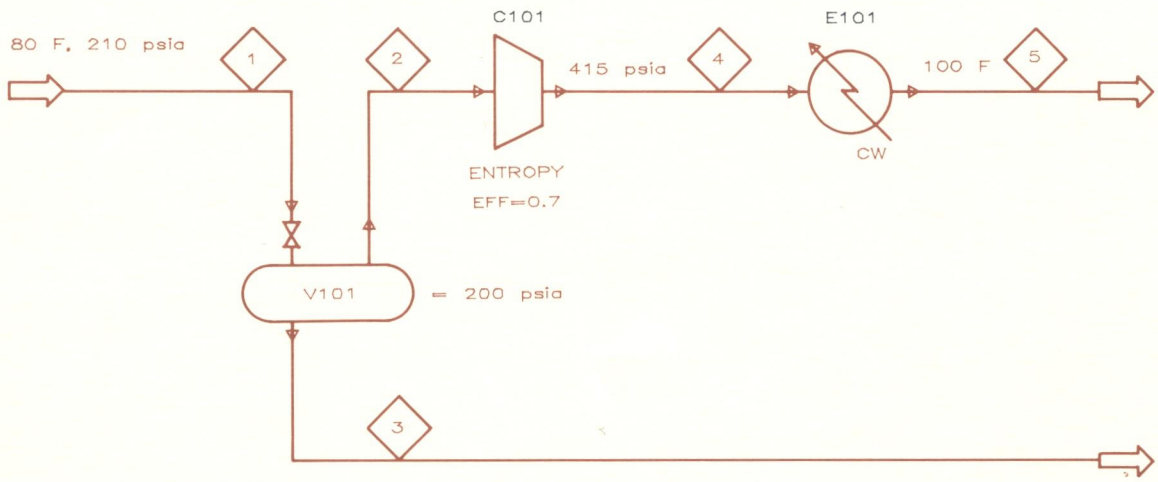


Figure 4. Simple Flowsheet

```
*COMPARE CASE REVA TO CASE REVB DATA MASFLO, WORK, DUTY
Tolerance (percent)?
*5

Item name    Data name    Units     First case     Second case     % change

Stream 1     MASFLO       lb/hr      107110.        125372.          17.0
Stream 2     MASFLO       lb/hr      70178.7        77960.1          11.1
Stream 3     MASFLO       lb/hr      36931.5        47412.0          28.4
Stream 4     MASFLO       lb/hr      70178.7        77960.1          11.1
Stream 5     MASFLO       lb/hr      70178.7        77960.1          11.1
Unit V101    - no differences found outside tolerance
Unit C101    WORK         HP        -1011.4        -1109.9           9.7
Unit E101    DUTY         Btu/hr   -4.3092E+06    -4.9238E+06        14.3
   7 datablocks compared
```

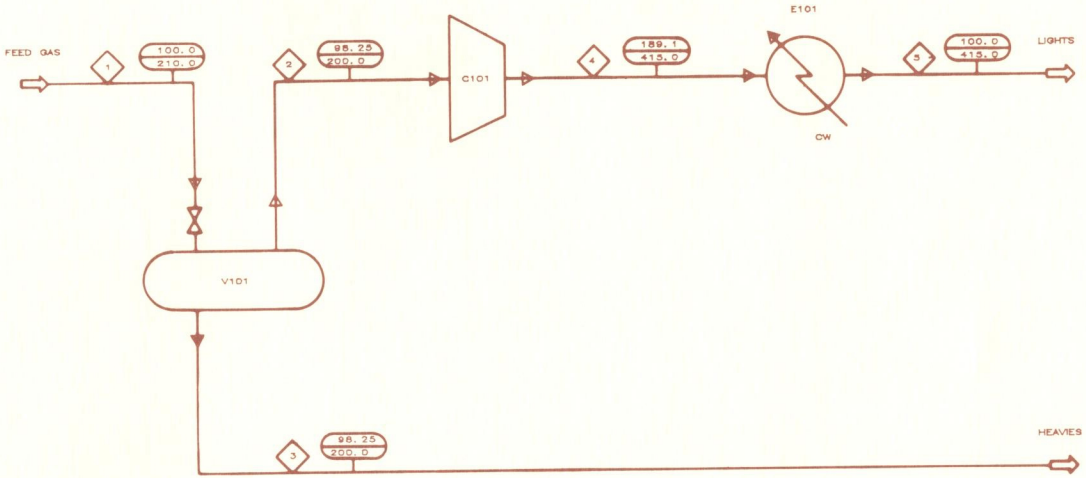
consider making up

Figure 4a. COMPARE Feature

After making the final energy and material balance, the process engineer may need to design individual items of equipment. DesignEQUIPMENT can access any set of stream properties from the database and pass these, in any format, to programs which perform equipment sizing and design calculations. Likewise, the results from these calculations are stored on the database.

The development of process flow diagrams (i.e. heat and material balance drawings) is particularly simplified with DesignDRAWINGS. All the calculated streams and equipment data is added to the flowsheet automatically from the database thus increasing productivity and minimizing errors in transmittal. See Figure 5 for a sample process flow diagram generated by DesignDRAWINGS.

Stream Name		1	2	3	4	5
Phase		2 Phase	Vapor	Liquid	Vapor	2 Phase
Vapor Mole Fraction		.8327	1.00	–	1.00	.9212
Temperature	(F)	100.03	98.25	98.25	189.08	100.03
Pressure	(psia)	210.00	200.00	200.00	415.00	415.00
Avg. Mol. Weight	(lb/lbmol)	38.19	29.91	80.50	29.91	29.91
Total Enthalpy	(Btu/hr)	-.2502E 7	.1321E 7	-.3822E 7	.3895E 7	-.4867E 6
Total Flow	(lb/hr)	.1071E 6	70178.78	38931.49	70178.78	70178.78
Total Flow	(lbmol/hr)	2805.00	2346.23	458.77	2346.23	2348.23
Comp. Flows	(lb/hr) Mol. Weight					
METHANE	16.04	.1604E 5	.1583E 5	213.4280	.1583E 5	.1583E 5
ETHANE	30.07	.2255E 5	.2120E 5	.1353E 4	.2120E 5	.2120E 5
PROPANE	44.09	.2205E 5	.1840E 5	.3652E 4	.1840E 5	.1840E 5
N-BUTANE	58.12	.1598E 5	.9949E 4	.6034E 4	.9949E 4	.9949E 4
N-PENTANE	72.15	.1299E 5	.4751E 4	.8235E 4	.4751E 4	.4751E 4
PCUT	175.0	.1750E 5	58.5444	.1744E 5	58.5444	58.5444



Unit Name		C101	E101	V101
AREA	(ft2)		2507.59	
U	(Btu/hr,ft2,F)		50.00	
DUTY	(Btu/hr)		-.4361E 7	
LMTD	(F)		34.78	
Water Flow Rate	(USgal/hr)		34904.09	
Outlet Pressure	(psia)	415.00		200.00
Efficiency	(frac)	.7000		
Power	(hp)	-1011.37		
CP/CV		1.20		

ok with tm

DESIGNMASTER™

PROCESS FLOW DIAGRAM

Title

Date | Engineer

Project : DEMO
Plant : COMPRESSION
Model : SINGLE STAGE
Case : REVA RESULTS
Drawing : 1 | Revision : A | Sheet 1 of 1

Figure 5. Process Flow Diagram

Also, equipment specification sheets and lists can be automatically produced by DesignSPEC in whatever format and dimensional units you require. The unit conversions are provided automatically by DesignMASTER. For example, an E & C firm can produce equipment specification sheets in its own format, or those of its client companies, or both. See Figure 6 for a sample vessel specification sheet.

Figure 6. Vessel Specification Sheet

```
                          PRESSURE VESSEL DATA SHEET
                          ==========================
Client   : ABC Chemicals                                Time       : 09:20
Unit     : Inlet Scrubber                               Date       : 01-MAR-85
Item no.: V101                                          Prepared by: JGS
Location: West Texas            Page 1 of 2             Revision   : A
-------------------------------------------------------------------------------
:Project: DEMO                Model: SINGLE STAGE      Unit   : V101          :
:Plant  : COMPRESSION         Case : REVA RESULTS      Design: V101 REVA      :
:-----------------------------------------------------------------------------:
:             MATERIALS                 :              GENERAL                 :
:-----------------------------------:-----------------------------------:
:Heads              : CARBON STEEL    :Vessel diameter, in - ID : 42         :
:                   :                 :                    - OD :            :
:Shell              : CARBON STEEL    :Length of vessel      ft : 10         :
:Supports           :                 :No. required             :  1         :
:                   :                 :Reference Drawing        :            :
:Flanges and covers:                  :-----------------------------------:
:Manway necks       :                 :          DESIGN DATA                :
:Nozzle necks       :                 :-----------------------------------:
:Bolting press,psig:                  :Operating pressure      psig:  215   :
:Manway gaskets     :                 :Req'd design pressure   psig:  240   :
:Tray supports      :                 :Max. allow. work press  psig:        :
:Trays              :                 :Design wind press,psf-Flat  :        :
:                   :                 :                     -Curved:        :
:Baffles            :                 :Operating temp     F -Top   :   98   :
:                   :                 :                     -Bottom:   98   :
:Internal piping    :                 :Design metal temp  F -Top   :  650   :
:                   :                 :                     -Bottom:  650   :
:Mist extractor     :6 IN DEMISTER PAD :Corrosion allow          in: .125   :
:                   :   304 SS        :Est. wt.,lbs - Empty        : 2156   :
:                   :                 :             - Full of water: 6501   :
:-----------------------------------------------------------------------------:
:           FABRICATION               :     CODE-INSPECTION-TESTING         :
:-----------------------------------:-----------------------------------:
:Type of heads            : 2:1       :Code                  : ASME V111    :
:Type of nozzles          :           :Stamping              : U-1A         :
:                         :           :   (Y/N)              : Y            :
:Type of lining           :           :Stress relieved (Y/N): N             :
:Type of trays            :           :Radiograph(Spot/100%): SPOT          :
:Sour service reqmts (Y/N): N         :Inspection by         :              :
:External insulation (Y/N): N         :Special examination   :              :
:Shop painting       (Y/N): Y         :                                     :
:-----------------------------------:-----------------------------------:
:       RELATED DRAWINGS              : REQ'D COPIES OF DRAWINGS & REPORTS :
:-----------------------------------:-----------------------------------:
:Trays              :                 :Prelim. drawings:                    :
:Ladder             :                 :Final drawings  :                    :
:Platforms          :                 :Mill reports    :                    :
:Lugs and clips     :                 :Mfr. reports    :                    :
:Auxiliary details  :                 :Other           :                    :
:Foundation drawing:                  :                                     :
-------------------------------------------------------------------------------
```

PRESSURE VESSEL DATA SHEET

Client : ABC Chemicals
Unit : Inlet Scrubber
Item no.: V101
Location: West Texas

Time : 09:20
Date : 01-MAR-85
Prepared by: JGS
Revision : A

VESSEL CONNECTIONS

Mk	No	Size	Rating	Facing	Service
A	1	8 IN	300 LB	R.F.	INLET
B	1	6 IN	300 LB	R.F.	VAPOR OUTLET
C	1	2 IN	300 LB	R.F.	LIQUID OUTLET
D					
E					
F					
G					
H					
K					
M					
N					
LC	2	2 IN	300 LB	R.F.	Level Control
LG	2	2 IN	300 LB	R.F.	Level Gage
PI	1	2 IN	300 LB	R.F.	Pressure Gage
TW	1	2 IN	300 LB	R.F.	Thermowell
HH					Insp. Opening
MN	1	18 IN	300 LB	R.F.	Manway w/Davit
V		2 in	Plain	Hole	Skirt Vents
W		8 in	Plain	Hole	Skirt Access
X		16 in	Plain	Hole	Skirt Manway

Install Trays - (Shop/Field) :
Insulation Support Rings Req'd (Y/N): N
Ladder (Y/N): Y Galv (Y/N): Y
Platforms (Y/N): N Galv (Y/N):

REMARKS:

Why do I need DesignMASTER?

DesignMASTER introduces quantifiable productivity gains and quality improvement. They result from the following:

- more process productivity
- saving time and money from fewer mistakes
- less cost than developing your own database system
- compatible with detailed engineering systems
- documentation can be standardized to your or your client's format
- interfaces to your company's own programs
- Integrated design systems have to be cost justified on their investment return. Table 2 illustrates the typical productivity improvement of using integrated process design systems.

TABLE 2

DesignMASTER Productivity Features

ACTIVITY	HOW	PRODUCTIVITY
Preparation for calculation	Menu driven input	2x
Calculation execution	Same as present	1x
Reviewing calculations	Computerized COMPARE	2x
Equipment Spec Sheets	Automated production Error-free	4x
Process Flow Diagrams	Screen prompted	5x
Heat/Mass Drawings	Screen prompted Error-free	10x

When these productivity gains are applied to the typical working pattern of a process engineer in an engineering or operating company, the time taken to perform the tasks is reduced by about one-third as shown in Table 3.

TABLE 3

Gains in Process Productivity

ACTIVITY	EXISTING METHODOLOGY % TIME	DESIGNMASTER PRODUCTIVITY BOOST	% TIME WITH DESIGNMASTER
Preparing for Calculations	10	2x	5
Execution of Calculations	20	1x	20
Review/Analyze Calculations	10	2x	5
Complete Equipment Spec Sheets	15	4x	4
Produce Process Drawings	15	10x	1.5
Others	30	-	30
Total	100		66

There are additional benefits which are harder to measure directly.

- Process engineers can do more (i.e. finish the job faster).
- Mistakes in transfer of process data are eliminated, thus shortening the review and re-review cycle.
- Productivity gains can also be used to optimize process design and hence make your company more competitive.

What's the bottom line?

Process design is a particularly important activity because of its effect on both plant operating costs and design/construction cost. The provision of an integrated, databased, process design and engineering system yields benefits on a broad scale, with returns on investment well in excess of 50%/year. This emerging technology offers new ways of working and the opportunity to apply corporate standards in order to achieve high organizational efficiency. DesignMASTER offers you this integrated database technology and is available to you now.

Is that all there is?

No. We have just barely touched on the capabilities of DesignMASTER. This system can be easily expanded to meet your future needs without expensive software development. DesignMASTER is flexible and open-ended.

If you want to know more about DesignMASTER, sign up now for a DesignMASTER presentation at your office or ours. Let us show you how to put DesignMASTER to work for you.

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Introducing DESIGN II/PC℠

DESIGN II input made quick and easy? No more plowing through manuals looking for a command you almost remember? Sound too good to be true? Well it isn't! ChemShare has a new, interactive program for the IBM PC-XT which will make creating or changing DESIGN II input files a snap. The initial release of this exciting product is March, 1985.

DESIGN II/PC is a menu driven, screen oriented system which allows you to enter your choices for required and optional data for equipments and streams for a flowsheet simulation. Data can be entered in any order which is convenient for you. DESIGN II/PC will assemble the data in the proper DESIGN II input format.

You can save the results of any session for later continuation. You can also review or modify previously entered data or create a DESIGN II input file. This input file is stored on the IBM PC disk and can be "uploaded" using any standard communications package to a mainframe computer for execution.

Call or write today for more details.

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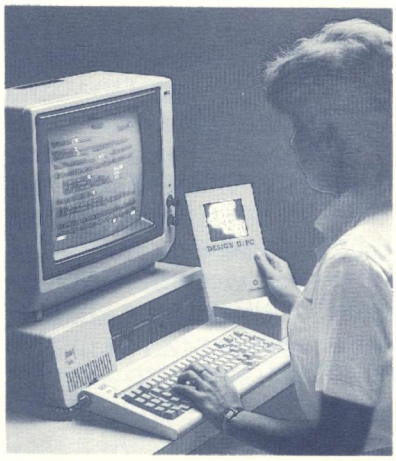
TWX: 910-881-2793

ChemShare Process Systems, Ltd.
Brook House, Church Street
Wilmslow, Cheshire
SK9 1AT
England
Tel: (0625) 532 113
TWX: 666 905



DESIGN II – New and Improved Features

We have been busy adding new capabilities and improving existing capabilities in the DESIGN II program. All of these features are currently available on ChemShare's PRIME 750 computer. They will be generally available in DESIGN II Version 2.0 which is scheduled for release beginning in March, 1985.

NEW	IMPROVED
Crude oil library	FLASH options increased
Depressuring analysis	PHASE MAP - new thermo allowed
Generalized equilibrium reactor	

Details and examples of these features are shown in the following pages. There is a complete set of documentation and/or sample problems for each of these new features which we will be happy to send to you. Please call or telex your sales representative at one of the following locations:

ChemShare Corporation
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311 Wassenaarseweg
2596 CV DEN Haag
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Tel: (07028) 1359
Telex: 33574

Taiwan Goodwinner Co. Ltd.
No. 8, 14 FL No 830 Hsin Yi Rd
Sec. 2, Taipei
Taiwan, Republic of China
Telex: 26875

ChemShare Process Systems, Ltd.
Brook House, Church Street
Wilmslow, Cheshire SK9 1AT
Tel: (0625) 532113
Telex: 666905

Computer Engineering Applications
8th Floor, 14 Queens Road
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D-7000 Stuttgart 80
West Germany
Tel: (0711) 7800495
Telex: 7255697

Soedarpo Service Bureau
J1 Let Jen S Parman 35
Jakarta, Barat
Indonesia
Telex: 45867

Seed H-K Ltd.
7/F Cheung Kong Building
661 Kings Road, North Point
Hong Kong
Telex: 780-60313

CRUDE OIL LIBRARY

ChemShare has implemented a library of crude oil distillations from Leo Aalund's "Guide to World Crudes" (*Oil and Gas Journal*). The following crudes were selected because sufficient TBP data was available. Others will be added as data becomes available.

To use these crudes, simply enter the FEED STOCK command in the CRUDE feed section of your DESIGN II input file. The following example shows how easy this feature is to use. The assay data which you get automatically from the program is shown for the U.K.-FORTIES feed.

Country-Place (Specific)

ABUDHABI-MURBAN
CEUTA-ZULIA
INDONESIA-ATTAKA, E. KALIMANTAN
IRAN-ARDESHIR
IRAN-DARIUS
IRAN-FEREIDOON BLEND
IRAN-HEAVY (BASRAH)
IRAN-LIGHT (BASRAH)
IRAN-SASSAN
KUWAIT-KUWAIT CRUDE
LATIN-OFICINA
LIBYA-AMNA (HIGH POUR)
LIBYA-BREGA
MALAYSIA-TEMBUNGO
NIGERIA-ESCRAVOS
NIGERIA-FORCADOS BLEND
NIGERIA-LIGHT (BONNY)
NIGERIA-MEDIUM (BONNY)
NIGERIA-PENNINGTON
NIGERIA-QUA IBOE
NORWAY-STATFJORD
QATAR-DUCKHAN
QATAR-MARINE
SAUDI-BERRI
SAUDI-HEAVY
SAUDI-LIGHT
SAUDI-MEDIUM
SAUDI-ZULUF
U.K.-BUCHAN, N. SEA
U.K.-FLOTTAMIX, N. SEA
U.K.-FORTIES
U.K.-MAGNUS, N. SEA
U.K.-NINIANBLEND, N. SEA
U.K.-TARTAN, N. SEA
U.S.A.-N. DAKOTA
U.S.A.-N. SLOPE
U.S.A.-ROCKY MOUNTAIN SWEET
VENEZUELA-LAGOMEDIO

```
AB123.
*CRUDE LIBRARY SAMPLE
MIX1=BLND,1,2,-3
CRUDE
FEE STK1=U.K.-FORTIES
FEE STK2=SAUDI-LIGHT
FEE(BBL/DAY)1=4000
FEE(BBL/DAY)2=6000
TP1=100,14.7
TP2=100,14.7
GEN,COM=62,2,3,4,5,6,7,8,
ESSOTAB,API
END
```

U.K. - FORTIES

GRAVITY DEG API	=	36.600
SULFUR WT %	=	0.28000
POUR POINT F	=	30.000
C4 & LIGHTER VOL%	=	3.8000
V, PPM	=	3.0000
NI PPM	=	2.0000
CAR.RESIDUE(CCR), WT %	=	2.2000
VISCOSITY SUS @ 100 F	=	40.700

PRODUCT NAME	TEMP F	YIELD VOL %	API	SULFUR WT %
LIGHT NAPHTHA	60- 167	6.7	79.8	0.001
HEAVY NAPHTHA	167- 347	18.3	54.8	0.001
KEROSENE	347- 482	12.9	41.8	0.016
LIGHT GAS OIL	482- 662	18.8	33.6	0.160
HEAVY GAS OIL	622- 977	23.7	25.8	0.410
RESIDUAL OIL	977+	15.8	14.3	0.780

SUPPLEMENTAL DATA FOR PRODUCTS

LIGHT NAPHTHA

PARAFFINS, VOL %	=	81.000
NAPHTHENES, VOL %	=	0.00000
AROMATICS, VOL %	=	2.0000
RON, CLEAR	=	74.000
RON + 3ML TEL	=	91.000

HEAVY NAPHTHA

PARAFFINS, VOL %	=	47.500
NAPHTHENES, VOL %	=	38.500
AROMATICS, VOL %	=	14.000
RON, CLEAR	=	51.000
RON [redacted] 3ML TEL	=	74.500
CHARACTERIZATION	=	11.800
ANILINE POINT, F	=	129.00

KEROSENE

SMOKE POINT, MM	=	20.000
FREEZE POINT, F	=	-44.000
ANILINE POINT, F	=	134.00
DIESEL INDEX	=	56.000
POUR POINT F	=	-60.000

LIGHT GAS OIL

CETANE INDEX	=	52.000
DIESEL INDEX	=	53.000
POUR POINT F	=	10.000
VISCOSITY SUS @ 100 F	=	39.800

HEAVY GAS OIL

NITROGEN(TOTAL) PPM	=	700.00
VANADIUM PPM	=	0.10000E 00
NICKEL, PPM	=	0.10000E 00
ANILINE POINT, F	=	186.00
POUR POINT F	=	95.000
VISCOSITY SUS @ 210 F	=	44.900

RESIDUAL OIL

CON CARBON, WT %	=	12.500
VANADIUM PPM	=	20.000
NICKEL, PPM	=	10.000
VISCOSITY SUS @ 210 F	=	850.00

CRUDE ASSAY 1 FEED 1

STREAM PROPERTIES

DEG API	=	36.60
SULFUR WT PCT	=	0.28

STREAM ASTM DATA		STREAM API DATA	
VOL PCT	ASTM F	VOL PCT	API
0.0	60.0	0.0	86.5
3.3	113.5	3.3	79.8
15.8	257.0	15.8	54.8
31.4	414.5	31.4	41.8
47.3	572.0	47.3	33.6
68.5	799.5	68.5	25.8
100.0	1197.7	100.0	3.1

STREAM PHYSICAL PROPERTIES

MID VOL	=	3.35	15.85	31.45	47.30	68.55
SULFUR WT PCT	=	0.00	0.00	0.02	0.16	0.41

CRUDE ASSAY 1 FEED 1 (CONTINUED)

VOL PCT	API	TBP F	ASTM F
0.0	86.50	-14.*	60.
3.3	79.80	67.*	113.
15.8	54.80	240.*	257.
31.4	41.80	425.*	414.
47.3	33.60	565.*	572.
68.5	25.80	813.*	799.
100.0	3.11	1382.*	1198.

* = AN EXTRAPOLATIVE VALUE

DETAILED FEED COMPONENT ANALYSIS OF FEED NO. 1 FEED 1

NO	COMPONENTS	CUM VOL	K WATSON	MOL WT.	API	LBMOL/HR
1	WATER	0.00	8.8	18.02	10.0	0.00
2	METHANE	0.00	19.5	16.04	339.4	0.00
3	ETHANE	0.00	19.4	30.07	265.8	0.00
4	PROPANE	0.00	14.7	44.09	147.5	0.00
5	I-BUTANE	1.44	13.8	58.12	120.0	8.14
6	N-BUTANE	2.97	13.5	58.12	110.8	8.97
7	I-PENTANE	5.07	13.1	72.15	95.1	10.59
8	N-PENTANE	5.54	13.0	72.15	92.8	2.37
9	108 F ABP	7.28	12.2	78.75	76.5	8.77
10	133 F ABP	9.08	12.2	84.20	73.2	8.63
11	158 F ABP	10.89	12.1	89.98	69.9	8.21
12	183 F ABP	12.69	12.1	95.99	66.5	7.83
13	208 F ABP	14.49	12.0	102.23	63.1	7.48
14	233 F ABP	16.37	12.0	108.64	59.7	7.47
15	258 F ABP	18.40	11.9	115.19	56.4	7.72
16	282 F ABP	20.51	11.8	121.87	53.1	7.74
17	307 F ABP	22.62	11.8	129.39	50.4	7.40
18	332 F ABP	24.73	11.8	137.77	48.6	7.02
19	357 F ABP	26.84	11.8	146.98	47.4	6.62
20	382 F ABP	28.95	11.8	156.29	45.8	6.28
21	407 F ABP	31.06	11.9	166.23	44.5	5.95
22	432 F ABP	33.76	11.9	176.67	43.2	7.21
23	457 F ABP	36.59	11.9	187.20	41.6	7.21
24	482 F ABP	39.42	11.9	198.22	40.1	6.86
25	507 F ABP	42.26	11.9	209.81	38.7	6.54
26	532 F ABP	45.09	11.9	222.01	37.5	6.22
27	557 F ABP	47.77	11.9	234.87	36.4	5.61
28	582 F ABP	49.91	11.9	248.19	35.2	4.26
29	607 F ABP	52.04	12.0	262.11	34.2	4.06
30	632 F ABP	54.18	12.0	276.57	33.1	3.87
31	657 F ABP	56.32	12.0	291.57	32.1	3.70
32	682 F ABP	58.46	12.0	307.12	31.1	3.53
33	707 F ABP	60.60	12.0	323.23	30.2	3.38
34	745 F ABP	64.88	12.1	348.44	28.8	6.32
35	795 F ABP	68.94	12.1	383.94	27.0	5.51
36	845 F ABP	71.70	12.1	420.23	24.9	3.47
37	895 F ABP	74.47	12.1	461.05	23.5	3.19
38	945 F ABP	77.23	12.1	502.60	21.9	2.96
39	995 F ABP	79.99	12.2	545.23	20.2	2.75
40	1070 F ABP	85.52	12.1	610.28	17.6	5.01
41	1170 F ABP	91.04	12.1	696.30	14.0	4.50
42	1270 F ABP	96.57	12.0	776.97	10.0	4.15
43	1370 F ABP	100.00	11.9	850.68	6.2	2.41
			12.1	214.49	35.8	229.91

	COMPONENT	LBMOL/HR	LB/HR	BBL/DAY
1	WATER	0.00000	0.00000	0.00000
2	METHANE	0.00000	0.00000	0.00000
3	ETHANE	0.00000	0.00000	0.00000
4	PROPANE	0.00000	0.00000	0.00000
5	I-BUTANE	8.1366	472.90	57.660
6	N-BUTANE	8.9747	521.61	61.288
7	I-PENTANE	10.588	763.88	83.941
8	N-PENTANE	2.3718	171.11	18.613
9	108 F ABP	8.7731	690.89	69.691
10	133 F ABP	8.6312	726.76	72.144
11	158 F ABP	8.2118	738.91	72.144
12	183 F ABP	7.8284	751.48	72.144
13	208 F ABP	7.4780	764.48	72.144
14	233 F ABP	7.4665	811.16	75.192
15	258 F ABP	7.7218	889.46	81.048
16	282 F ABP	7.7408	943.36	84.425
17	307 F ABP	7.3954	956.93	84.425
18	332 F ABP	7.0154	966.50	84.425
19	357 F ABP	6.6201	973.01	84.425
20	382 F ABP	6.2819	981.77	84.425
21	407 F ABP	5.9512	989.27	84.425
22	432 F ABP	7.2135	1274.4	107.96
23	457 F ABP	7.2062	1349.0	113.24
24	482 F ABP	6.8650	1360.8	113.24
25	507 F ABP	6.5382	1371.8	113.24
26	532 F ABP	6.2248	1382.0	113.24
27	557 F ABP	5.6073	1317.0	107.20
28	582 F ABP	4.2633	1058.1	85.550
29	607 F ABP	4.0627	1064.9	85.549
30	632 F ABP	3.8745	1071.6	85.550
31	657 F ABP	3.6979	1078.2	85.549
32	682 F ABP	3.5320	1084.7	85.550
33	707 F ABP	3.3759	1091.2	85.549
34	745 F ABP	6.3181	2201.5	171.10
35	795 F ABP	5.5095	2115.3	162.55
36	845 F ABP	3.4675	1457.1	110.52
37	895 F ABP	3.1888	1470.2	110.52
38	945 F ABP	2.9560	1485.7	110.52
39	995 F ABP	2.7549	1502.1	110.52
40	1070 F ABP	5.0089	3056.8	221.05
41	1170 F ABP	4.5011	3134.1	221.05
42	1270 F ABP	4.1451	3220.6	221.05
43	1370 F ABP	2.4149	2054.3	137.18
44	1438 F ABP	0.00000	0.00000	0.00000
		229.91	49315.	4000.1

CRUDE ASSAY 1 FEED 1 (CONTINUED)

COMPONENT PHYSICAL PROPERTIES

	COMPONENT	SULFUR W T PCT
1	WATER	0.0000
2	METHANE	0.0000
3	ETHANE	0.0000
4	PROPANE	0.0000
5	I-BUTANE	0.0000
6	N-BUTANE	0.0000
7	I-PENTANE	0.0000
8	N-PENTANE	0.0000
9	108 F ABP	0.7153E-03
10	133 F ABP	0.7153E-03
11	158 F ABP	0.7153E-03
12	183 F ABP	0.7153E-03
13	208 F ABP	0.7153E-03
14	233 F ABP	0.7153E-03
15	258 F ABP	0.9612E-03
16	282 F ABP	0.1420E-02
17	307 F ABP	0.2094E-02
18	332 F ABP	0.3061E-02
19	357 F ABP	0.4433E-02
20	382 F ABP	0.6362E-02
21	407 F ABP	0.9046E-02
22	432 F ABP	0.1336E-01
23	457 F ABP	0.2061E-01
24	482 F ABP	0.3160E-01
25	507 F ABP	0.4767E-01
26	532 F ABP	0.7072E-01
27	557 F ABP	0.1022
28	582 F ABP	0.1225
29	607 F ABP	0.1347
30	632 F ABP	0.1480
31	657 F ABP	0.1628
32	682 F ABP	0.1789
33	707 F ABP	0.1967
34	745 F ABP	0.2267
35	795 F ABP	0.2727
36	845 F ABP	0.3172
37	895 F ABP	0.3585
38	945 F ABP	0.4051
39	995 F ABP	0.4579
40	1070 F ABP	0.5501
41	1170 F ABP	0.7026
42	1270 F ABP	0.8974
43	1370 F ABP	1.094
44	1438 F ABP	1.650
		0.2800

DEPRESSURING ANALYSIS

Depressuring systems are used extensively in process plants for protecting vessels from overpressure. There are many causes for overpressuring, such as external fire, exothermic reactions, loss of power, inadequate cooling, and blocked lines. Depressuring systems are needed to prevent equipment from rupturing and to provide safety for plant personnel. API RP-520 recommends that vessel pressure should be reduced to 100 PSIG or 50% of design pressure, whichever is lower, in 15 minutes.

This depressuring analysis is based on a vessel which is exposed to an external fire. The program calculates the pressure buildup in the closed vessel until the pressure reaches the set pressure of the valve. The conditions during the blowdown period after the opening of the depressuring valve are also calculated. The blowdown period is divided into several intervals with important variables reported for each time interval.

Three assumptions are made for the depressuring analysis:

1. Flow to vessel is stopped (i.e. no fresh feed).

2. The heat involved is provided externally either at a constant rate (ΔQ = constant Btu/time period) or as a function of wetted surface area ($\Delta Q = 21000 \times F \times AW^{.82}$)
   where F is an environmental factor (recommended by API RP-520)
   AW is wetted surface area.

3. The vapor flow through the valve is either a choking flow or subsonic flow due to sufficiently large back pressure.

The depressuring module should be coded with one inlet and one outlet stream. There is only one required command for the module:

CROss sectional area of valve (L units) =	Enter the cross-sectional area for the valve.

You have two choices for entering the heat involved in the depressuring analysis: heat added at a constant rate or heat as a function of wetted surface area.

HEAT absorbed (H units/t units) =	Enter the constant rate of external heat which will be applied to the vessel.
or	
DIAmeter (L units) =	Enter the diameter of the vessel.
and	
HORizontal **VER**tical **SPH**erical	Enter one of the vessel configurations for calculation of wetted surface area. Default is VERtical.

You can use any of the following optional commands.

ENVironment factors =	Enter an environmental factor for type of installation. Default is 1. See TABLE 1 for typical values.
REDuced pressure (P units) =	Enter the reduced pressure. Default is 100 PSIG or 50% of operating pressure, whichever is *lower*.
BACk pressure (P units) =	Enter a value if a sub-sonic flow condition is desired (non-choking flowrate). If the back pressure is higher than critical-flow pressure, the resulting vapor flowrate will be lower. Default is 14.696 PSIA.
SET pressure (P units) =	Enter the pressure at which the valve is to open. Default for set pressure is 10% above operating pressure.
COEfficient of discharge =	Enter manufacturer's specification. Default is 1.0.

The composition of the vessel contents is determined from the inlet stream. The default volume for the vapor and liquid phases in the vessel is the rate of the inlet stream. If the depressuring analysis will be calculated with heat as a function of wetted surface area, you can enter commands which will cause the program to adjust the rate of the vapor and liquid portions of the stream (using inlet compositions). Enter the following commands:

LENgth (L units) =	Enter the length of the vessel for horizontal or vertical vessel configuration.
LIQuid **HEI**ght (L units) =	Enter the height of the liquid from the bottom of the vessel.

Method of Calculation

The temperature and pressure of the inlet stream are assumed to be the operating conditions of the vessel. A flash is performed to determine vapor and liquid compositions and initial flow rates.

For calculations performed using heat as a function of wetted surface area, length for a cylindrical vessel, if not entered, is determined from the initial volume of vapor and liquid and the given diameter. If the vessel is spherical, the diameter is calculated using the initial volume of contents. The calculated diameter is checked against the input diameter. If there is a discrepancy, the calculated diameter will be used in the depressuring analysis. If you enter LENgth and LIQuid HEIght commands, the liquid and vapor rates are adjusted (using inlet compositions) until the vessel is full.

Once the contents and size of the vessel are known, the depressuring analysis begins. The pressure build-up in the closed vessel due to the external heat source is calculated until the set pressure of the valve is reached. The conditions of the blowdown period are then calculated until the reduced pressure or back pressure is reached. A table of results for the depressuring analysis will be printed in the "NOW CALLING" section of the output. The outlet stream composition and flow rate will be identical to the inlet stream.

TABLE 1. Environment Factors

Type of Installation

	Factor F
1. Bare vessel	1.0
2. Insulated vessels (arbitrary insulation conductance values are shown as examples and are in BTU/HR/FT2/° F):	
a. 4.0	0.3
b. 2.0	0.15
c. 1.0	0.075
3. Water-application facilities, on bare vessel	1.0
4. Depressurizing and emptying facilities	1.0
5. Underground storage	0.0
6. Earth-covered storage, above grade (from American Petroleum Institute RP-520, Page 11)	0.03

Coding:

```
NN999.
*DEPRESSURE V101
DEP1=V101,1,-2
VERT
CRO(IN2)=2.7648
SET PRE=650
BACK PRE=25
DIA(FT)=13
REDUCED PRE=200
GEN,COM=46,2,3,4
FLO(FRA)1= .05, .4, .325, .225
TOT FLO 1= 1749.645
TP1=-35,610
APISOAVEH,APISOAVEK,
END
```

Results from this sample input are shown below.

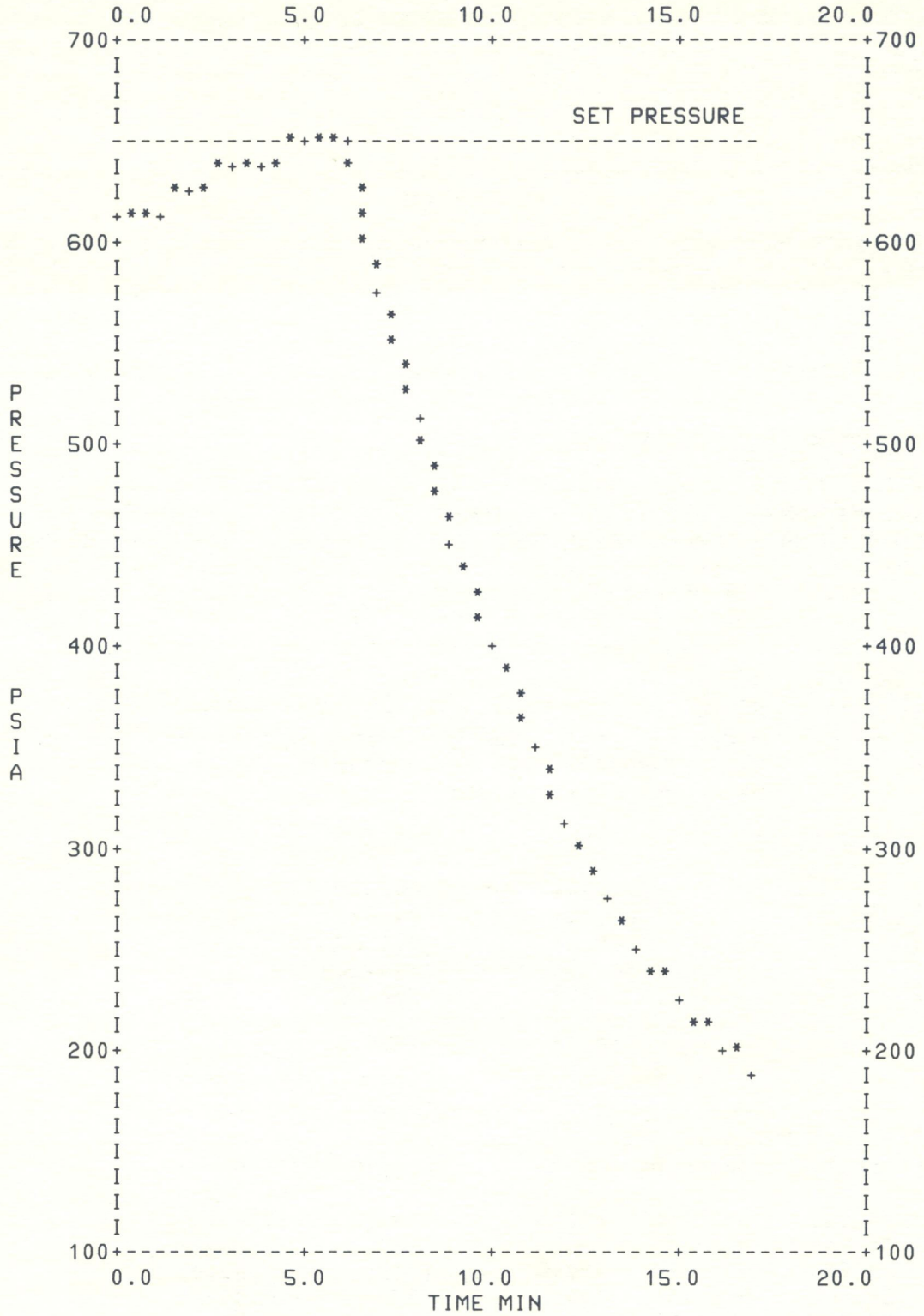
```
NOW CALLING EQUIPMENT   1  + DEP     (DEPS) +
ASOA KVALUES  ASOA ENTHALPY  ASOA DENSITY

VERTICAL     VESSEL FOR DEPRESSURING SYSTEM,
                    RADIUS =          6.5000    FT
                    LENGTH =          29.524    FT

INITIAL CONDITION: TEMPERATURE  = -35.000    F
                   PRESSURE  =     610.00    PSIA
                   MOLES  =        1749.6    LBMOL/HR
                   SET PRESSURE =  650.00    PSIA
                   BACK PRESSURE=  25.000    PSIA

  INITIAL COMPOSITION       VAPOR          LIQUID
  LBMOL/HR
  ------- -----------     ------------   ------------
  NITROGEN                  60.441         27.041
  METHANE                   289.21         410.65
  ETHANE                    58.134         510.50
  PROPANE                   11.305         382.36
                          --------------  --------------
                            419.09         1330.6


                    DEPRESSURING ANALYSIS TABLE
                    ------------ -------- -----
 TIME  TEMPERATURE  PRESSURE  VAPOR       LIQUID       VENT
  MIN
  1.00   -33.291    617.136   422.9       1327.      0.0000
  2.00   -31.585    624.302   426.8       1323.      0.0000
  3.00   -29.883    631.493   430.6       1319.      0.0000
  4.00   -28.184    638.714   434.5       1315.      0.0000
  5.00   -26.489    645.962   438.5       1311.      0.0000
  6.00   -24.798    653.236   442.4       1307.      0.0000
  7.00   -28.037    580.073   519.7       1230.       122.2
  8.00   -31.237    513.401   464.7       1163.       110.9
  9.00   -34.402    452.636   413.0       1103.       96.60
 10.00   -37.323    399.900   367.1       1053.       84.06
 11.00   -40.017    354.007   327.0       1009.       73.85
 12.00   -42.491    314.066   291.6       970.3       65.03
 13.00   -44.693    279.849   260.0       936.9       56.46
 14.00   -46.676    250.128   233.2       907.2       50.06
 15.00   -48.474    224.194   209.7       880.7       44.51
 16.00   -50.091    201.566   189.0       856.9       39.68
 17.00   -51.537    181.818   170.9       835.3       35.48
```



References

1. API Recommended Practice 520, "Recommended Practice for the Design and Installation of Pressure-Relieving Systems in Refineries, Part I-Design", 4th Ed., American Petroleum Institute, Washington, D.C., 1976.
2. API Recommended Practice 521, "Guide for Pressure Relief and Depressuring Systems", 1st Ed., American Petroleum Institute, Washington, D.C., 1969.

GENERALIZED EQUILIBRIUM REACTOR

This generalized equilibrium reactor module calculates gas-phase reactions of multi-component systems. Chemical equilibrium can be calculated isothermally or adiabatically. Isothermal calculations are the default. This module is not restricted to a specific type of reaction as is the REActor module which can model CO Shift, methanation, methanol and ammonia synthesis, and primary and secondary reformer reactions only. Heat and entropy of formation data at 25 °C are required for all components. This data is available automatically for the first 98 components in the **PURE COMPONENT DATA BASE**.

To enter this data for other components, simply enter the following commands in the GENeral section of your input file:

HEAt of **FOR**mation (H units/molar Q unit)i =

ENTropy of **FOR**mation (H units/molar Q units/T units)i =

where i is the component ID number.

For ENTropy of FORmation, the allowable units are as follows:

BTU/LBMOL/R (default)
KCAL/KGMOL/K
CAL/GMOL/K
J/GMOL/K

For example,

```
GEN,COM=2,49,48,62,1021
ENT FOR (BTU/LBMOL/R) 1021 = -30.9907
HEA FOR (BTU/LBMOL) 1021 = -86544
```

You can enter product constraints or stoichiometric coefficients for reactions occurring at conditions away from equilibrium such that extent of reaction or temperature approach specification can be used. Since these are gas-phase reactions, one of the following equation of state techniques should be used:

APISOAVEK	LKPK*
BWRK	PENK
BWRSK	RKK

*Leo-Kesler-Ploecker equation. See Thermodynamics section of this newsletter.

The following commands are used to enter general reaction information:

GUEssed products (Q units/t units) =	Enter product flows for each component in the same order as they appear in the COMponents list.
INErt =	Enter the ID numbers of the components which are not involved in the reaction(s). These components must be completely inert.
PROduct constraint (molar Q units/t units)i =	Enter the flow of component i in the product stream, where i is the component ID number. This sets the maximum amount of component i allowed in the product.
TEMperature **APP**roach (T units) =	Enter the approach to equilibrium temperature for all reactions in this module.

The GUEssed product and INERT commands have the effect of speeding up calculations.

Reaction j =	Enter the stoichiometric coefficients for reactants, component ID numbers for reactants, stoichiometric coefficients for products, and component ID numbers for products for reaction j, where j is the reaction number (multiple reactions are allowed per EQUilibrium REActor module).
EXTent of reaction j =	Enter the percent completion of reaction j, where j is the reaction number.
TEMperature approach for **REA**ction j (T units) =	Enter the approach to equilibrium temperature for reaction j, where j is the reaction number.

To use either the EXTent of reaction or TEMperature approach for REAction commands, you must enter a Reaction command. This command is of the form:

Rj = (a1*r1 + a2*r2 + ... = b1*p1 + b2*p2 + ...)

where a1,a2 are the stoichiometric coefficients for the reactants,
r1,r2 are the component ID numbers for the reactants,
b1,b2 are the stoichiometric coefficients for the products,
p1,p2 are the component ID numbers for the products,
and j is the reaction number.

The stoichiometric coefficients are entered on a molar basis. Fractions are allowed. For the following reaction,

CH4 + H2O — -> CO + 3H2

you would enter the following Reaction command:

R1 =(1*2 + 1*62 = 1*48 + 3*1)

Note: Although reactions are described with stoichiometric coefficients on a molar basis, the reactions are not necessarily equi-molar. Reactions will always be in mass balance.

No specifications are required for the generalized equilibrium reaction module other than heat and energy of formation date at 25 °C for all components. Several example problems are shown below:

Example 1. Using product constraint.

```
NN999.
*METHANATOR
EQU REA1 = C1FM, 1, -2, -3
C-PRODUCT CONSTRAINT FOR METHANE
PRO  CON2 = 1.514
GEN, COM = 2,  49,  48,  1,  62,  46
FLO1 = 15,  14,  0,  0,  2,  84.07,  59
TP(K)1 = 1066.67,  179.12
BWRK
END
```

Example 2. Using extent of reaction.

```
AB123.
*NITROGEN IS AN INERT
EQU REA10 = C1FM,  1,  -2,  -3
EXT2=13.8
R1=(1*2 + 1*62 = 1*48 + 3*1)
R2=(1*48 + 1*62 = 1*49 + 1*1)
INERT=46
GEN,COM=2, 49, 48, 1, 62, 46
FLO1=15, 14, 0, 0, .2, 84.07, .59
TP(K)1=1066.7, 179.12
APISOAVEK
END
```

Example 3. Using temperature approach for reaction 1.

```
NN999.
*ADIABATIC REACTION
EQU REACTOR 7=ADIA, 1,-2,-3,  ADIABATIC
TEM REA1 = 45
R1=(1*2 + 1*62 = 1*48 + 3*1)
R2=(1*48 + 1*62 = 1*49 +1*1)
GEN, COM=2,49,48,1,62,46
FLO1=15.14,0,0,.2,84.07
TP(K)1=1066.67,179.12
PENK,PENH,BIN PAR=PENG1
END
```

Example 4. Multi-component system at equilibrium.

```
AB123.
*THE BIG REACTOR
EQU REA 75=BIG,1, -2
GUESSED PRODUCTS=2,20,10,10,3*5,3*10,15
GENERAL
COM=1, 2, 3, 4, 5, 6, 7, 49, 48, 62, 47
FLO1=2, 20, 10, 10, 5, 5, 10, 10, 15
TP1=600,100
LKPK,LKPH
END
```

Improvements

GENERALIZED FLASH ALGORITHM

ChemShare has incorporated the flash algorithm used for the MULtiFLAsh module in the regular FLAsh (phase separation) module. This allows you to request phase separation in addition to the following pairs of calculation options:

TEMperature **OUT**(T units) =	Enter the outlet temperature for the flash.
PREssure **OUT**(P units) =	Enter the outlet pressure for the flash.
ADIabatic	Specifies an adiabatic (constant enthalpy) calculation.
ISOthermal	Specifies an isothermal calculation using the multiflash algorithm rather than the default FLAsh calculation.
HEAt(Q units/t units) =	Enter the amount of heat added to (positive value) or removed from (negative value) the calculation.
ISEntropic	Specifies an isentropic calculation.
BUBble point	Requests calculation of bubble point temperature or pressure. Default is temperature.
DEW point	Requests calculation of dew point temperature or pressure. Default is temperature.
LIQuid **FRA**ction (MOLar/MASs) =	Enter the fraction of liquid desired in the outlet stream. Options are MOLar or MASs. Default is MOLar.
LIQuid	Specifies that all components go to the liquid phase.
VAPor	Specifies that all components go to the vapor phase.

One inlet stream and up to three outlet streams are allowed.

Example. Set temperature and pressure for flash calculation.

```
AB123.
*FLASH
FLA1 = SEP, 1, -2, -3, VERTICAL
TEM OUT =120, PRE OUT  =380
GEN, COM=2,3,4,5,6,7,8,10,12,100
AMB100= 350, API100=36, AMW100=210
FLO1=1000, 750, 400, 275, 200, 76, 87, 50, 62, 400
TP1=100, 350
END
```

PHASE MAP MODIFICATION

The capabilities of the PHAse MAP module have been extended to include

- use of SOAVE, APISOAVE or PENg-Robinson equations of state with or without interaction parameters (e.g. BINPAR = PENG1).
- No limit on the number of components (previously the maximum number was 30).

In addition, the calculation algorithm has been modified to provide faster convergence while maintaining accuracy.

Thermodynamics

The Lee-Kesler-Ploecker equation of state for calculating K-values, enthalpies and densities has been added to DESIGN II. This correlation includes the Lee-Kesler modification of the BWR equation for thermodynamic properties of normal fluids as applied to mixtures. Vapor-liquid equilibria at high pressures are calculated using a one-fluid theory with a new mixing rule for the pseudo-critical temperature. This mixing rule appears to be applicable for mixtures whose components differ appreciably in molecular size, such as synthesis gas from coal or heavy petroleum feedstocks. Binary constants calculated by Ploecker, Knapp and Prausnitz for a large number of binary pairs containing light gases are included. See Table 1 for an alphabetical list of the binary pairs for which a binary constant is included.

TABLE 1

Component ID No.	Name 1st Component	Component ID No.	Name 2nd Component
65	ACETYLENE	22	ETHYLENE
63	AMMONIA	1171	ARGON
		46	NITROGEN
		62	WATER

TABLE 1 (CONTINUED)

Component ID No.	Name 1st Component	Component ID No.	Name 2nd Component
1171	ARGON	63	AMMONIA
		2	METHANE
		46	NITROGEN
		47	OXYGEN
40	BENZENE	6	n-BUTANE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		3	ETHANE
		22	ETHYLENE
		11	n-HEPTANE
		10	n-HEXANE
		2	METHANE
		13	n-NONANE
		82	i-OCTANE
		12	n-OCTANE
		8	n-PENTANE
		4	PROPANE
28	1,3-BUTADIENE	6	n-BUTANE
		24	1-BUTENE
5	i-BUTANE	6	n-BUTANE
		49	CARBON DIOXIDE
		3	ETHANE
		50	HYDROGEN SULFIDE
		2	METHANE
		46	NITROGEN
		4	PROPANE
		23	PROPYLENE
6	n-BUTANE	40	BENZENE
		28	1,3-BUTADIENE
		5	i-BUTANE
		27	1-BUTENE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		3	ETHANE
		22	ETHYLENE
		11	n-HEPTANE
		10	n-HEXANE
		1	HYDROGEN
		2	METHANE
		46	NITROGEN
		13	n-NONANE
		12	n-OCTANE
		7	i-PENTANE
		8	n-PENTANE
		4	PROPANE
		23	PROPYLENE
27	i-BUTENE	28	1,3-BUTADIENE
		49	CARBON DIOXIDE
		23	PROPYLENE

TABLE 1 (CONTINUED)

Component ID No.	Name 1st Component	Component ID No.	Name 2nd Component
49	CARBON DIOXIDE	40	BENZENE
		5	i-BUTANE
		6	n-BUTANE
		27	1-BUTENE
		38	CYCLOHEXANE
		14	n-DECANE
		3047	DIFLUOROMETHANE
		3	ETHANE
		1005	ETHYL ETHER
		1176	FREON 12
		11	n-HEPTANE
		10	n-HEXANE
		1	HYDROGEN
		50	HYDROGEN SULFIDE
		2	METHANE
		1021	METHANOL
		39	METHYLCYCLOHEXANE
		46	NITROGEN
		1043	NITROUS OXIDE
		13	n-NONANE
		12	n-OCTANE
		7	i-PENTANE
		8	n-PENTANE
		4	PROPANE
		23	PROPYLENE
		41	TOLUENE
		62	WATER
		43	m-XYLENE
48	CARBON MONOXIDE	1	HYDROGEN
		50	HYDROGEN SULFIDE
		2	METHANE
		46	NITROGEN
1036	m-CRESOL	2	METHANE
1122	CHLOROPENTAFLUOROETHANE	1154	FREON 22
1155	CHLOROTRIFLUORMETHANE	1114	FLUOROFORM
		1176	DICHLORODIFLUORO-METHANE
38	CYCLOHEXANE	40	BENZENE
		6	n-BUTANE
		49	CARBON DIOXIDE
		7043	CYCLOHEXENE
		14	n-DECANE
		1028	1,2-DICHLOROETHANE
		3	ETHANE
		11	n-HEPTANE
		10	n-HEXANE
		2	METHANE
		13	n-NONANE
		12	n-OCTANE
		8	n-PENTANE
		4	PROPANE

TABLE 1 (CONTINUED)

Component ID No.	Name 1st Component	Component ID No.	Name 2nd Component
7043	CYCLOHEXENE	38	CYCLOHEXANE
		1028	1,2-DICHLOROETHANE
12	DECANE	40	BENZENE
		6	n-BUTANE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		3	ETHANE
		11	n-HEPTANE
		10	n-HEXANE
		50	HYDROGEN SULFIDE
		2	METHANE
		46	NITROGEN
		13	n-NONANE
		12	n-OCTANE
		8	n-PENTANE
		4	PROPANE
1176	DICHLOROFIFLUOROMETHANE	1155	CHLOROTRIFLUORO-METHANE
		1154	FREON 22
1028	1,2-DICHLOROETHANE	38	CYCLOHEXANE
		7043	CYCLOHEXENE
3047	DIFLUOROMETHANE	49	CARBON DIOXIDE
54	2,2-DIMETHYLBUTANE	3004	1-PENTANOL
55	2,3-DIMETHYLBUTANE	3004	1-PENTANOL
4178	DIPHENYLMETHANE	2	METHANE
3	ETHANE	40	BENZENE
		5	i-BUTANE
		6	n-BUTANE
		49	CARBON DIOXIDE
		48	CARBON DIOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		22	ETHYLENE
		11	n-HEPTANE
		10	n-HEXANE
		1	HYDROGEN
		50	HYDROGEN SULFIDE
		2	METHANE
		1021	METHANOL
		46	NITROGEN
		13	n-NONANE
		12	n-OCTANE
		7	i-PENTANE
		8	n-PENTANE
		4	PROPANE
		23	PROPYLENE

TABLE 1 (CONTINUED)

Component ID No.	Name 1st Component	Component ID No.	Name 2nd Component
1012	ETHANOL	4	PROPANE
22	ETHYLENE	65	ACETYLENE
		40	BENZENE
		6	n-BUTANE
		3	ETHANE
		11	n-HEPTANE
		1	HYDROGEN
		2	METHANE
		46	NITROGEN
1005	ETHYL ETHER	49	CARBON DIOXIDE
1114	FLUOROFORM	1155	CHLOROTRIFLUORO-METHANE
		1052	TETRAFLUORO-METHANE
1176	FREON 12	49	CARBON DIOXIDE
1154	FREON 22	1176	DICHLORODIFLUORO-METHANE
		1122	CHLOROPENTAFLUORO-ETHANE
11	n-HEPTANE	40	BENZENE
		6	n-BUTANE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		3	ETHANE
		22	ETHYLENE
		10	n-HEXANE
		1	HYDROGEN
		2	METHANE
		13	n-NONANE
		82	i-OCTANE
		12	n-OCTANE
		8	n-PENTANE
		4	PROPANE
10	n-HEXANE	40	BENZENE
		6	n-BUTANE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		3	ETHANE
		11	n-HEPTANE
		1	HYDROGEN
		2	METHANE
		46	NITROGEN
		13	n-NONANE
		12	n-OCTANE
		8	n-PENTANE
		3004	1-PENTANOL
		3005	t-PENTANOL
		4	PROPANE

TABLE 1 (CONTINUED)

Component ID No.	Name 1st Component	Component ID No.	Name 2nd Component
1	HYDROGEN	6	n-BUTANE
		49	CARBON DIOXIDE
		48	CARBON MONOXIDE
		3	ETHANE
		22	ETHYLENE
		11	n-HEPTANE
		10	n-HEXANE
		2	METHANE
		3175	METHYLNAPHTHALENE
		46	NITROGEN
		8	n-PENTANE
		4	PROPANE
		23	PROPYLENE
		3147	TETRALIN
		41	TOLUENE
50	HYDROGEN SULFIDE	5	i-BUTANE
		49	CARBON DIOXIDE
		48	CARBON MONOXIDE
		11	n-HEPTANE
		39	METHYLCYCLOHEXANE
		46	NITROGEN
		8	n-PENTANE
		41	TOLUENE
		43	m-XYLENE
1174	KRYPTON	47	OXYGEN
2	METHANE	1171	ARGON
		40	BENZENE
		5	i-BUTANE
		6	n-BUTANE
		49	CARBON DIOXIDE
		48	CARBON MONOXIDE
		1036	m-CRESOL
		38	CYCLOHEXANE
		14	n-DECANE
		4178	DIPHENYLMETHANE
		3	ETHANE
		22	ETHYLENE
		11	n-HEPTANE
		10	n-HEXANE
		1	HYDROGEN
		3175	1-METHYL-NAPHTHALENE
		46	NITROGEN
		1043	NITROUS OXIDE
		13	n-NONANE
		12	n-OCTANE
		7	i-PENTANE
		8	n-PENTANE
		4	PROPANE
		23	PROPYLENE
		3147	TETRALIN
		41	TOLUENE
		43	m-XYLENE

TABLE 1 (CONTINUED)

Component ID No.	Name 1st Component	Component ID No.	Name 2nd Component
1021	METHANOL	49	CARBON DIOXIDE
		62	WATER
39	METHYLCYCLOHEXANE	49	CARBON DIOXIDE
		50	HYDROGEN SULFIDE
3175	1-METHYL NAPHTHALENE	1	HYDROGEN
		2	METHANE
52	2-METHYLPENTANE	3004	1-PENTANOL
53	3-METHYLPENTANE	3004	1-PENTANOL
46	NITROGEN	63	AMMONIA
		1171	ARGON
		40	BENZENE
		5	i-BUTANE
		6	n-BUTANE
		49	CARBON DIOXIDE
		48	CARBON MONOXIDE
		3	ETHANE
		22	ETHYLENE
		1176	FREON 22
		10	n-HEXANE
		1	HYDROGEN
		50	HYDROGEN SULFIDE
		2	METHANE
		1043	NITROUS OXIDE
		47	OXYGEN
		7	i-PENTANE
		8	n-PENTANE
		4	PROPANE
		23	PROPYLENE
1043	NITROUS OXIDE	2	METHANE
		46	NITROGEN
		47	OXYGEN
13	n-NONANE	40	BENZENE
		6	n-BUTANE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		3	ETHANE
		11	n-HEPTANE
		10	n-HEXANE
		2	METHANE
		12	n-OCTANE
		8	n-PENTANE
		4	PROPANE

TABLE 1 (CONTINUED)

Component ID No.	Name 1st Component	Component ID No.	Name 2nd Component
82	i-OCTANE	40	BENZENE
		11	n-HEPTANE
12	n-OCTANE	40	BENZENE
		6	n-BUTANE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		3	ETHANE
		11	n-HEPTANE
		10	n-HEXANE
		2	METHANE
		13	n-NONANE
		8	n-PENTANE
		4	PROPANE
47	OXYGEN	1171	ARGON
		1174	KRYPTON
		46	NITROGEN
		1043	NITROUS OXIDE
7	i-PENTANE	6	n-BUTANE
		49	CARBON DIOXIDE
		3	ETHANE
		2	METHANE
		46	NITROGEN
		8	n-PENTANE
		4	PROPANE
8	n-PENTANE	40	BENZENE
		6	n-BUTANE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		3	ETHANE
		11	n-HEPTANE
		10	n-HEXANE
		1	HYDROGEN
		50	HYDROGEN SULFIDE
		2	METHANE
		46	NITROGEN
		13	n-NONANE
		12	n-OCTANE
		7	i-PENTANE
		4	PROPANE

TABLE 1 (CONTINUED)

Component ID No.	Name 1st Component	Component ID No.	Name 2nd Component
3004	1-PENTANOL	10	n-HEXANE
		54	2,2-DIMETHYU-BUTANE
		55	2,3-DIMETHYL-BUTANE
		52	2-METHYLPENTANE
		53	3-METHYLPENTANE
3005	t-PENTANOL	10	n-HEXANE
4	PROPANE	40	BENZENE
		5	i-BUTANE
		6	n-BUTANE
		49	CARBON DIOXIDE
		38	CYCLOHEXANE
		14	n-DECANE
		3	ETHANE
		11	n-HEPTANE
		10	n-HEXANE
		1	HYDROGEN
		2	METHANE
		46	NITROGEN
		13	n-NONANE
		12	n-OCTANE
		7	i-PENTANE
		8	n-PENTANE
		23	PROPYLENE
1019	2-PROPANOL	10	n-HEXANE
23	PROPYLENE	5	i-BUTANE
		6	n-BUTANE
		27	i-BUTENE
		3	ETHANE
		2	METHANE
		46	NITROGEN
		4	PROPANE
3058	TETRACHLOROETHANE	41	TOLUENE
1052	TETRAFLUOROMETHANE	1114	FLUOROFORM
3147	TETRALIN	1	HYDROGEN
		2	METHANE
41	TOLUENE	1	HYDROGEN
		50	HYDROGEN SULFIDE
		2	METHANE
		3058	TETRACHLOROETHANE
62	WATER	63	AMMONIA
		49	CARBON DIOXIDE
		1021	METHANOL
43	M-XYLENE	49	CARBON DIOXIDE
		2	METHANE

General

Improving Process Engineering Productivity with the Use of Flowsheet Simulation Programs

With the gracious permission of the Abu Dhabi National Oil Company, we are reprinting in its entirety, a paper by Fadi Z. Jarjur which was presented at the Gas Processors Association European/ London Chapter held in London on 18 January 1984.

This article describes several areas where flowsheet simulation capabilities can be of benefit to an operating company, whether in daily operations or in feasibility studies and planning. By using computerized flowsheet calculations, 40-75% of the engineering man-hours assigned for daily operations could be reallocated to other essential projects.

Since the time this paper was presented, in-line Fortran capabilities in DESIGN II allow an engineer to integrate his economic (or other calculations) into the flowsheet simulation.

UTILIZING PROCESS ENGINEERING SIMULATION PROGRAMS FOR IMPROVING PROCESS ENGINEERING PRODUCTIVITY

PREPARED BY: FADI Z. JARJUR
ABU DHABI NATIONAL OIL COMPANY
ABU DHABI
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ABSTRACT

The ABU DHABI NATIONAL OIL COMPANY "ADNOC" is the major share holder or the sole owner of most of the oil and gas production, transportation, processing and refining industries within the Emirate of Abu Dhabi. These industries include:

Gas processing plants
Refineries
LNG Plant
Oil fields surface facilities plants
Gas fields surface facilities plants.

The production operations in all these plants and facilities are interrupted by modification, upgrading, expansion, optimization and revamping. This non steady production pattern is amplified by the continually fluctuating market demands. This environment prompted the engineer for more alert and close monitoring operations. The ChemShare Process Engineering Computer Simulator was acquired in 1979. This simulator helped the engineers to do this close monitoring more timely, improve their productivity and address any plant operations upset more quickly. This improvement on the productivity resulted in mantime savings which was diverted towards new essential planning and futuristic activities.

1.0 INTRODUCTION

During the period 1972 -1979, the computing power was limited within ADNOC'S Companies. The computer was overloaded with the companies' business applications leaving little computing power for the technical applications. The only Process engineering computer programs available were those that could perform flash calculations with few thermo options and little physical properties data. ADNOC'S investigated and pilot tested some of the available process engineering computer simulation software in the world-market. After comparative analysis in 1979 the decision was made to acquire the ChemShare process engineering computer simulaton software which was closest to meeting the predetermined selection criteria.

Training was provided to acquaint the engineers with the facilities of the software and train them in using it in the different process engineering applications.

Several enhancements to the software were later implemented and its use grew to cover the following applications areas:

Natural Gas Production and Handling

- Natural and associated gas production and field facility operations.
- Gas processing plants.
- Gas liquefaction and cryogenic operations.

Oil Production and Handling

- Oil production and field facilities' operation.
- Crude sweetening and crude stabilization.
- Refinery operation.

Studies and Planning

- Vendors assumptions and proposal verification.
- Production facilities optimization.
- Production planning.

2.0 Natural Gas Production and Handling

ADNOC produces associated and natural gas from its hydrocarbon reservoirs both from the onshore fields and offshore fields.

2.1 Production

Natural gas is produced from gas reservoirs, cap gas and associated gas. ADNOC spared no effort to ensure the maximum utilization of the produced associated gas and to avoid any wastage or flare of this valuable source of energy. For this purpose several gas processing plants and a gas liquefaction plant were constructed.

The cutdown in the crude production rates forced an increase in the production of the cap gas which is not favoured by reservoir engineers. This lead to the decision of developing field facilities for producing the natural gas reservoirs in Abu Dhabi. Figures 1-3 presents the current and future Gas/oil production and handling systems.

Some small gas field facilities already exist and the development of new facilities is on going. These developments go through the normal phases of any project construction:

- Feasibility study
- Process design phase, engineering and equipment design, and procurement
- Construction
- Commissioning and start up

For such projects, in the past, all the phases were contracted out and most of the work, except for the last two phases, were carried out in the contractor's home offices. ADNOC adopted computerization to meet the ADNOC engineers requirements for performing and conducting most of the phases locally. In addition to the process engineering computer simulation software, other software packages were acquired. Some of these software packages covered the disciplines: of reservoir simulation , pipelines fluid flow simulation, pipeline design and laying simulation and pipe stress analysis simulation. The end result has been that ADNOC engineers are now conducting the global feasibility studies starting from the reservoir, moving to the pipelines and covering the surface handling facilities. In addition, they are in a position to analyze the process design and verify both the design and the assumptions made by the contractor. Also this software was useful during the start up of the facilities especially most of the facilities did not start and still not operating at their design capacities.

All of the software acquired meets the technical needs but nevertheless most of them have the folowing shortcomings:

- the economic aspects of projects are not covered.
- they require special input data preparation for each run.
- produce only one format of output that cannot be transferred to other simulators except through a manual interface.
- do not provide one run planning capabilities.

2.2 Gas Processing Plant Operations

Since the acquisition of these computer simulation software packages no new plants have been constructed. Nevertheless, they were acquired just in time for the commissioning of several gas processing plants. Also, they were just the right tools for the engineers to carry out their day to day operations. The process simulation software was used in the commissioning and running operations of the gas plants and also is used for:

- setting up a total plant process model so that at any moment in time they would be able to predict the effect of one or several changes in the plant operation and total plant performance.

- performing production trouble shooting and predicting bottlenecks.

- checking the feasibility of by-passing or modifying the operations of some unit-equipment.

- answering many types of "what-if" questions and their impacts on the plant performance.

The statistics showed that for this work the engineers made a minimum of 40% mantime saving and in some cases the saving reached as high as 75%. The extra mantime saved was diverted to other essential projects, for example, studying the feasibility of total or partial plant expansion, diversifying the feed sources, injecting materials into the process lines, and most important gave the engineers a better insight into the total plant operation and enhanced the back up capability of the engineers to each other.

2.3 Gas Liquefaction/Cryogenic Operations

The process simulation software is frequently used for refrigerant requirements, and compression power requirement calculations for both multi-component and single component refrigerant systems. Lately these requirements are not readily predicted because of the continuous variation in both the feed flowrates and composition. In this area, engineers saved a sizable amount of mantime and are able to rigorously simulate the total refrigeration cycles including the refrigeration towers, which cannot be done manually. In this area, the engineers have to make some assumptions because the system currently predicts the same outlet temperature for the tube side streams in the LNG chiller module. An important and not available facility, which is to exit from the program to perform economic calculations and re-enter it again for optimizing the operation, would have been a definite advantage.

3.0 OIL PRODUCTION AND HANDLING

ADNOC produces oil from both its onshore and offshore fields. Currently the situation is that the market demands are not steady and the oil production profile keeps fluctuating. The production/process engineers are confronted with many types of questions that require hard and long working hours to answer. Very often, some of these questions would have become a project that requires a task force to answer if it were not for the available computer aided simulation tools. These tools (mainly the process engineering and fluid flow simulators) are used to evaluate the effect of the oil production fluctuations on the gas rates and qualities, on the lines and on the surface facilities.

3.1 Production and Facility Operations:

In the fields, the engineer's main concern and objective is to meet the crude market demands and provide the field facilities energy supply requirements to maintain smooth operations. The process simulation software is used for simulating the gas oil separation stations, the crude transmission and simulating the associated gas handling facilities. This software is also used for simulating the complete gas oil separation stations, by-passing one or more stages, operating the stages at different conditions to achieve a specified product split and evaluate the effect of the changes on the total field performance. All of these simulations were helpful to the engineers in identifying what it takes to meet their objective under the different operating or problem conditions.

3.2 Crude Stabilization and Sweetening

The crude stabilization stations are simulated to identify the optimum operating conditions to meet the export crude specifications with minimum loss of materials.

Also the crude sweetening units are being simulated, more frequently than before, to do closer monitoring of the stripping gas consumption. This new trend is the result of a study performed on some of the oil fields which revealed that the sweet gas rates were not reduced sufficiently as a result of the cut in the crude production. Consequently, the crude was over-stripped and the H2S contents in the crude fell below the maximum allowed. It is true the crude quality became better but no additional revenue was incurred while extra expensive sweet gas was unnecessarily lost (on the average 5-8 million standard cubic feet per day, per sweetening unit).

3.3 Refinery Operations

The Crude column performance is simulated to study the changes in the product's qualities as a consequence of variation in the blending feeds and conditions. Also the software is used to characterize the feed and specify the

operating conditions to meet product specifications.

4.0 STUDIES AND PRODUCTION PLANNING:

Without the assistance of computers, it was not feasible for the engineers to conduct studies and produce accurate production plans. This is because of the complexity and size of the operation and because these activities cannot be handled manually within a reasonable time and manpower force. The situation has changed over the past four years and dependance upon the consulting firms is reduced for small and medium size engineering activities and trouble shooting.

4.1 VENDOR'S ASSUMPTIONS AND PROPOSAL VERIFICATION:

In the past the engineers had the limited ability to verify vendors proposals and almost no checking was done on the assumptions made. With computer facilities more rigorous checking is being carried out and simulation of the existing and proposed facilities is made to verify each assumption. As a result, changes to the sizing were requested (which resulted in capital investment cutdown) or the implementation was broken into phases where some phases were delayed until the need for those facilities arose.

4.2 PRODUCTION FACILITIES OPTIMIZATION:

With the computer aided facilities available, the Production, Petroleum, Reservoir and Planning engineers are able to conduct studies to optimize the production facilities in the fields. The objective is to re-design the layout of the lines networks, manifolds, pumping, separation and safety facilities. These studies are aimed at maximizing the utilization of the crude pressure as a driving force through the transmission lines, minimize power consumption and optimize the Gas oil separation.

4.3 PRODUCTION PLANNING:

Due to their design, the use of the simulators have been limited to the technical simulation. As a result, the simulators, in the planning applications, have been used for answering the "what-if" questions and production forecasting for a specific assumption per run.

The oil and gas handling, processing and industries in Abu Dhabi depend totally on the local Oil and Gas production. Because of this close association, it is now ADNOC'S intention to more closely monitor the planning function of the production, handling and processing of the natural oil and gas resources. This is a big advance which is under consideration.

The process engineering simulation package can simulate the production handling and facilities; it is able to simulate the industries and their production; it is even able (to a lesser extent) to simulate the transmission lines between the two. However, for any global production handling and process planning, two other functions are missing: the capability to simulate the Well Head production (before the handling and surface facilities and linking this production to the industries' production rates) and the economics of the production pattern. The last two functions would be the basis for the production optimization section of any Natural Resources Production Planning systems which may be considered.

5.0 BENEFITS FROM USING PROCESS ENGINEERING SIMULATORS:

In this paper, there is no attempt to give a Dollar value to the benefits that can be withdrawn from utilizing computer based process engineering simulators. The process engineering simulators are used as tools to:

- help the engineers improve the quality and efficiency of their work
- perform activities that cannot be performed without the aid of such simulators.

In general the benefits are:

5.1 Higher Productivity

The engineer's efficiency, at the beginning dropped a little as the engineers spent some time to:

- Explore the capabilities of the simulators.
- Practice running the simulator to gain confidence in its use and attempting to construct models for non-standard applications that are specific to the engineers operations.

The drop in the efficiency may be minimized by a sound and well planned training programme.

Figure 4 is an average presentation of the productivity improvement and the time needed to reach optimum utilization.

The following table gives the annual mantime saving during the years 1981 and 1982.

INDUSTRY	Man-days/ Year	%*
1. Gas Processing Industries	**	65%
2. Gas Liquification Industries	180	50%
3. Gas/Oil Production & handling	600	60%
4. Refining	30	30%

* % of the time needed to do the same job manually.

** No specific figure was given since most of the work done through using the package, would not have been carried out in-house. It was estimated that for smaller jobs, it would take three times as long to do the same job manually.

5.2 Better Product Quality

The produced figures became more accurate since the engineers do not have to make approximations and they have more confidence in their judgement. Also, to more accurately reflect reality, the engineers made many history-matching simulation runs to generate appropriate correction factors to the simulation results. This even gave them an advantage over the consulting engineers.

5.3 Faster Results

The engineers are able to address emerging problems immediately and results obtained quickly. This reduced the production interruption time and increased the production rate per unit cost.

5.4 Low Risk Testing

All tests were simulated rather than experimenting on the plant and results were predicted without upsetting the plant operations.

5.5 Additional Activities carried out by Company Engineers

By using the process engineering simulator, the engineers are able to carry out new activities that were not feasible to be performed manually. The following table shows the activities performed by the engineers with the aid of the computer simulation facilities that would not be done manually.

INDUSTRY	NEW ACTIVITIES
1. Gas Processing	(1.1) Total Plant production simulation, (1.2) simulation of by-passing Plant-Sections, (1.3) Re-injection of condensates into the main crude lines.
2. Gas Liquification	(2.1) MCR- Refrigeration Cycle simulation (2.2) Total Plant material balance, (2.3) Expansion Simulation, (2.4) studies.
3. Gas Oil Production	(3.1) Total Gas availability and Handling calculations (3.2) Cap-Gas production calculation, (3.3) pseudo-oil gas lift simulation, (3.4) simulation of the water gas lift facilities, (3.5) crude sweetening simulation, (3.6) Sour water stripping simulation, (3.7) surface facility optimization.
4. Refining	(4.1) Crude column - Rigorous simulation, (4.2) Meeting products specification, (4.3) Crude Blend characterization, (4.4) Maximization of ATK production.

5.6 Implication-Forecasting

The implications of any addition, bypassing, deletion, alteration or changes in the plant operations are forecasted and only feasible changes are physically tested and implemented.

5.7 Computer Usage Costs

The computer utilization costs became bigger, but this increase is justified. The increased staff productivity and the higher production rate per cost unit, by far outweigh the increase in the computer charges. Besides, these charges are internal and cover the usage of already available facilities.

6.0 Future enhancements

In general, the available process simulators addressed the technical needs of the engineers. With these needs being met, the engineers became more sophisticated and their scope of work widened and a good portion of their effort is redirected to new activities. These new activities are mainly planning, studies and optimization. With this sophistication and new activities, the engineers' requirements are no longer the same, however they did not reduce in magnitude and in fact they often increased in size. Planning, studies and optimization are functions which to a great extent depend upon economic analysis. All of this calls for additional features to be provided by the process engineering simulators. The more pressing features are:

- Technical optimization.
- Facilities for linking the oil production simulation to the plant production simulation in the same system.
- Costing information.
- Economic information.
- If the costing and economic facilities are outside the scope of these simulators, then these simulators need to be redesigned to easily interact with other systems by providing the technical information needed for the costing and economic analysis.
- Interactive graphics capability and to a lesser extent, animated process graphical presentation.

7.0 SUMMARY

Powerful and Comprehensive Process Engineering Computer Simulators have expanded their original scope of being limited to simulating Petroleum, Petrochemical and Chemical industries to becoming very useful and necessary tools to the Natural Gas and Oil Production Engineering simulation. The process engineering simulator has been equally used by engineers from the Natural Gas and Oil Process industries, Gas and Oil production and their transmission and handling within ADNOC and its group of companies. The availability and the use of the process engineering simulation package have resulted in mantime saving, improvement in the engineer's efficiency, improvement in the engineers' products quality, faster trouble shooting,improvement in the products' quality, minimization in the material and resource loss. It also was the right tool that enabled the process engineers to pick additional activities that resulted in some saving on consultant's fees. This simulator is one of the major computer systems that became the back-bone of the studies and planning functions within ADNOC. This added a new perspective into the engineering function and made the engineers' approach more sophisticated and futuristic. This new trend and sophistication has brought forward new demands which prompted new additional capabilities to be provided by such simulators.

Figure 1. Current off-shore oil and gas production and handling.

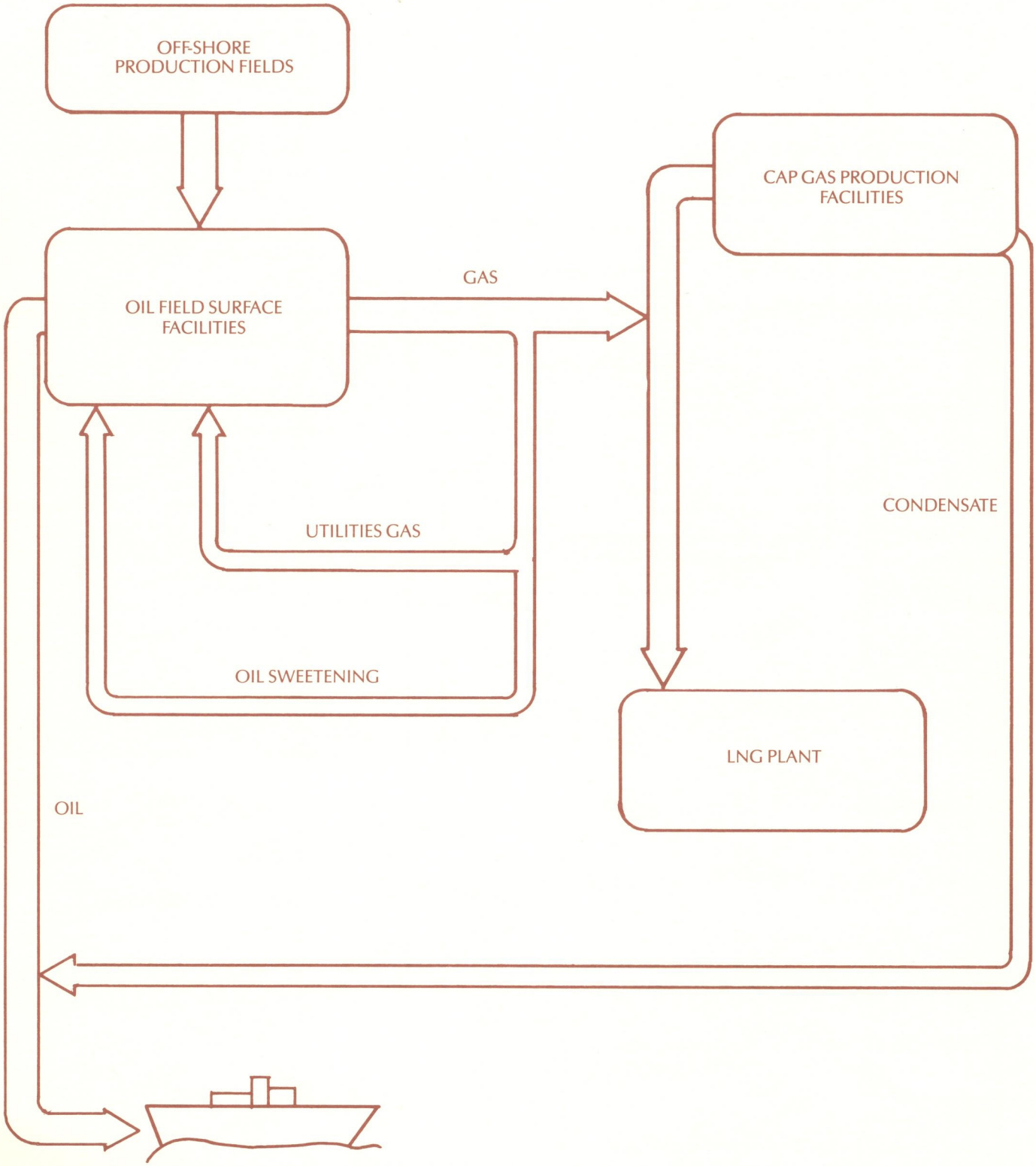


Figure 2. Future off-shore oil and gas production and handling. The cap gas field surface facilities will become gas injection facilities.

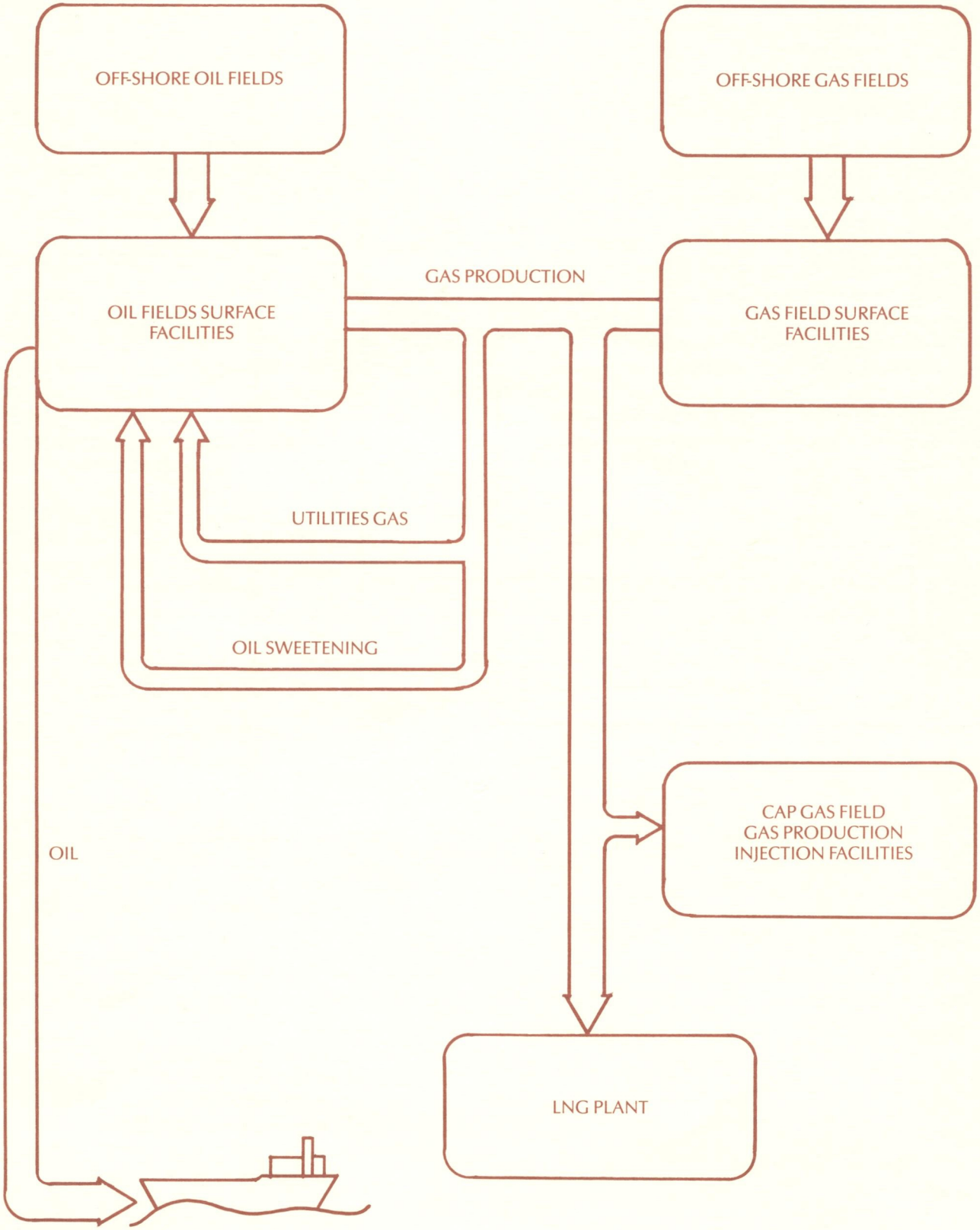


Figure 3. On-shore oil and gas production and handling.

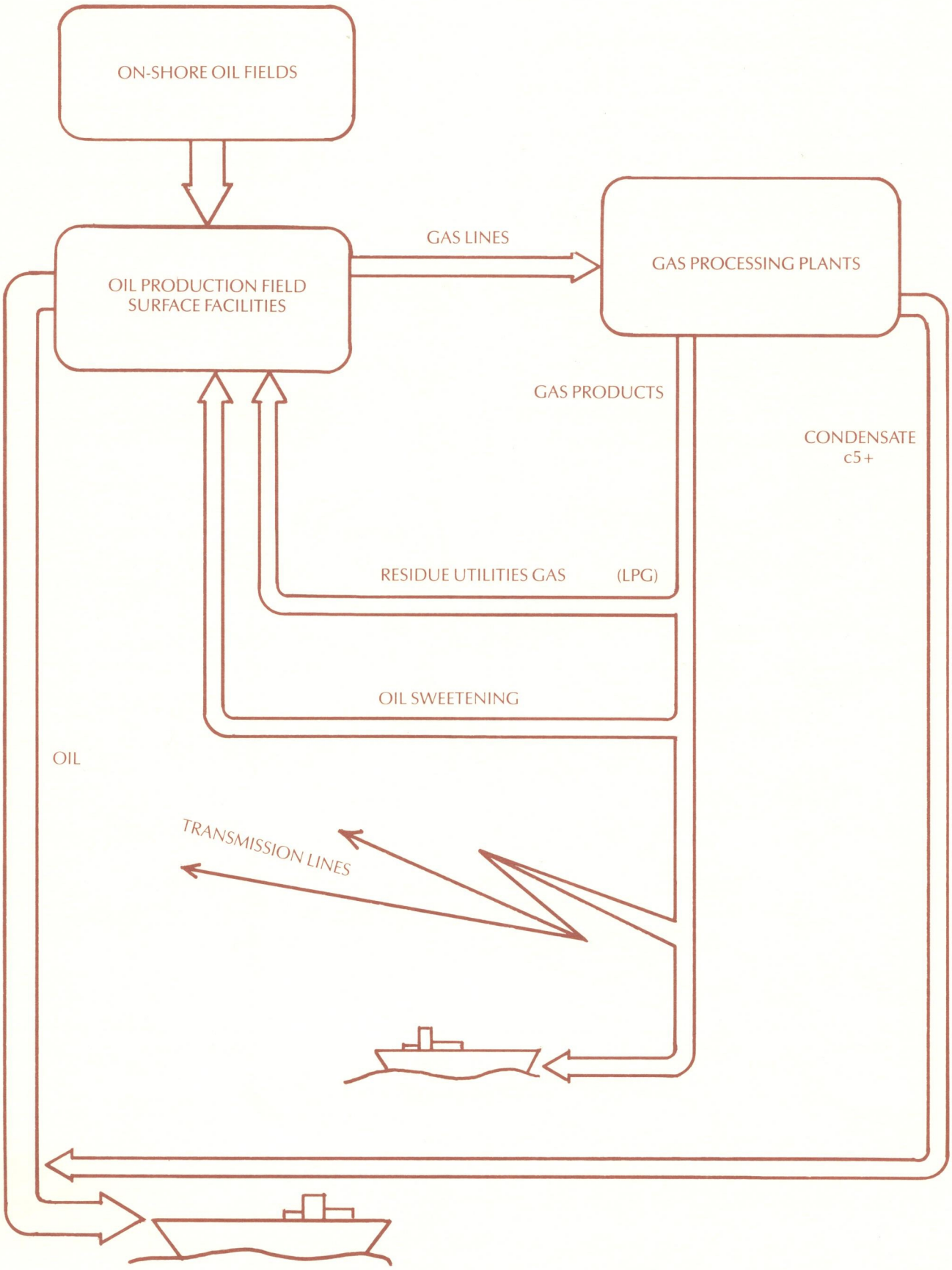
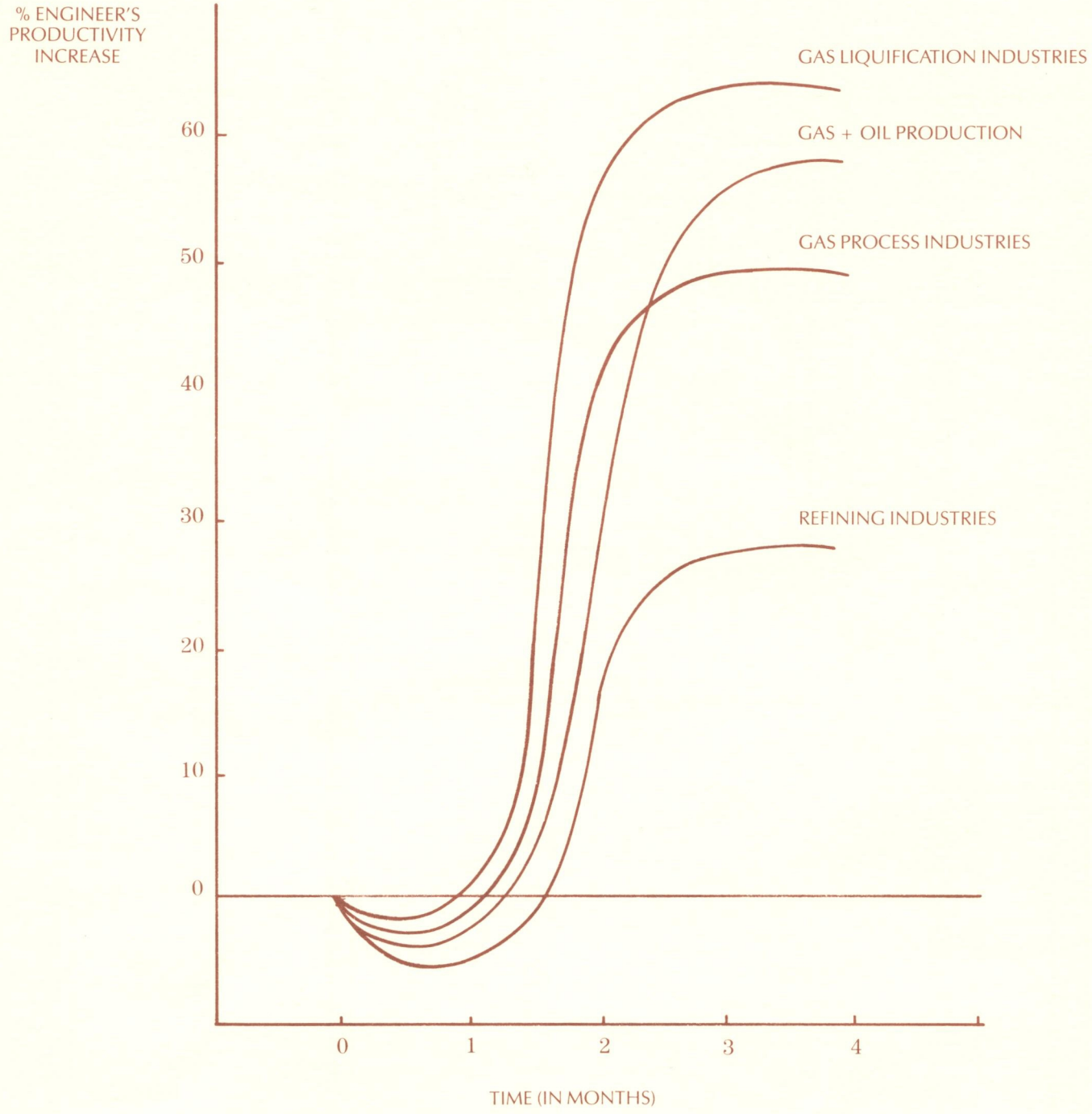


Figure 4. Profile of engineer's productivity improvement (including the learning period)



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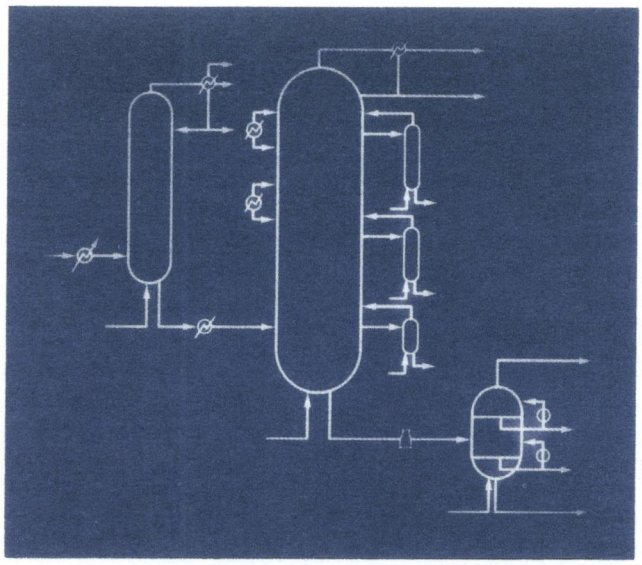

DESIGN II is a powerful process engineering tool that solves all refinery distillation columns . . . fast. For the first time, you can model columns with an essentially unlimited number of stages, pumparounds, strippers, and total products. Even difficult columns, such as vacuum, quench, coker and cat cracker fractionators,can be solved.With DESIGN II, all limits are off.

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ChemShare®

The ChemShare Corporation
1900 Lummus Tower • Houston, Texas 77056
Phone: 713/627-8945 • TWX: 910-881-2793
Hot Line: 713/627-1760

ChemShare Process Systems Ltd.
Brook House Church Street • Wilmslow, Cheshire SK9 1 AT England
Phone: 0625-532113 • Telex: 666905