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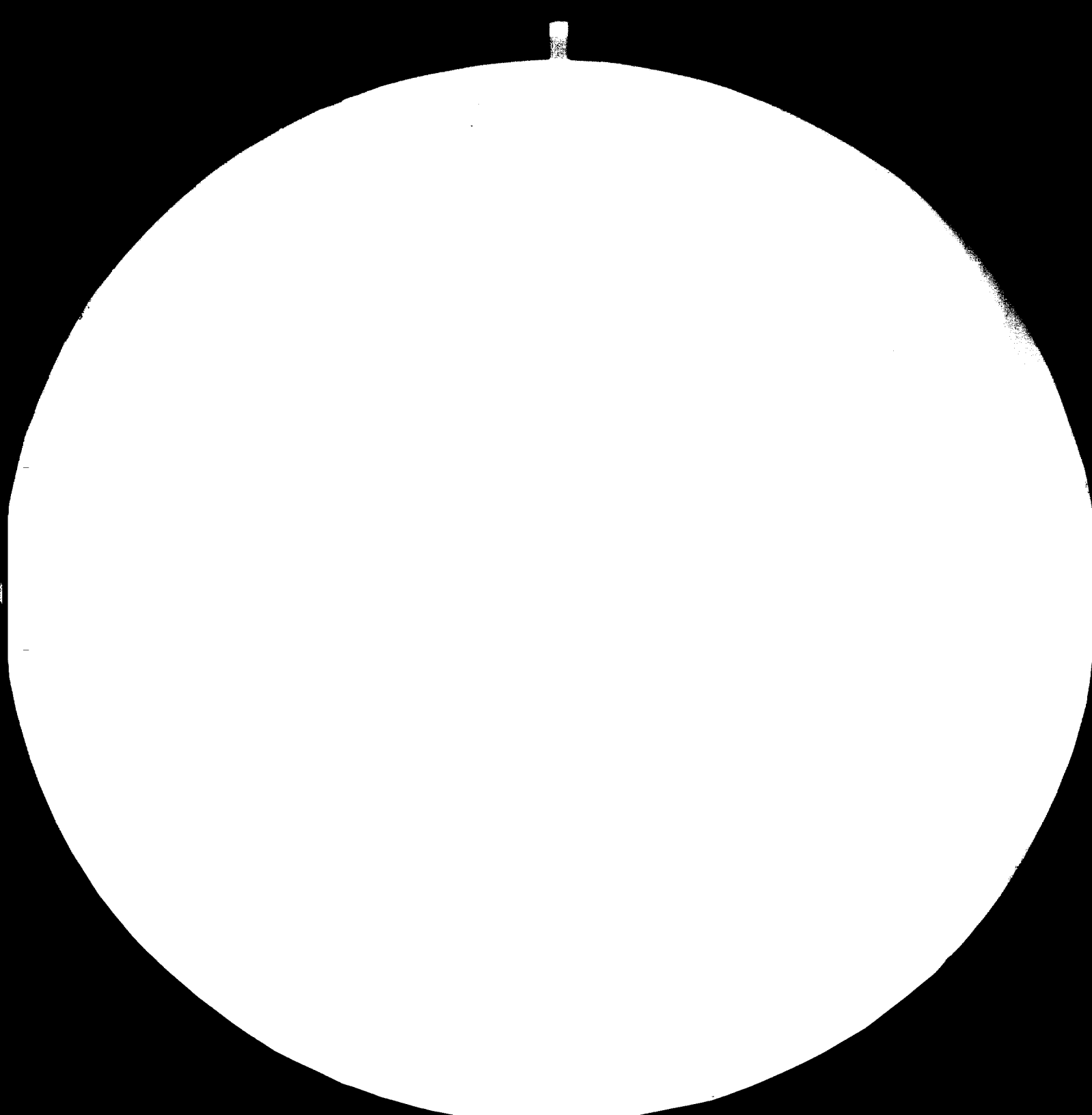

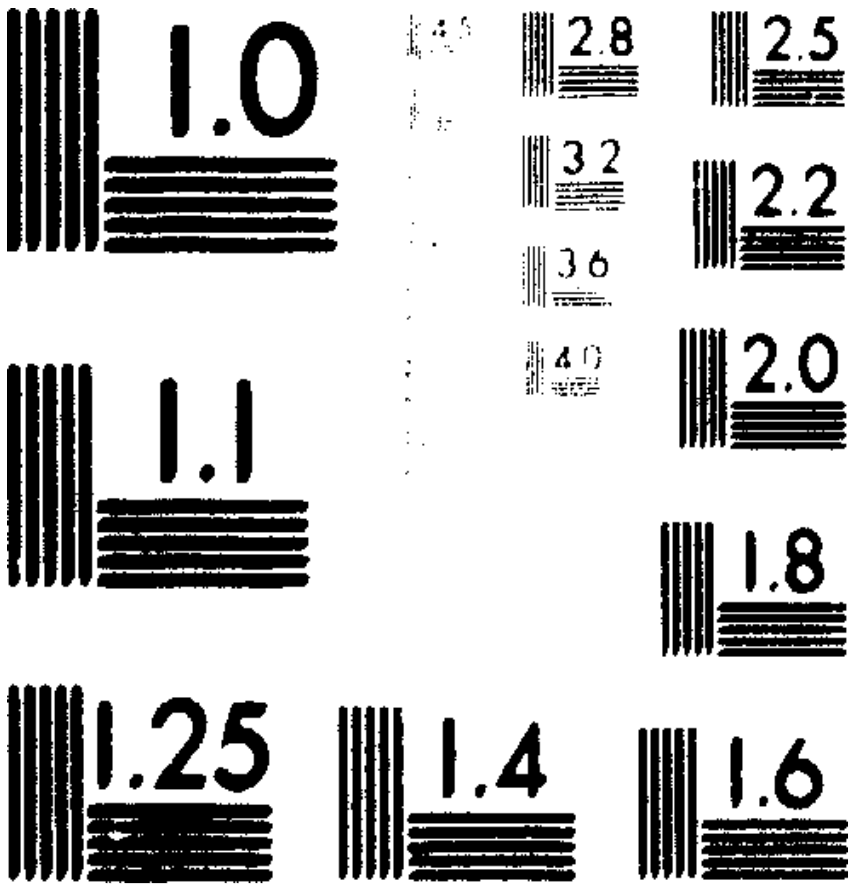

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Subcontract Report:

COMPUTER SOFTWARE FOR DISTILLATION SIMULATION AND DESIGN

DP/ARG/75/021/80.38.DR.

Visit to Planta Piloto de Ingenieria Química,
Universidad Nacional del Sur, Bahía Blanca, Argentina.

Report prepared for

UNITED NATIONS INDUSTRIAL DEVELOPMENT ORGANIZATION

by

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(Consultant, Chemical Engineering)

UNIDO Expert

June 1980

SUMMARY OF CONTENTS

Report by Professor Wayne C. Edmister, on his visit to the Planta Piloto de Ingeniería Química, Universidad Nacional del Sur, Bahía Blanca, Argentina, May - June 1980.

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1. Introduction

The purpose of this visit was to deliver a magnetic tape, containing new computer programs, to PLAPIQUI and give assistance in adding these new programs to the software library of the PDP 11/70 in Bahía Blanca.

These new computer programs are for multistage, multicomponent distillation calculations and were prepared by the writer after returning home from his lecture-consulting visit to PLAPIQUI in 1979.

In addition, work on two of the class projects (water-hydrocarbon phase equilibria and chemical reaction equilibria) was reviewed.

2. Travel Dates - 1980

9 May Lv San Rafael, California
12 May Ar Bahía Blanca, Argentina
10 June Lv Bahía Blanca, Argentina
10 June Ar Buenos Aires, Argentina
14 June Lv Buenos Aires, Argentina
15 June Ar San Rafael, California

3. Industrial Visits

Gas del Estado, Bahía Blanca (June 2)
YPF - Florencio Varela (June 11)
Gas del Estado, Buenos Aires (June 12)
Petrochemical General Mosconi - Buenos Aires (June 13)

4. Preparatory Work

At the 2nd International Meeting on Petrochemical Technology (held in Bahía Blanca July 16 and 17, 1979) the writer outlined a versatile short-cut method for making multistage, multicomponent separation process calculations. This proposed method was shown to be applicable to complex columns, i.e. more than one feed and more than two products. The development of computer programs for making such calculations and the integration of the resulting new subroutines into SIPREQ was discussed in July 1979.

A listing of SIPREQ was taken home by the writer and used in doing the preliminary work on this project. During the fall 1979 quarter, while teaching part time at University of California, Santa Barbara, the writer prepared another version of SIPREQ that would be suitable for batch operations on large computers, such as the IBM 370/158, the machine available for the writer's work in California.

During the winter quarter (Jan - Mar 1980), the writer continued work on the development of an enlarged SIPREQ that contained the short-cut distillation calculation capabilities, working at Kaiser Engineers (Oakland, California), where the writer does occasional consulting work. The SIPREQ work at KE continued on a part-time basis, until May 8th (the day before departure for Argentina).

The most significant difference between the "batch" version of SIPREQ, for use on large computers, and the version required for the "communicative" type operation employed on the PDP 11/70 at PLAPIQUI is the difference in the ways the physical properties data are stored and recalled for use. In the batch version the data banks are part of the program, while in the PLAPIQUI version the data are kept in a separate file and only those items needed are read and transmitted into the core memory for operations.

5. Magnetic Tape Delivered

The SIPREQ program put on tape on May 8th was about 5000 cards in length. These were loaded onto a 9 track magnetic tape at 1600 b.p.i. for delivery.

For convenience, the material was divided into three sections, containing 32, 33 and 31 blocks of 50 lines in each block. In this arrangement it is easy to locate and retrieve any desired portion of the program.

Subroutines of the program delivered follow. A complete listing is attached as Appendix II.

SECTION 1

MAIN	CONVT
NHULI	CONTEM
COFBIN	BUFT
CONS	BUBP
SPEQN	DEWP
FUGAS	FLASHT
NORM	FLASHP
CONP	FLASHL
CONV	GUESS
CONVPR	ENTHS

SECTION 11

BUBBT	MFLASH
BUBBP	PFLASH
DEWWT	GASFLO
DEWWP	COMPR
FLSHT	EXPAND
FLSHP	KHFIT
HEAD	INVER
ANS2	REACK
ANSWER	

SECTION 111

SHORT	ASFPH
UNDER	FRACT
SHODIS	

The subroutines in Sections 1 and 11 are for basic thermodynamic properties predictions and for simple equilibrium processes. Those of Section 1 are also in the PLAPIQUI version of SIPREQ. Those in the lefthand column of Section 11 are likewise in the PLAPIQUI version. All other programs, i.e. the right hand column of Section 11 and Section 111 are new to PLAPIQUI.

ASFPH and FRACT are the programs that use the absorption and stripping factor functions, referred to in the July 1979 presentation mentioned above. Background literature on this method were assembled and two copies made for PLAPIQUI use.

6. PLAPIQUI Computer Systems

The hardware and software systems of the PDP 11/70 computer are rather small for such a large program as the expanded SIPREQ. Additional core memory and a new, more powerful compiler will be obtained in the future. These will increase capacity. For the present two things are being done to operate all parts of the new SIPREQ. These are: make SIPREQ into two programs instead of one. SIPREQ 1 would be composed of the subroutines in Sections 1 and 11 and would be for all applications except multistage separation calculations. SIPREQ 2 would be composed of the subroutines in Sections 1 and 111 and part of those in Section 11 and would be for distillation simulation and design calculations.

Because of the size of the program and the length of multistage calculations, SIPREQ 2 might require using an overlay technique

wherein the thermodynamic subroutines are first used to obtain property values for the mixture; then these and other data are filed on the disc for use in the second part of the program which is put in core, overlaying the thermodynamic subroutines.

Another limiting feature of the PLAPIQUI PDP 11/70 system is the terminal only operation while having too few terminals. More terminals will be available in the future and this will make it possible for more users to work at the same time.

7. Thermodynamic Properties

An alternate method for finding the liquid and vapour roots of the equation of state has been added to PLAPIQUI's SIPREQ thermo pack. The alternate is an iterative procedure, as compared to the analytical procedure that has been used previously. This option has been found to be preferable in some cases by U.S. workers in the field. To date users at PLAPIQUI have had no trouble with the analytical method, however. Both give the same results for problems solved in Bahia Blanca to date.

In the prediction of equilibrium temperatures (B.P., D.P. or FLASH) for mixtures at high pressures, the calculations are very sensitive to the starting values of temperature and unknown phase compositions that are given in the input data. If assumed temperature values are too high or too low, the calculations might not converge or there might be a false convergence, with all K values equal to unity as if at the critical state.

This is partly due to using the same equation (the SRK or the PR EOS) for both phases. Accordingly, it was proposed that a two-equation technique for predicting the vapor-liquid distribution ratios be put into SIPREQ. The Lee-Erbar-Edmister method is such a procedure.

In the L.E.E. method vapor fugacities are found by an EOS and liquid fugacities by using an activity coefficient expression and a pure state reference fugacity. As the writer had a listing of this method, it was keyed into the system.

Preliminary tests indicate that this two-equation method, when used for intermediate estimates of temperature and compositions starting values for the one-equation method, does improve the predictions.

A similar problem might arise in the prediction of pressure. If so, the same two-equation package can be tried for estimating better starting values of pressure and unknown phase compositions for starting data in the one-equation method.

The one-equation method, when it works, which is most of the time, is better than the two-equation method. It is more sensitive however and we hope to get around this by the above intermediate predictions by a less sensitive method.

From experience we have found that the above trouble occurs only at higher pressures, not at lower pressures. Based on this finding, a method has been proposed for estimating the BP or DP temperature for a high pressure by making predictions at two lower pressures and then extrapolating to find a reasonable temperature at the desired high pressure.

Subroutine REACK was reviewed with Campaña, who had derived the missing constants in his class project last year. Corrections to these constants were made and a first draft of a manuscript for publication was prepared.

8. Simple Equilibrium Processes

New programs were prepared for multiple flashes, flashes with heat

balances, compression, expansion, gas flow, and curve fitting the K and H values for use in distillation calculations. Some of these simple process programs were also done at PLAPIQUI. Time has not permitted comparing these duplicates, however.

The writer's MFLASH and KHFIT programs are inter-related and necessary for the operation of the distillation programs. For this reason it was decided to use them in the thermodynamic calculations made to prepare for distillation calculations.

Subroutines REACK and GASFLO were not integrated into SIPREQ and tested. Both have operated successfully previously, so there should be no difficulty, if and when they are needed.

9. Distillation Simulation and Design

Section 111 subroutines SHORT, UNDER, ASFPH, SHODIS and FRACT are all concerned with multistage separation calculations. SHORT and UNDER, which are short-cut design procedures for simple fractionators (one feed and two products), will find the required reflux or equilibrium stages, given one or the other, for a specified separation. This method uses the limiting conditions, i.e. minimum reflux with infinite number of stages and minimum stages at total reflux.

ASFPH is for absorbers, reboiled absorbers and strippers and uses the A and S factor functions of the writer. As SHORT and UNDER and ASFPH have been used previously as separate programs, integration into SIPREQ should be a routine programming job.

The two new subroutines SHODIS and FRACT were recently prepared. SHODIS is the program that reads the starting information, i.e. the compositions and conditions of the feeds and the configuration of the

separation process to be simulated or designed. Feed information is then transmitted to MFLASH where flashes are made at three temperatures to obtain K and H values, which are then sent to KHFIT where polynomial equations are derived.

All this information is then used in the separation calculations that follow. For this application the information is made available in a data file that is set up on the disc. In this way most of the thermodynamic parts of SIPREQ can be removed from core memory to make space for the required separation calculation subroutines. Using polynomials as sources of K and H values in the separation calculations should save calculation time and require less memory.

Subroutine FRACT covers many configurations of distillation columns, i.e. one or more feeds, two or more products, with or without side-stream strippers, reboilers or steam stripping, and intermediate heat removal or addition. This makes FRACT a very long program, which would present no problems on a large size computer. For use on the PDP 11/70 it is better to divide FRACT into several shorter programs. This was done and the new programs were named $FRACT_1$, $FRACT_2$, etc.

With this organization, the user will indicate the FRACT subroutine wanted, i.e. the one that fits the configuration for the problem being solved. In future simulation work, other FRACT subroutines may be added.

Each distillation process configuration in FRACT is divided into sections (2 to 6 or more). Each separation section contains several (two or more) equilibrium stages, which must be specified by the user in setting up the simulation problem in SHODIS. The effect of the number of stages on the separation is included in the calculations, of course.

FRACT calculations are started with assumed temperatures and liquid-vapor flow rates for tops and bottoms of each section. The calculations find the rates, temperatures and compositions of the products and the internal streams.

Temperatures are revised by equilibrium bubble and dew point calculations and rates are revised by heat balance calculations. When values of temperature and flow rates do not change from one iteration to another, the solution is converged.

Similar procedures are followed in ASFPH except that the heat balances are used to revise temperatures and equilibrium calculations to revise flow rates.

In the design procedures of SHORT there are no convergence steps, although these could be added later if desired.

Background literature, covering the A and S Factor method, was assembled and bound in convenient form and copies given to Brignole and Mabe. Copies of the equation derivations were made for Mabe and Fornari.

10. Other Activities

In addition to working with G. Mabe on developing computer software for distillation simulation and design, the writer did the following:

10.1. Worked with H. Campaña on the completion of the reaction equilibrium calculation project, including: (a) data bank of constants for the free energy of formation equation for the same 49 components that appear in the SIPREQ data bank, (b) completing a computer program for calculating free energies and equilibrium constants for chemical reactions of the components in the data bank, (c) preparation of a

manuscript for publication on the work done.

10.2. Reviewed with E.A. Brignole and J. Festa the work being done on three phase equilibrium predictions for hydrocarbon - water systems. This project was started in 1979 as a class project in the writer's lecture course on applied thermodynamics and properties prediction. It is a more difficult problem than originally expected. Apparently two sets of binary interaction coefficients are required, one for the vapor and water-rich liquid phases and another for the vapor and the hydrocarbon-rich phases. Brignole and Festa have been working together on the problem. A worthwhile publication should be forthcoming from this effort.

10.3. Assistance has been given to the Metallurgical Consultant, Ing. Sterling Booth, by helping him prepare, send and receive the telex communications required to obtain the additional information from his office in California.

11. Conclusions and Recommendations

Following are this Consultant's suggestions:

11.1. Besides the additional core memory and terminals and the new compiling system that are being obtained for the PDP 11/70, it is recommended that an alternate "batch" method of operating be prepared. It might also be desirable to have a card punch and card reader in the system for more flexibility.

11.2. A flow sheet simulation program is needed. This might be CHESS with some modules replaced by those of SIPREQ or another system. Professor Guillermo Aguayo (University of Puerto Rico - Mayaguez) is recommended as one to help develop this simulator. Aguayo already has such a program running.

11.3. A future addition to the SIPREQ software library might be the UNIFAC - UNIQUAC method for aqueous chemical solutions. The writer has a copy of this program, in card form, that could be put on tape and installed in the PLAPIQUI system.

11.4. Another future addition might be a rigorous matrix general method for multistage separation calculations. The writer also has such a program in a form that could be transmitted to Bahia Blanca.

12. Acknowledgement

The friendly cooperation and helpful assistance of PLAPIQUI faculty and staff during this mission are appreciated. The administrative help of Esteban Brignole and the technical help of Guillermo Mabe were of great importance in this project. Others contributing to the writer's efforts were Rosa Fornari, Jorge Ardenghi and Guillermo Simari.

Respectfully submitted

Wayne C. Edmister

Bahia Blanca
June 1980

A P P E N D I X I

DP/ARG/75/021

SUBCONTRACT JOB

Subject: Develop computer software for simulation and design of Complex Multicomponent Destillation columns using short cut methods.

Requirements: The programmes should be written in Fortran IV and should be compatible with a PDP 11/70 with 256 Kb of CPU and a 67 Mb storage disk.

- The programs should be recorded in magnetic tape of 9 tracks (800 - 1600 bpi).
- A thermodynamic properties prediction system and data bank for light hydrocarbons and related products, should be provided together with the programs.
- The subcontract should include a four week stay at PIDCOP, Bahía Blanca, Argentina, of the software writer for the final implementation, testing and training of systems users.
- The computer package should be delivered within the 45 days after the awarding of the subcontract. The four week stay should be scheduled for March 1980.

Description: The computer package should be able to compute the following:

1) Columns with up to 5 feeds and two products.
   Number of component: 15. Compute product distribution or number of plates depending on specification.
2) Columns with up to 5 feeds and 5 liquids or vapor lateral extractions. Compute product distribution or number of plates depending on specifications.
3) Complex absortions of stripping columns up to 15 components.