MODIFICATION AND EXPANSION OF A COMPUTER AIDED DESIGN PACKAGE FOR PROCESS FLOWSHEET DEVELOPMENT

by

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ABSTRACT

An interactive design calculation package (DESPAC), prepared under the direction of Prof. A. Westerberg at Carnegie-Mellon University, contains flash, distillation and absorption routines. In this study DESPAC was firstly modified from the DEC-20 computer system to the CDC Cyber 170/815 computer system and then expanded by adding the multicomponent liquid-liquid extraction and the shell-and-tube heat exchanger computation modules. The new package (DESPAC2) is capable of solving steady-state problems for various process flowsheets on a unit by unit basis.

DESPAC2 has a library file which comprises some thermophysical properties for ninety-one chemical species. This file can be extended defining new properties and components. In addition to this, it is possible to introduce new unit computations into DESPAC2. The methodology required for this purpose, is explained in detail.

In order to present the flexibility of DESPAC2, various examples are solved. Firstly six problems involving single operation units are studied. Secondly various flowsheets are proposed and tested for a separation problem as an example of flowsheet development using DESPAC2.

This package is simple to use and can be employed for wide range of applications including flowsheet development, process design, in research and education.

ÖZET

Carnegie-Mellon Üniversitesi'nde Prof. A. Westerberg'in yönetiminde hazırlanan etkileşimli tasarım hesaplamaları paketi (DESPAC) flaş, distilasyon ve absorpsiyon altprogramlarını kapsar. Bu çalışmada, DESPAC öncelikle DEC-20 bilgasayar sisteminden, CDC Cyber 170/815 bilgisayar sistemine adapte edilmiş, sonra çok bileşenli sıvı-sıvı ekstraksiyonu ve borulu ısı değiştiricisi hesaplama modülleri eklenerek genişletilmiştir. Yeni paket DESPAC2, çeşitli proses akım şemalarını ünite bazında, kararlı hal problemleri için çözebilmektedir.

DESPAC2, doksan bir kimyasal maddenin termofiziksel özelliklerini içeren bir veri kütüphanesine sahiptir. Bu termofiziksel özellikler kütüphanesi, yeni özellikler ve maddeler eklenerek genişletilebilir. Buna ek olarak DESPAC2'ye yeni ünite hesaplamaları eklenebilir. Bu amaçlar için gereken yöntemler tüm ayrıntılarıyla açıklanmıştır.

DESPAC2'nin çok amaçlılığını gösterebilmek için çeşitli örnekler çözülmüştür. Önce bağımsız operasyon üniteleri için altı problem ele alınmıştır. Daha sonra akım şeması geliştirilmesine örnek olarak bir ayırma problemi için değişik akım şemaları önerilmiş ve DESPAC2 ile sınanmıştır.

Kullanımı kolay olan bu paket, akım şeması geliştirilmesi, proses tasarımı, araştırma ve eğitimde geniş bir uygulama alanına sahiptir.

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a_s	Cross area for flow (m^2)
A	Heat transfer area (m^2)
B	Baffle spacing (mm)
CMTD	Corrected Mean Temperature Difference (°K)
C_p	Heat capacity of fluid (J/kg-°K)
d_i	Inside diameter of tube (mm)
d_o	Outside diameter of tube (mm)
D_e	Equivalent diameter (mm)
D_s	Shell inner diameter (mm)
f_i	Pure component fugacity of component i
$\hat{f}_i$	Fugacity of a component i in a mixture
F	Correction factor
G_s	Fluid mass velocity on the shell side (kg/s-m^2)
G_t	Fluid mass velocity on the tube side (kg/s-m^2)
h_{di}	Inside thermal resistance of scale deposits (W/m^2-°K)
h_{do}	Outside thermal resistance of scale deposits (W/m^2-°K)
h_i	Inside resistance (W/m^2-°K)
h_{io}	Inside resistance based on the outside diameter (W/m^2-°K)
h_o	Outside resistance (W/m^2-°K)
k	Thermal conductivity (W/m-°K)
K_i	Equilibrium ratio of component i
l	Total length of tubes (m)

LMTD	Logarithmic Mean Temperature Difference (°K)
L1	Heavy-phase overall flow rate(kmol/h)
L2	Light-phase overall flow rate (kmol/h)
m	Flow rate of fluid (kg/s)
N_t	Number of tubes
P	Pressure (bar)
P_t	Tube pitch (mm)
Q	Heat transferred per unit time (J/s)
SL1	Heavy-phase side stream flow rate (kmol/h)
SL2	Light-phase side stream flow rate (kmol/h)
t	Temperature (°K)
t_A	Average fluid temperature of cold stream (°K)
t_W	Temperature at the tube wall (°K)
T	Temperature (°K)
T_A	Average fluid temperature of hot stream (°K)
T_r	Reduced temperature
U_D	Overall heat transfer coefficient (W/m^2-°K)
x_i	Component mole fraction in liquid phase
X1	Component mole fraction in heavy-phase
X2	Component mole fraction in light-phase
y	Clearance between tubes (mm)
y_i	Component mole fraction in vapor phase
z_i	Component mole fraction in feed

Greek Letters:

ε	Epsilon
γ_i	Activity coefficient of component i in the mixture
θ	Viscosity constitutional constant of Thomas' equation
μ	Viscosity (centipoise)
μ_W	Viscosity of the fluid at the tube wall (centipoise)
ρ_L	Density (g/cm^3)
τ	Time

I. INTRODUCTION

DESPAC2 is the modified and expanded form of DESPAC [42] which operates on the CDC Cyber 170/815 computer system at Boğaziçi University.

The original package, DESPAC, has the capability to solve steady-state problems for flash, distillation and absorption units. Seven different flash calculations can be performed by changing the temperature and the pressure of the flash, heat added to the flash, and the specified fraction of the feed to be vaporized. Bubble and dew points of mixtures may be calculated by the PHASE routine. Also DESPAC has different methods for distillation calculations, namely, McCabe-Thiele binary distillation, shortcut multicomponent distillation (adjacent and non-adjacent keys), and rigorous multicomponent distillation. Edmister method is employed for the design of gas-liquid absorbers.

DESPAC2, the DESPAC expansion aimed at this study, contains multicomponent, multistage liquid-liquid extraction and shell-and-tube heat exchanger routines in addition to the above mentioned unit computation modules. The algorithms of these routines are prepared in accordance with the structure of DESPAC and are presented in Section 3.2.1. Furthermore, the technique to introduce new unit computations into the existing software has been deciphered and explained in detail in Section 3.2.2. Following the procedure presented in this section, preparation and addition of new unit calculation routines for additional process equipment into DESPAC2 becomes an almost routine and easy programming job.

DESPAC2 contains a library file of thermophysical properties of ninety-one chemical species. The technique to expand the library file either by adding new components or by introduction of additional properties of the existing components is explained in the Section 3.2.3. Consequently, the range of application of DESPAC2 can now easily be extended with a reasonable effort. In its final form DESPAC2 contains 143 routines.

DESPAC2 is a program package which may be used for flowsheet synthesis and development. DESPAC2 philosophy and the philosophy underlying the design of flowsheeting packages like FLOWTRAN, PROCESS, etc. are quite different. In the well-known programs (as in FLOWTRAN), usually the flowsheet is quite fixed at the beginning of calculations and once the calculations start the flowsheet is almost inflexible. Thus, in flowsheet synthesis these programs have to be used for mostly calculating the results of hypothetical flowsheet configurations foreseen a priori. However, the DESPAC2 philosophy is based on flowsheet computations on a unit by unit basis under a unified program structure. Thus, the foreseen alternative flowsheet configurations may be tested for processing conditions, operating flexibility and various flowsheet configurations one by one. In these calculations the input data are supplied by the user for each unit. Only after testing each unit and its relation with the following units that the use of, and hopefully a more economical and efficient use of complete flowsheeting program may be made. Furthermore, results of DESPAC2 can be fed as initial guesses to the well-known packages such as FLOWTRAN, in order to reduce the computer time (CPU).

DESPAC2 may be employed as a powerful tool for process design courses. The user can enter the operational parameters into DESPAC2 interactively and obtain results in a very short period of time. The speed of the run enables the user to change the operation parameters and/or the proposed process flowsheet easily.

In this study to test the capability of DESPAC2, solutions of various example problems are shown. All examples are obtained from Chemical Engineering literature. Firstly, six different examples are solved for single operation units, and then to illustrate the utility of DESPAC2 for flowsheet synthesis and development, a separation process containing various operation units is studied.

Establishment of the approriate process flowsheet can be achieved by employing either of the two following routes:

In the first route to obtain the optimum process flowsheet for the problem under consideration, a known process pattern is employed and tested by changing the process specifications.

In the second route, various flowsheets which are applicable to the problem solution are developed. Later, the most appropriate configuration(s) may be selected.

Once a flowsheet has been selected by either one of the two routes explained above, the processing conditions of each unit in the flowsheet are decided upon either in the order of the process flow or, more intelligently, these exploratory calculations are initiated from the most critical unit in the accepted flowsheet by employing DESPAC2. These calculations are then continued with the other units in the order of the decreasing importance in the process flowsheet.

II. GENERAL APPROACH FOR COMPUTER-AIDED DESIGN AND SIMULATION

Design of chemical plants and process equipment can be achieved in two ways:

a. Manually (hand calculation)
b. Employing digital computers.

Rapid developments in processes and process equipment technologies increases the number of design alternatives drastically. Furthermore, processes are elobarated on in order to increase their effectiveness. As processes and equipment become more complex, there will be a greater need for the digital computer solutions.

Before computer usage became popular, instruction in engineering analysis was restricted to simple systems which were of little practical value, and most of the effort was devoted to solve the few elementary equations. But, most industrial problems fall into advanced mathematics which can only be solved by computers [15].

A model of a typical chemical process will often involve some or all of the following:

1. Fluid flow
2. Equilibrium
3. Mass transfer
4. Heat transfer
5. Kinetics
6. Process dynamics and control calculations.

The general procedure for conducting an analytical study, covering all six categories above, is shown in Fig. 2.1 [15].

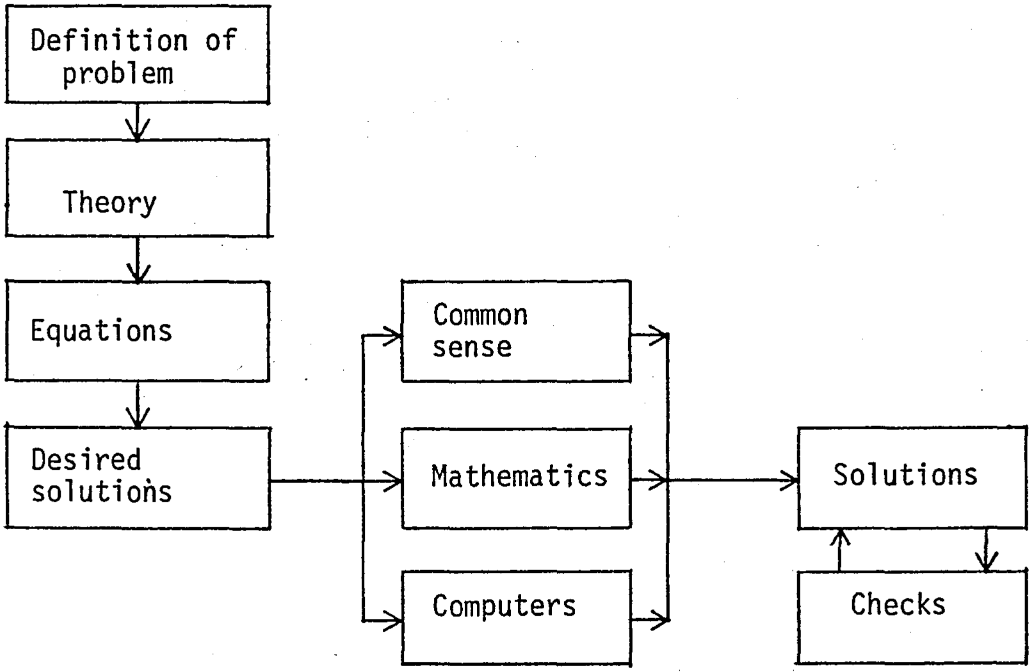


Figure 2.1 - Procedure for analytical approach.

The first step is the definition of the problems which are to be solved.

The second step is comprised of the definition of the theories which will be employed for the solution of the above mentioned problems.

One of the advantages of the computerized approach is the facility of rapidly obtaining solutions to various cases; this makes comparisons between alternate theories possible.

Next, the fundamental concepts, relevant to the problem in hand are expressed in the form of mathematical equations.

The computational phase offers several alternate routes for the solution. The method selected depends upon the complexity of the equations to be solved and the desired accuracy of the solution. If, the equations required are simple the solutions desired can be obtained by inspection. For the more complex cases, the equations can be solved by analytical techniques. Digital computation is the advanced method to solve, even the most complex equations.

The last phase is the verification of the solution obtained from the mathematical model [15].

The most rapid solution method is that of digital computers which can successfully be used in

- Process Design, and
- Process Simulation [9].

With the help of computer-aided design and simulation the engineer obtaines more accurate results in a shorter period of time. Hence, on modelling and economy of a given process [31].

Design is defined as the sizing and the combination of devices to achieve a required change from input to output stream variables; on the other hand in simulation, the output stream variables are calculated, given the inputs and the characteristics of the devices. Although design and simulation are different, they are closely interrelated. The results of the preliminary evaluation of process simulators can be used as estimates for input data to the final design situation.

The simulation has the data set, and the sets of mathematical models called unit computations [9].

The engineer can use a set of unit operations to devise a new process or he can patch together unit computations to calculate an existing process. This can be represented by building blocks. Each "block" or unit computation refers to only one Unit Operation. e.g. Distillation Unit Computation, Absorber Unit Computation.

In Fig. 2.2, a process and its block representation are depicted [40].

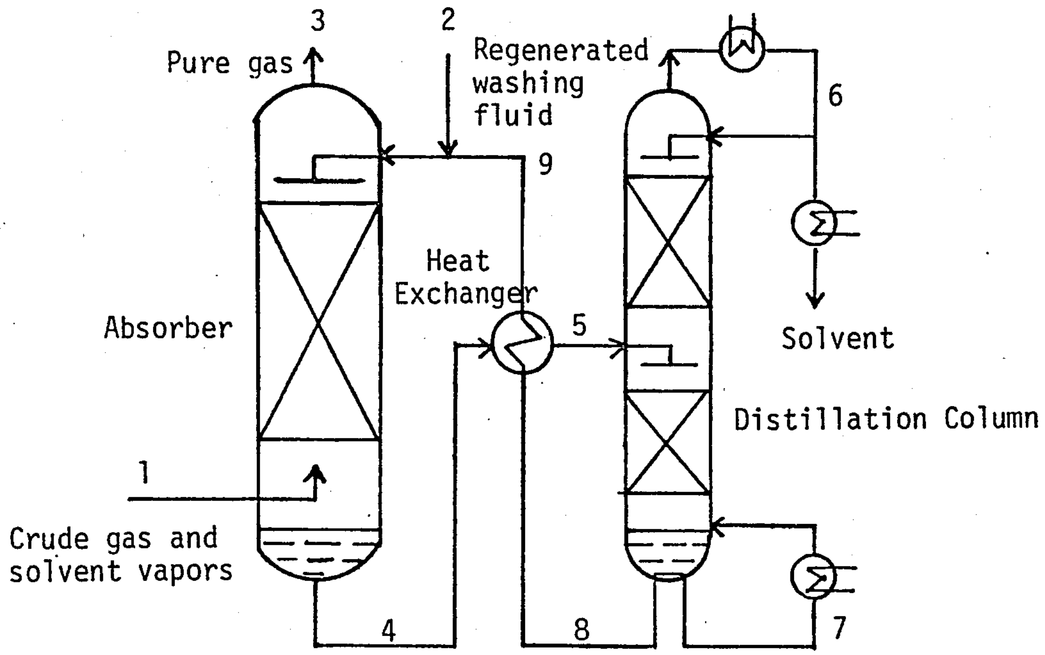
Simulation can also be applied to the transient (dynamic) or steady-state processes. The following programs are some examples of dynamic and steady-state flowsheet simulators available to engineers.

Dynamic - System Simulators:

1. DYNSYS [2]
2. PRODYC [22]
3. REMUS [19]
4. FLEX [39]
5. KARDASZ [23]

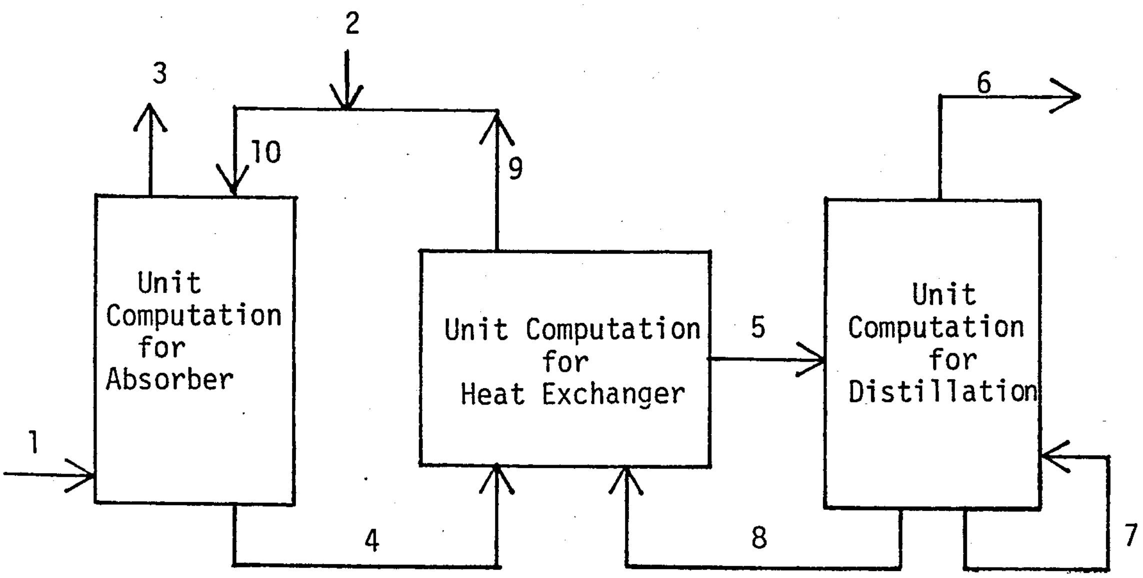
Steady-State Material & Energy Balance Programs:

1. PACER [38]
2. FLOWTRAN [12]
3. CHESS [8]
4. GIFS [16]
5. PROCESS



Methanol recovery from exhaust air

a) A process flow diagram.



b) Block representation of the process flow diagram.

Figure 2.2 - A process and its block representation.

On the other hand, DESPAC2 (Interactive Design Calculation Package) is also a collection of programs that are applicable to the design of separation processes under steady-state conditions on a unit by unit basis.

DESPAC2 can solve problems for single operation units. It is also possible to develop a flowsheet for a complet process using this package. The user proposes several possible flowsheets by patching the necessary operation units together. In DESPAC2, the data transfer between units must be handled by the user. On the contrary, complex simulators such as FLOWTRAN has an executive program which calls upon different unit computations and calculates the values of operating variables for all streams in the system.

Computer core requirement is low and convergence in the unit computation modules is speedy in DESPAC2. Input data required are less than that of the complex packages, since the process flow diagram along with process data must be supplied to complex simulators. The results of DESPAC2 can be fed to complex packages as initial guesses to reduce the computation time.

DESPAC2 operates interactively and gives results in a very short period of time. This capability of DESPAC2 offers the user to change operation parameters easily. The user can obtain results quickly by changing the process flowsheets, because of the flexibility of DESPAC2. Hypothetical flowsheets may be checked whether they are properly defined and suitable alternatives may be selected with the aid of DESPAC2.

The heart of this study is to use the above mentioned property of DESPAC 2, and in the following chapters the steps to reach that kind of usage of this package are explained in detail.

Operation of DESPAC2 is more practical than the other complex packages which are quite clumsy for the development of flowsheets and for process design. For this reason, DESPAC2 is also a powerful tool for education and training purposes.

Entry of the input data into DESPAC2 may be achieved interactively and by computer library file simultaneously. DESPAC2 contains a library file of thermophysical properties of ninety-one chemical species.

DESPAC2 can be expanded by adding new unit computations. The thermophysical property library file can be enlarged by introducing new components and thermophysical properties which are not present.

Consequently, DESPAC2 can either design and evaluate the feasibility of a new process or predict and improve the operation of an existing process.

Contents and the organization of DESPAC2 are explained in Appendix A.

III. DEVELOPMENT OF DESPAC2

3.1 MODIFICATION OF DESPAC

DESPAC is a FORTRAN program which is developed to run on TOPSC, a DECSYSTEM-20 computer under the TOPS-20 operating system at Carnegie Mellon University [42].

Although FORTRAN is said to be standardized, various computer system companies have different FORTRAN compilers. During the compilation of DESPAC on the CDC Cyber 170/815 at Boğaziçi University, numerous problems were encountered. Therefore, DESPAC is modified to run on the CDC Cyber 170/815 system.

3.1.1 Computer Language Standards and Program Portability

FORTRAN was introduced as a programming language originally in the late 1950's and was further developed through the 1960's mostly for scientifically oriented problem solution. It is one of the oldest of what may be called "foundation languages" (FORTRAN, COBOL, ALGOL, and BASIC) which is still very popular even after the introduction of "structural languages" such as PASCAL [35].

A fully portable program, or a source code, is the one which may be transported from a computer to another without any necessary modifications. This may be achieved if the compiler in question all abide by the standard set by ISO - International Standard Organization and/or ANSI - American National Standard Institute. However, unfortunately most compiler designers succumb to a compelling urge to provide "better" features in their compilers in a quite competitive field. These "better" features generally are implemented before the standards have been set and are therefore non-standard at the point of their applications. It is also true that various compilers exist for a machine model, but all machines of the same model may employ somewhat different compiler versions. So in reality most active compilers are located near but not really at the ISO or ANSI standards [35].

These variations among compilers, as expected cause problems in computer program portability. As it would be expected these problems generally are more serious among the machines of different manufacturers. If the source code has employed only very well accepted and standard features of a language, like FORTRAN, portability problems may be minimal or none. The problems start multiplying in numbers and degree of severity when non-standard features of a compiler have been used and these features do not exist in the new compiler where the program is desired to be transported. In such cases new but different standard or non-standard route have to be employed in place of the non-standard features which have to be replaced.

On the other hand, efficiency of a source code might decrease after transportation, i.e. CPU time required and/or the memory requirement might increase.

A major part of the effort spent in the present study was to convert the DESPAC routine originally prepared for the DECSYSTEM-20 computer running under the TOPS-20 operating system to the CDC Cyber 170/815 Computer system.

In the following parts some examples of the important differences between the routes shown by the two different compilers are shown in contrast. At this point probably it is neither proper nor justified to call some differences important, since this might mean some others are not. Naturally, it is well known to all that even the most minor looking alteration, if not done, will be detrimental for the functioning of the package in the new machine/compiler combination.

3.1.2 Major Differences Between FORTRAN Compilers of the DEC-20 and the CDC Cyber 170/815 Computer Systems

Since CDC 170/815 has a different FORTRAN compiler from the DEC-20 system, the compilation of DESPAC or CDC Cyber 170/815 has caused numerous problems. Consequently, the modification of DESPAC has been deemed necessary. For this purpose the following major modifications and conversions were performed:

a) The INCLUDE statement of the DEC-20 system is refused by the CDC since it does not have any equivalent statement. If a certain group of Common Blocks has to appear in more than one routine, INCLUDE statement of the DEC-20 system is a practical solution to convey this information. On the DEC-20 system INCLUDE statement with its group name is sufficient to transfer the complete information of Common Block among routines. On the other hand, all Common Blocks (Refer to Appendix D) have to be declared in the respective subroutines on the CDC version.

b) On the DEC-20 system, the PARAMETER statement does not require its arguments to be declared in paranthesis. On the CDC system the arguments of the PARAMETER statement must be declared in paranthesis.

c) All comments and syntax (e.g. ";", ":") after an executable statement in the same line is accepted on the DEC-20 system. On the contrary, CDC compiler accepts such declarations between the 73rd and 80th columns only. Otherwise, they should be deleted on the CDC version.

d) CHARACTER, INTEGER, LOGICAL, DOUBLE PRECISION and REAL variables can be equalized to each other on the DEC-20 compiler. This kind of usage is refused by the CDC, since it equalizes the same type of variables to each other. Hence, such contradictory usage should be corrected for the CDC system.

e) All variable names starting with letters I, J, K, L, M, N are automatically assumed as INTEGER variables on the CDC. All REAL variables of DEC-20 system starting with I to N should be declared as REAL variables on the CDC system. Alphanumeric variables should be declared in a CHARACTER statement on the CDC.

f) Certain characters (e.g. "$") may be used in a FORMAT statement on the DEC-20 system. But such characters are refused by the CDC compiler and cause errors.

g) Certain characters (e.g. "," or ")", comma or right paranthesis, respectively) which fulfill certain functions on the DEC-20 system are useless and cause errors on the CDC compiler.

h) All non-executable statements in a routine must precede all of the executable statements on the CDC system since the opposite kind of usage is frequently detected on the DEC-20 system, each of them is rearranged on the CDC version in order to prevent FORTRAN compilation errors.

i) Certain statements on the DEC-20 system (e.g. SKIP RECORD, TYPE) are not defined on the CDC. Instead of SKIP RECORD and TYPE, REWIND and PRINT statements may be used, respectively on the CDC system.

j) Very frequent and complicated usage of OPEN and CLOSE statements, on the DEC-20 compiler, can be removed by the definition of the tapes for the file management at the beginning of the PROGRAM DESPAC on the CDC version.

k) Declaration of field width of format descriptor is different on the DEC-20 and on the CDC systems.

```
e.g.  DEC-20  accepts  FORMAT (2I)
      CDC     refuses  FORMAT (2I)
```

l) On the CDC system only 19 continuation lines for a single statement is permitted. On the other hand, on the DEC-20 system there is no such limitation.

m) End of file (EOF) and end of record (EOR) statements must be packed on the CDC version.

n) On the DEC-20 system, "!", "]", or "C" in the first column are accepted for comments. If "!", "]" appears in the middle of the line, the rest is interpreted as a comment. For all explanations and comments, "C" must be written in the first column of the respective line on the CDC version.

Also the data section of the original program on the DEC-20 system, must be separated from the rest and transferred to a new data file. If data file will be left in the program, (just to give information), unless "C" is written in the first columns, fatal errors will be encountered on the CDC system during the compilation of the program.

Table 3.1 presents the main differences between FORTRAN compilers of the DEC-20 and the CDC Cyber 170/815 computer systems.

There are 135 subroutines and a total of 17 000 lines in DESPAC. Consequently, any correction completed in any one of the subroutine, causes new errors in the linked subroutines. Fig. 2 in Appendix A shows the linked subroutines of just one modelling routine (FLSHPQ), in order to indicate the complexity of interrelated routines. Hence, any correction completed in the program must systematically, carefully and patiently be introduced into the linked subroutines.

TABLE 3.1 - Main Differences Between FORTRAN Compilers of the DEC-20 and the CDC Cyber 170/815 Computer Systems

	DEC-20	CDC Cyber 170/815
a)	Accepts INCLUDE	Refuses INCLUDE
b)	PARAMETER arg=const	PARAMETER (arg=const)
c)	Accepts ";" ":" after an executable statement	Refuses ";" ":" after an executable statement
d)	INTEGER = CHARACTER etc.	INTEGER = INTEGER CHARACTER = CHARACTER
e)	all variables' types must be specified	default INTEGER for I-N, rest REAL
f)	Accepts certain characters in FORMAT such as "$"	Refuses certain characters in FORMAT such "$"
g)	Accepts "," ")" to fulfill certain functions	Refuses "," ")" to fulfill certain functions
h)	Executable statement may precede non-executable statements	Non-executable statement must precede executable statements
i)	Employs SKIP RECORD and TYPE for certain functions	Employs REWIND and PRINT for certain functions
j)	Employs OPEN and CLOSE for file management	Employs tape declaration in the PROGRAM statement for file management
k)	Accepts FORMAT (2I)	Refuses FORMAT (2I)
l)	Unlimited number of continuation lines	19 continuation lines
m)	-	EOF and EOR must be packed
n)	"!", "]" or "C" in the first column for comments	"C" in the first column for comments

3.2 EXPANSION OF THE CAPABILITIES OF DESPAC

DESPAC already covers flash, distillation and absorption unit computations, and a thermophysical library file-of 91 components. DESPAC can be expanded by adding new unit computations and also the contents of library file can be enlarged by adding either new components and/or new thermophysical properties of components. The modified version of DESPAC which operates on CDC-system has been extended by introducing "Multicomponent Liquid-Liquid Extraction" and "Shell-and-Tube Heat Exchanger" unit computation modules. This final form of DESPAC is named as DESPAC2. In this chapter, the preparation of new unit computation algorithms and the procedure of inserting new unit computations into DESPAC and enlargement of library file will be explained in detail. Following the procedures mentioned, it becomes an almost routine activity to expand the capability of DESPAC2.

3.2.1 Preparation of New Unit Computation Software

Two new modelling routines are included in DESPAC2; namely:

a. Shell-and-Tube Heat Exchanger (HEX),

b. Multicomponent, Multistage Liquid-Liquid Extraction (EXT).

3.2.1.1 Algorithm for the Design of a Shell-and-Tube Heat Exchanger

An algorithm to design a multipass, counter current, shell-and-tube heat exchanger is developed following the method presented in Backhurst & Harker [3], and employing references Afgan and Schlunder[1], Blackwell [4], Fraas and Özışık [13], Frank [14], Kays and London [24], Kern [25], Peters and Timmerhaus [32] and Reid et al. [36].

The main assumptions for the preparation of the algorithm are as follows:

1. The overall heat-transfer coefficient is constant through the heat exchanger.
2. The flowrate of each fluid is constant.
3. The specific heat of each fluid is constant.
4. There is no condensation of vapor or boiling of liquid in any part of the exchanger.
5. Heat losses are negligible.
6. The heat-transfer surface in each pass is equal.
7. The temperature of the shell-side fluid in any shell-side pass is uniform over any cross section.
8. Pressure loss is negligible.

The detailed explanation of the theory applied is presented in Appendix B.

The main aspects of the iteration cycle are listed below:

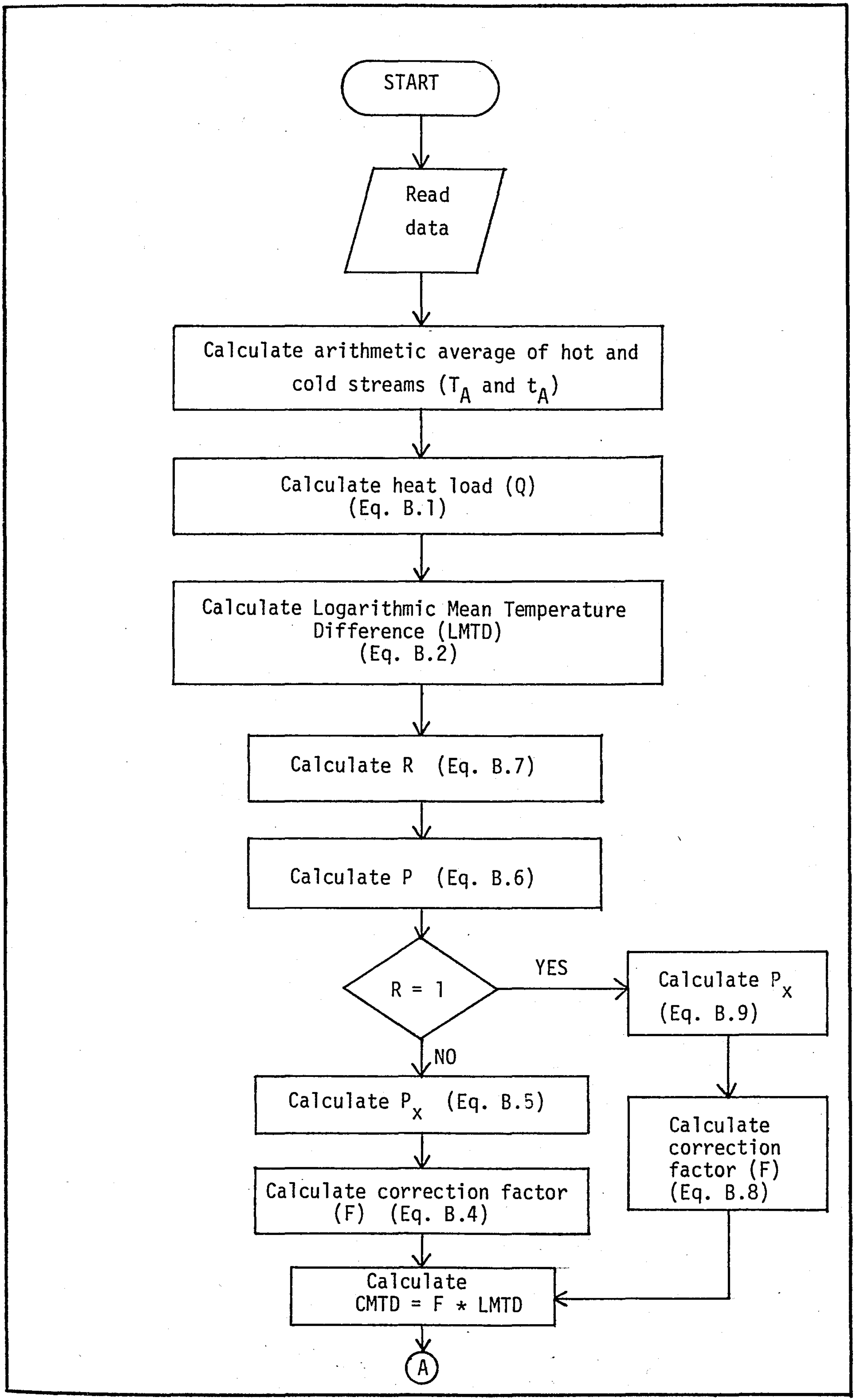
1. The input data required are submitted.
2. The amount of heat transferred per unit time is calculated.

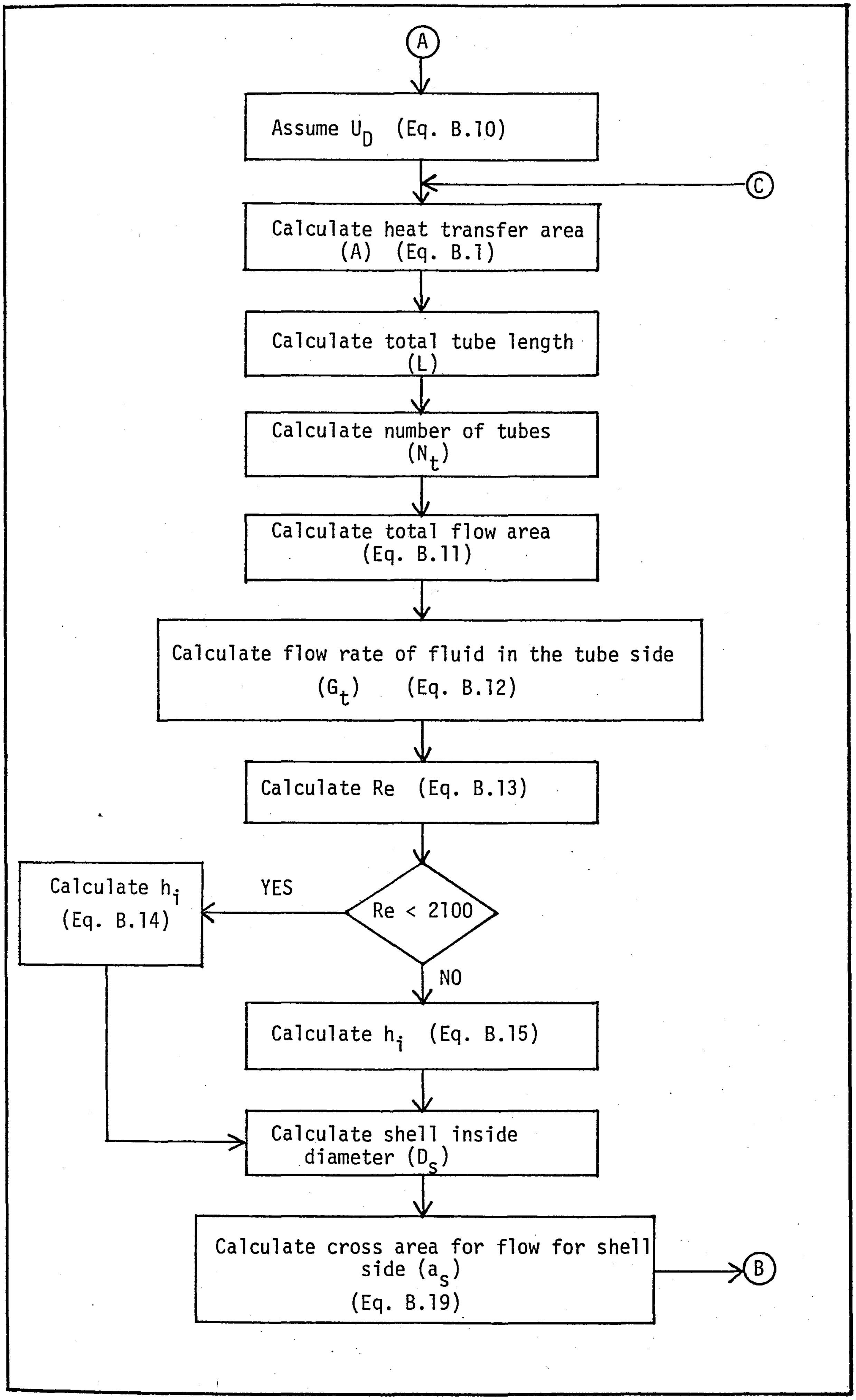
3. Upon calculation of Logarithmic Mean Temperature Difference and Correction Factor, the Corrected Mean Temperature difference is obtained.
4. Routine estimates the initial overall heat transfer coefficient employing initially assumed heat transfer coefficients.
5. Total number of tubes and the flow rate of fluid in the tube side are calculated.
6. Heat transfer coefficients inside tubes are evaluated.
7. The flow rate of the fluid in the shell side is computed.
8. Heat transfer coefficient in the shell side is calculated.
9. The overall heat transfer coefficient is obtained using the tube and shell side heat transfer coefficients calculated in steps 6 and 8, respectively.
10. If the difference between the overall heat transfer coefficients computed in steps 4 and 9 is less than the present tolerance, the algorithm stops. If not the next guess is evaluated and the steps between 5 and 10 are reiterated.

The logical flow diagram of the algorithm depicted in Fig. 3.1.

3.2.1.2 Algorithm for the Simulation of a Multicomponent, Multistage Liquid-Liquid Extraction Column

Liquid-Liquid extraction is a separation process which can be carried out either in packed or staged columns.


START
Read data
Calculate arithmetic average of hot and cold streams (T_A and t_A)
Calculate heat load (Q) (Eq. B.1)
Calculate Logarithmic Mean Temperature Difference (LMTD) (Eq. B.2)
Calculate R (Eq. B.7)
Calculate P (Eq. B.6)
R = 1
YES
Calculate P_x (Eq. B.9)
Calculate correction factor (F) (Eq. B.8)
NO
Calculate P_x (Eq. B.5)
Calculate correction factor (F) (Eq. B.4)
Calculate CMTD = F * LMTD
A


A
Assume U_D (Eq. B.10)
C
Calculate heat transfer area (A) (Eq. B.1)
Calculate total tube length (L)
Calculate number of tubes (N_t)
Calculate total flow area (Eq. B.11)
Calculate flow rate of fluid in the tube side (G_t) (Eq. B.12)
Calculate Re (Eq. B.13)
Re < 2100
YES
Calculate h_i (Eq. B.14)
NO
Calculate h_i (Eq. B.15)
Calculate shell inside diameter (D_s)
Calculate cross area for flow for shell side (a_s) (Eq. B.19)
B

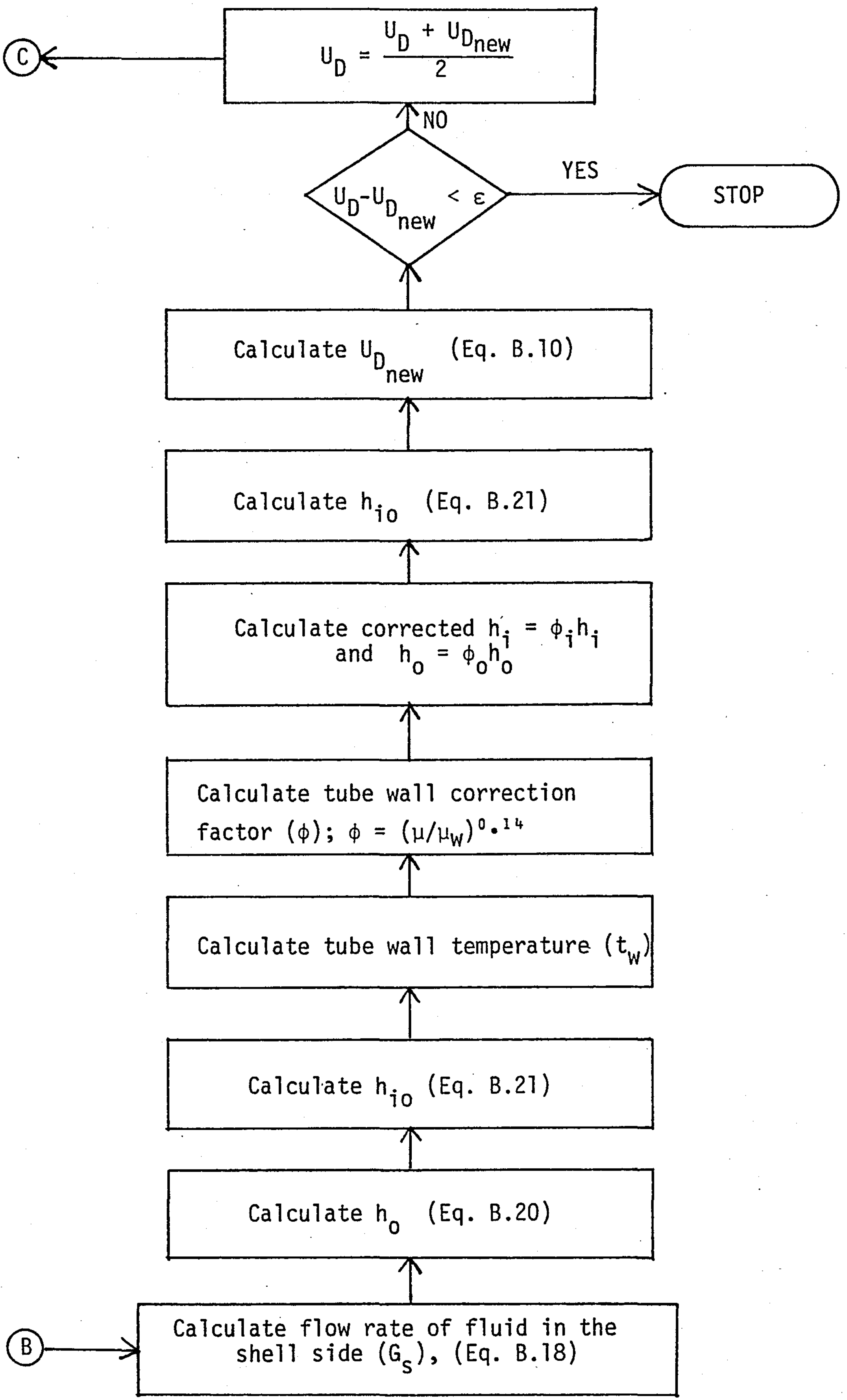


Figure 3.1 - Logical flow diagram of the iteration cycle of the Shell-and-Tube Heat Exchanger Algorithm.

The algorithm to simulate multicomponent, multistage equilibrium-stage liquid-liquid extraction is obtained from Sen [37]. The algorithm is based on the relaxation technique, i.e., it uses the transient model equations to reach the steady-state solution.

The detailed explanation of the theory applied can be found in Appendix C.

The main aspects of the iteration cycle are presented below:

1. The algorithm parameters, composition and overall flow rate profiles of light and heavy phases are assumed initially.

2. Activity coefficients of component i in both of the phases are calculated by a thermodynamic model, such as the 3-suffix Morgules, NRTL, or UNIFAC equations. Then the equilibrium ratios are calculated.

3. Substituting the assumed overall stage flow rates and the calculated equilibrium ratios into the linearized equation sets, the resulting equations may be solved by a tridiagonal matrix algorithm to yield the heavy-phase mole fractions at the incremented time $(\tau + 1)$.

4. The calculated heavy-phase mole fractions are normalized.

5. Light-phase mole fractions are calculated from the heavy-phase mole fractions and the equilibrium ratios.

6. The calculated light-phase mole fractions are normalized.

7. New values of the overall stage flow rates are calculated.

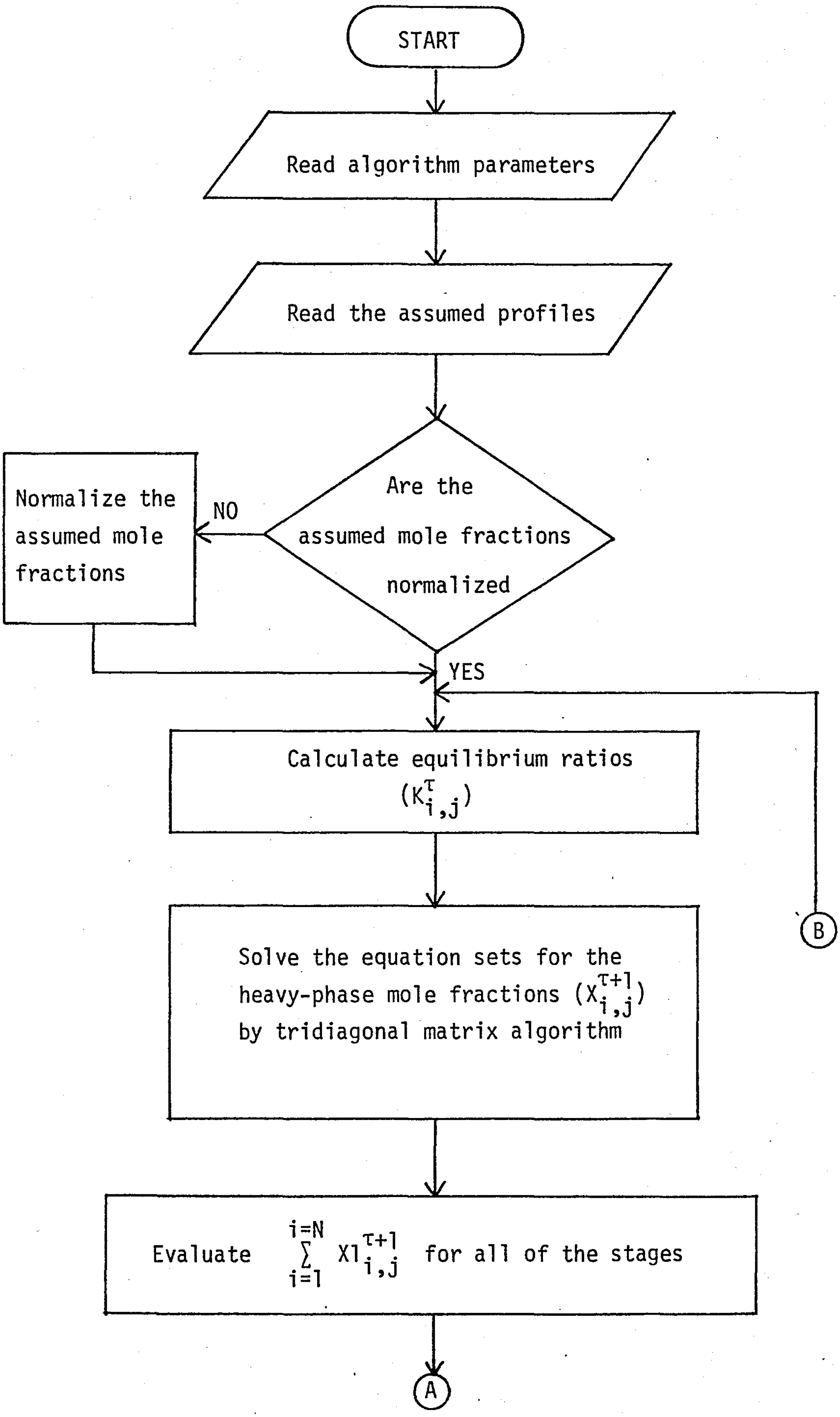
8. If the difference between the heavy phase mole fractions at time (τ) and at the incremented time ($\tau + 1$) is less than the preset tolerance, the algorithm stops. If not another iteration is performed between the steps 2 and 8.

The logical flow diagram of the algorithm is given in Fig. 3.2.

The above mentioned algorithm which was actually available on the UNIVAC 1106 computer, is introduced into DESPAC to increase its capabilities. For the implementation of this algorithm the following modifications are performed:

1. The original algorithm operates on the UNIVAC 1106. It is modified to operate on the CDC Cyber 170/815 eliminating the differences between the FORTRAN compilers of two systems.

2. The original algorithm is modified to fit into the DESPAC structure. For this reason, the modelling routine (EXT) and the executive routine (XEXT) are prepared which are consistent with the structure of DESPAC. The executive routine (XEXT) calls the modelling routine (EXT). XEXT routine also enables the user to operate the EXT routine interactively. XEXT routine contains NAMELIST features (Refer to Appendix A) which allow the user to enter the input data.


START
Read algorithm parameters
Read the assumed profiles
Are the assumed mole fractions normalized
NO
Normalize the assumed mole fractions
YES
Calculate equilibrium ratios ($K_{i,j}^{\tau}$)
Solve the equation sets for the heavy-phase mole fractions ($X_{i,j}^{\tau+1}$) by tridiagonal matrix algorithm
Evaluate $\sum_{i=1}^{i=N} X1_{i,j}^{\tau+1}$ for all of the stages
A
B

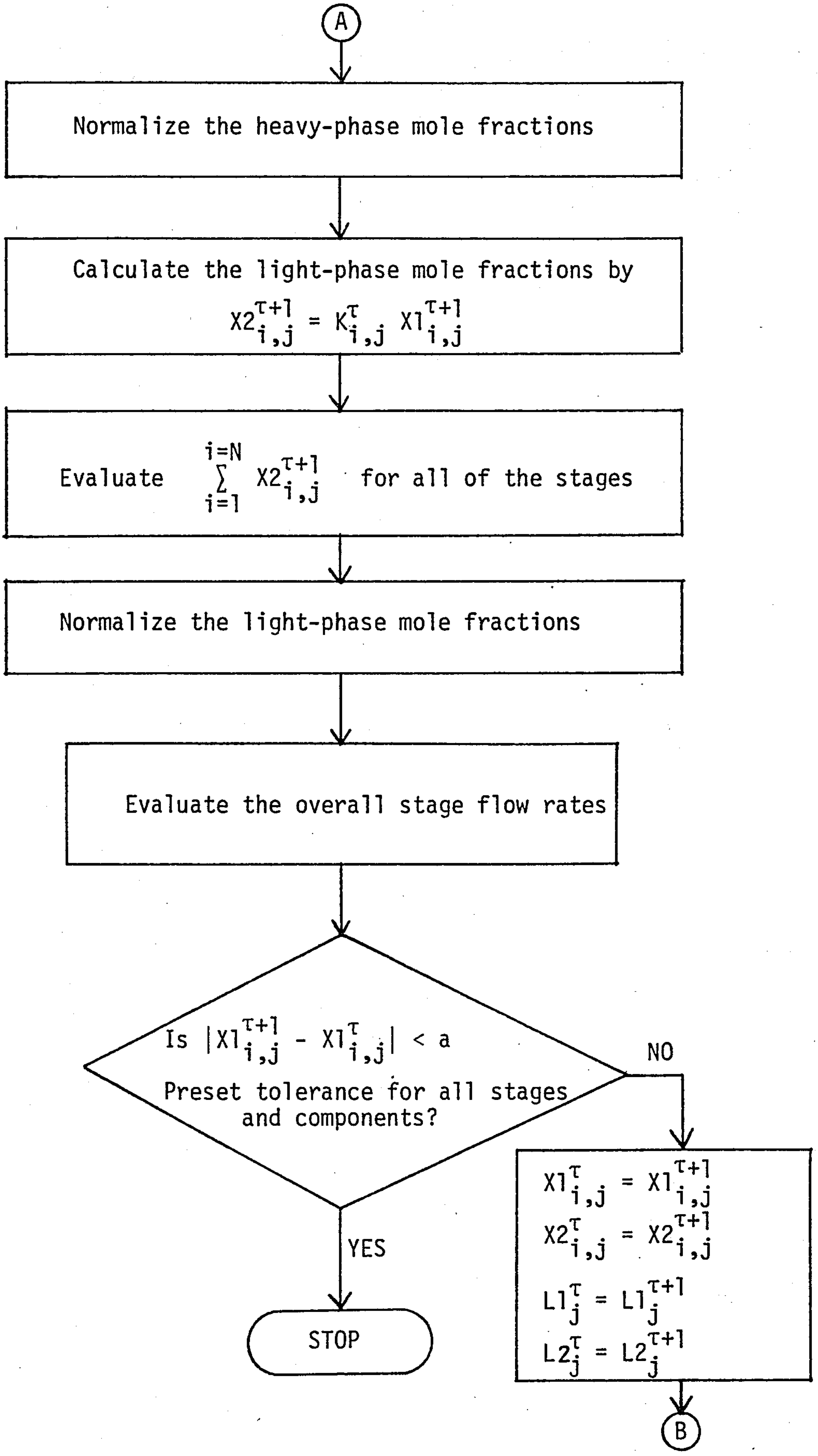


Figure 3.2 - Logical flow diagram of the iteration cycle of the Multicomponent Liquid-Liquid Extraction Algorithm.

3.2.2 The Procedure for the Addition of New Unit Computation Routines Into the DESPAC Structure

In this section, addition of new unit computations into the DESPAC structure is explained in detail and examples for additions are given for the shell-and-tube heat exchanger (HEX) and the multi-component liquid-liquid extraction (EXT) routines.

The procedure required to insert a new modelling routine is presented below.

1. The executive routine(s) which calls the modelling routine must be prepared.

   e.g.

Executive Routine		Modelling Routine
XHEX	⟷	HEX
XEXT	⟷	EXT

2. The executive routine(s) should be prepared in the INTERACTIVE mode. The dialogue between the user and the program is performed by the INPUT and OUTPUT statements which are consistent with the PARAM Common Blocks (In Appendix D, the function of PARAM is explained).

3. The executive routine(s) must also contain NAMELIST features (Refer to Appendix A), and it has to call Subroutine READNL (Refer to Appendix A) which introduces NAMELIST properties [30].

   e.g.

   ```
   NAMELIST/DATA/A,B,C
   CALL READNL ('DATA')
   READ (2, DATA)
   ```

4. The executive routines must contain PARAM, NCOMP and IDENT Common Blocks, and the modelling routines must contain PARAM, NCOMP, PHYS and IDENT (if necessary) Common Blocks (Appendix D presents the functions of these Common Blocks) for the shell-and-tube heat exchanger and the liquid-liquid extraction routines, where XHEX and XEXT are executive routines and HEX and EXT are modelling routines.

e.g.

XHEX	⟷	HEX
PARAM		PARAM
NCOMP		NCOMP
IDENT		PHYS

XEXT	⟷	EXT
PARAM		PARAM
NCOMP		NCOMP
IDENT		PHYS
		IDENT

5. The executive routines are called by PROGRAM DESPAC which prompts the user a menu containing all of the modelling and some of the auxiliary routines (Refer to Appendix A for the contents of the menu). The user selects the code number of the respective routines. The additional modelling routines and their code numbers must be inserted into the menu. PROGRAM DESPAC calls the relevant executive routines using the selected numbers.

Table 3.2 presents the summary of the procedure for the addition of new unit computations into the DESPAC structure.

TABLE 3.2 - Addition of New Unit Computations Into DESPAC (Summary Procedure)

1. Executive routine calls Modelling routine
2. Executive routine allows the user to run interactively
3. Executive routine contains NAMELIST features
4. Executive and Modelling routines contain the relevant Common Blocks
5. PROGRAM DESPAC calls Executive routine

3.2.3 Enlargement of the Thermophysical Library File

The library file contains some of the thermophysical properties of ninety-one chemical species (Refer to Appendix E which explains the DESPAC2 Library File).

This file can be extended by adding new components and/or new properties for the existing components.

3.2.3.1 Addition of New Properties Into the Thermophysical Library File for the Existing Components

As in the case of the shell-and-tube heat exchanger routine, density of a component may be required. Hence the procedure to insert a new physical property into the library file is explained below. For this purpose, density (RHO) is selected as an example.

1. Any additional property to be added (i.e. RHO) must be defined in the LIB Common Block and PHYS Common Block (Refer to Appendix D for LIB and PHYS Common Blocks). LIB and PHYS Common Blocks should be modified whenever they are used in DESPAC2. The form of these definitions are shown in Appendix D.

2. Some modifications must be performed in the relevant Auxiliary Subroutines (Refer to Appendix A), as explained below:

   a) Subroutine LOADLB:

   This subroutine copies data for a component from a file into the library.

   A new prefix must be defined using DECODE features in subroutine LOADLB.

   e.g.
   ```
   IF (PREFIX. EQ. '$') DECODE (75,540, LINE) RHO(I)
   540 FORMAT (F15.6)
   ```

   Library file must contain the prefix mentioned in accordance with the FORMAT.

   b) Subroutine SYSTEM:

   In subroutine SYSTEM, data are transferred from /LIB/ to /PHYS/ and /IDENT/ Common Blocks.

   I refers to component I of user (his Ith component)
   II refers to component I in the library /LIB/.

The user has to define the transfer of data as follows:

```
DENS(I) = RHO(II)
```

c) Subroutine DEFINE:

DEFINE allows the user to enter new values (and new components) into the library. Firstly, the information for pure component property is obtained from the user. The definition in the subroutine DEFINE is in the form below:

```
DENS = RHO(I)
```

Then, this value will be transferred to the library file. The necessary definition for this step is as follows:

```
RHO(I) = DENS
```

d) Subroutine STORE:

This subroutine copies data for selected components from library /LIB/ to a disk file named by the user.

In the additional STORE, a WRITE statement for the additional physical properties must be introduced.

```
e.g.    WRITE(UFIL,580)   RHO(I)
   580  FORMAT('$b̸STb̸`,5A5,1Pb̸E12.5)
```

e) Subroutine ERASE:

It erases all data in /LIB/ for component I. The required definition is shown below:

RHO(I) = 0.0

3.2.3.2 Addition of New Components Into the Thermophysical Library File

The user may insert new components into the library file selecting RETREV, DEFINE and STORE routines from the menu. Subroutine RETREV retrieves physical properties from disk files. Subroutine DEFINE allows the user to enter new components into the library and then subroutine STORE stores the values of new components on the library file.

Table 3.3 presents the summary of the procedure for the enlargement of the thermophysical library file of DESPAC.

TABLE 3.3 - The Enlargement of the Thermophysical Library File of DESPAC (Summary Procedure)

Addition of New Properties	Addition of New Components
1. New property must be defined in LIB and PHYS Common Blocks 2. Modifications must be performed in the relevant Auxiliary Routines i.e. LOADLB, SYSTEM DEFINE, STORE, ERASE	New component may be introduced into the Library File employing the Auxiliary Routines RETREV, DEFINE and STORE

IV. APPLICATIONS OF DESPAC2

DESPAC2 can solve steady-state problems for single operation units under a unified structure developed in DESPAC [42]. Complex processes which require more than one unit may be handled on a unit basis as long as the computational routines in DESPAC2 fit the needs of the process. In this chapter, firstly an example run is performed for phase and flash calculations to show the operation of DESPAC2 in detail. Then, six examples involving single operation units are presented. Finally, in order to utilize the full applicational capability of DESPAC2 development of a separation flowsheet consisting of various unit computations, will be attempted.

4.1 AN EXAMPLE RUN TO SHOW THE OPERATION OF DESPAC2

As shown in Appendix G immediately after the executive command statement, DESPAC2 prompts the user a menu with several options to select from. Firstly, the user has to retrieve physical constants from the library file by entering "11" from the menu to operate subroutine RETREV. Then, the name of the library file of thermophysical properties of components must be entered (i.e. PUBDAT, VLE).

After this step the user has to supply the names of the components required. The program is conducted by selecting "12" from the menu which employs subroutine SYSTEM. This subroutine presents three models for vapour enthalpy, four models for liquid enthalpy and three models for vapor-liquid equilibrium calculations. The user has to select one model for each calculation. Components involved are selected by their codes, i.e. 001002 etc. After these steps it is possible to select the unit computation required. For phase calculation the user has to select "3" from the menu. DESPAC2 requests values of parameters by typing the ":" in column 1. To assign values to these parameters, the user enters a list of required parameters followed by a ";". If the user is interested in changing one or more parameters be can repeat the whole calculation supplying the new value of the parameter(s). To operate another modelling routine the user has to enter "N" to negate the "REPEAT? (Y or N)" question, and then enter the code of the desired modelling routine, i.e. "4" for FLASH. The necessary steps are the same as before and their details can be followed in the computer output of the sample run and data file simultaneously which are presented in the following pages.

The italic characters on the computer output represent the response of the user during the interactive run of the program. The INPUT data file (which follows the example run) can also be prepared for the batch run of the program (Refer to Appendix G).

If the user selects "18" from the menu the program is stopped.

It is recommended that Appendix F which explains the input and output symbol descriptions of the computer output(s) and data file(s) is referred to before reviewing the example(s).

EXAMPLE RUN
PHASE AND FLASH CALCULATIONS

```
DESPAC.5.8 (6-APR-81)

PROCEDURES:
 1.KVALUE       7.SHTCUT      11.RETREV      17.HELP
 2.ENTHALPY     8.COLUMN      12.SYSTEM      18.STOP
 3.PHASE        9.CERDA       13.DEFINE      19.TIME AND DATE
 4.FLASH       10.COLCST      14.STORE
 5.ABSEDM      21.HEX         15.ACTFIT
 6.MCCABE      22.EXT

SELECT PROCEDURE:  11

RETREV - RETRIEVE PHYSICAL CONSTANTS FROM DISK FILES

ENTER NAME OF FILE (RETURN FOR PUBLIC DATA):PUBDAT
+DATA WILL BE RETRIEVED FROM FILE PUBDAT
RETRIEVE ALL COMPONENTS FROM FILE? (Y OR N): N

NAME COMPONENT TO BE RETRIEVED (RETURN TO END): WATER
+COMPONENT  1 IS WATER

NAME COMPONENT TO BE RETRIEVED (RETURN TO END): METHANOL
+COMPONENT  2 IS METHANOL

NAME COMPONENT TO BE RETRIEVED (RETURN TO END): ETHANOL
+COMPONENT  3 IS ETHANOL

NAME COMPONENT TO BE RETRIEVED (RETURN TO END): -
LIBRARY IS REDEFINED.  SYSTEM IS UNDEFINED.

PROCEDURES:
 1.KVALUE       7.SHTCUT      11.RETREV      17.HELP
 2.ENTHALPY     8.COLUMN      12.SYSTEM      18.STOP
 3.PHASE        9.CERDA       13.DEFINE      19.TIME AND DATE
 4.FLASH       10.COLCST      14.STORE
 5.ABSEDM      21.HEX         15.ACTFIT
 6.MCCABE      22.EXT

SELECT PROCEDURE:  12

SYSTEM - DEFINE COMPONENTS IN SYSTEM

MODELS FOR VAPOR ENTHALPY HV:
  1. IDEAL SOLUTION OF PERFECT GASES.
  2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
  3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR LIQUID ENTHALPY HL:
  1. IDEAL SOLUTION OF SATURATED LIQUIDS.
  2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
  3. EXCESS ENTHALPY FROM WILSON EQUATION.
  4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR VLE CALCULATIONS:
  1. LIQUID: WILSON ACTIVITY;VAPOR: VIRIAL EQN OF STATE.
  2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
  3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

SELECT MODELS FOR HV,HL,VLE (    BLANK THEN RETURN FOR 1 1 1): 113
SELECT COMPONENTS (0 FOR HELP):  001002003
```

```
SELECTED COMPONENTS:
  1. WATER
  2. METHANOL
  3. ETHANOL

VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
K-VALUES: RAOULT'S LAW.

PROCEDURES:
 1.KVALUE        7.SHTCUT       11.RETREV       17.HELP
 2.ENTHALPY      8.COLUMN       12.SYSTEM       18.STOP
 3.PHASE         9.CERDA        13.DEFINE       19.TIME AND DATE
 4.FLASH        10.COLCST       14.STORE
 5.ABSEDM       21.HEX          15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE: 3

PHASE - BUBBLE POINT AND DEW POINT CALCULATION

ENTER INPUT PARAMETERS (P,T,Z, TLO,TUP,PLO,PUP  ;  )

+:  P = 1,  T = 350,   Z = 2,3,5;


PHASE RESULTS          -BUBBLE POINT-     --DEW  POINT--
 P =    1.000          BT  =  348.839     DT  =  354.401
 T = 350.000           BP  =    1.046     DP  =    .8408

 I  COMPONENT          YBT(I)  YBP(I)     XDT(I)  XDP(I)       Z(I)
 1. WATER               .0794   .0796      .4014   .4038       .2000
 2. METHANOL            .4649   .4638      .1585   .1560       .3000
 3. ETHANOL             .4558   .4566      .4401   .4402       .5000


REPEAT? (Y OR N): Y
ENTER INPUT PARAMETERS (P,T,Z, TLO,TUP,PLO,PUP  ;  )

+:  P = 2;


PHASE RESULTS          -BUBBLE POINT-     --DEW  POINT--
 P =    2.000          BT  =  367.820     DT  =  373.337
 T = 350.000           BP  =    1.046     DP  =    .8408

 I  COMPONENT          YBT(I)  YBP(I)     XDT(I)  XDP(I)       Z(I)
 1. WATER               .0835   .0796      .3922   .4038       .2000
 2. METHANOL            .4480   .4638      .1683   .1560       .3000
 3. ETHANOL             .4685   .4566      .4395   .4402       .5000


REPEAT? (Y OR N): N

PROCEDURES:
 1.KVALUE        7.SHTCUT       11.RETREV       17.HELP
 2.ENTHALPY      8.COLUMN       12.SYSTEM       18.STOP
 3.PHASE         9.CERDA        13.DEFINE       19.TIME AND DATE
 4.FLASH        10.COLCST       14.STORE
 5.ABSEDM       21.HEX          15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE: 4
```

```
 FLASH CALCULATIONS

 SELECT TYPE OF FLASH:

+1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :  7
 ENTER INPUT PARAMETERS
+(T,P,Z,(GUESS,X,Y,V) ;   )

+:  T = 350,     P = 1,     Z = 2,3,5;


 FLASH RESULTS
  HF = -2.5313E+05      T  = 350.000
  HL = -2.6499E+05      P  =   1.000
  HV = -2.1849E+05      V  =    .2550

  I  COMPONENT          X(I)     Y(I)     Z(I)     XI(I)       K(I)
  1. WATER             .2350    .0978    .2000    .1248       .4164
  2. METHANOL          .2592    .4191    .3000    .3562      1.617
  3. ETHANOL           .5058    .4831    .5000    .2463       .9550


 REPEAT? (Y OR N):  Y
 ENTER INPUT PARAMETERS
+(T,P,Z,(GUESS,X,Y,V) ;   )

+: P = 1.5;


 FLASH RESULTS
  HF = -2.6316E+05      T  = 350.000
  HL = -2.6316E+05      P  =   1.500
  HV = -2.1688E+05      V  =    .0000

  I  COMPONENT          X(I)     Y(I)     Z(I)     XI(I)       K(I)
  1. WATER             .2000    .0796    .2000    0.          .2776
  2. METHANOL          .3000    .4638    .3000    0.         1.078
  3. ETHANOL           .5000    .4566    .5000    0.          .6367


 REPEAT? (Y OR N): N
+1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE : 8

 PROCEDURES:
  1.KVALUE       7.SHTCUT       11.RETREV       17.HELP
  2.ENTHALPY     8.COLUMN       12.SYSTEM       18.STOP
  3.PHASE        9.CERDA        13.DEFINE       19.TIME AND DATE
  4.FLASH       10.COLCST       14.STORE
  5.ABSEDM      21.HEX          15.ACTFIT
  6.MCCABE      22.EXT

 SELECT PROCEDURE: 18
   PROGRAM IS STOPPED
```

```
11
PUBDAT
N
WATER
METHANOL
ETHANOL

12
113
001002003
3
P=1,T=350,Z=2,3,5;
Y
P=2;
N
4
7
T=350,P=1,Z=2,3,5;
Y
P=1.5;
N
8
18
21.05.38.UCLP, BU, P04     ,       0.241KLNS.
```

INPUT data file for the batch run of the program.

4.2 EXAMPLES FOR SINGLE OPERATION UNITS

DESPAC2 can solve steady-state problems for single operation units. In order to illustrate this capability of DESPAC2, six examples are tested for single operation units. Two of them are for the multicomponent liquid-liquid extraction and one for the shell-and-tube heat exchanger. For binary distillation, one example is studied. One example is tested for the shortcut multicomponent distillation. The results of the shortcut multicomponent distillation are used to calculate the size and the cost of the calculated column.

The methods and the routines employed for each example can be listed as follows:

	Method	Routine
Example 1:	McCabe Thiele Binary Distillation	MCCABE
Example 2:	Shortcut Multicomponent Distillation	SHTCUT
Example 3:	Shortcut Multicomponent Distillation and Sizing and Costing of the Calculated Column	CERDA
Example 4:	Multicomponent Liquid-Liquid Extraction	EXT
Example 5:	Multicomponent Liquid-Liquid Extraction	EXT
Example 6:	Shell-and-Tube Heat Exchanger	HEX

4.2.1 Example 1

McCabe-Thiele Binary Distillation (MCCABE)

Problem Statement:

This example is taken from McCabe and Smith [29] *(page 560).*

A fractioning column is to be designed to separate a mixture of benzene and toluene. The feed rate is 350 lbmol/hr and it contains 0.44 percent benzene. Benzene percentage in the overhead product is 0.974 and overhead product rate is 153.4 lbmol/hr. A reflux ratio of 3.5 moles to 1 mole of product is to be used.

a) Calculate the moles of bottom product per hour, and benzene percentage in the bottom product.

b) Determine the number of ideal plates and the position of the feed plate, if the feed is saturated liquid.

As explained in the previous example run, routines RETREV and SYSTEM must be supplied to select the components, e.g. benzene and toluene, and the models required to calculate the liquid enthalpy, vapor enthalpy and vapor-liquid equilibrium calculations. In order to employ the McCabe-Thiele calculation method (MCCABE) the user has to choose procedure number "6" from the menu. Routine MCCABE requires RATIO, ALPHA, Q, ETA, XF, XD, F and D parameters to execute the method. Appendix H presents the particular values of the above parameters and the computer output of DESPAC2 for this application. Symbol descriptions can be found in Appendix F.

In Table 4.1 results of DESPAC2 and of McCabe and Smith [29] are tabulated. Results of DESPAC2 are in close agreement with that of McCabe and Smith [29] as shown in Table 4.1 below.

TABLE 4.1 - Results of the McCabe-Thiele Method

	DESPAC2	McCabe & Smith [29]
x_ω	0.0233	0.0235
ω (kmol/h)	196.6	196.6
L	905.93	not available (n.a.)
V	1059.3	n.a.
LB	1255.9	n.a.
VB	1059.3	n.a.
NT	7	7
NB	5	5

4.2.2 Example 2

Shortcut Multicomponent Distillation (SHTCUT)

Problem Statement:

This example is obtained from Perry and Chilton [31], page. 13.27.

A large butane-pentane splitter is to be shut down for repairs. Some of its feed will be diverted temporarily to a smaller column has only 11 bubble-cap trays plus a partial reboiler. The feed enters on the middle tray. Past experience on similar feeds indicates that the 11 trays plus reboiler are equivalent to 10 equilibrium stages and the column has a maximum top vapor capacity of 1.75 times the feed rate on a mole basis. Column will operate at a pressure of 120 lb/in^2 *(8.271 bar). The feed will be at its bubble point (*$q = 1.0$*) at temperature of 185*^{o}*F (358*^{o}*K). The feed has the following composition.*

Component	*FXF (mole%)*
C_3	5
$i\text{-}C_4$	15
$n\text{-}C_4$	25
$i\text{-}C_5$	20
$n\text{-}C_5$	35
	100

The original column normally has less than 2 mole percent $i\text{-}C_5$ *in the overhead and less than 3 mole percent* $n\text{-}C_4$ *in the bottom product. Can these product purities be produced on the smaller column?*

After calling RETREV and SYSTEM routines to select the components and models required, procedure number "7" from the menu must be selected to employ the shortcut multicomponent distillation method (SHTCUT). The user has to specify the column, the method to find reflux ratio and whether the relative volatilities are calculated automatically or not. Depending on the combination of the above mentioned specifications, which are presented in Appendix F, the user may enter the parameters required. In this particular example a new column is specified. Reflux ratio is found as a function of VMAX. Relative volatilities will be calculated by calling the routine FLSHTP. Depending on the selections above for this problem the user has to enter F, LKEY, Q, XF, VFMAX, T, P, FTL and FBH (Information on these computer abbreviations are given in Appendix F). The computer output for this problem and the relevant data file are presented in Appendix H.

Results of DESPAC2 and that of Perry and Chilton [31] are tabulated in Table 4.2.

Results of DESPAC2 and Perry and Chilton [31] close to each other, the deviations should be resulting from the relative volatilities employed in the two calculations.

Recalling the calculated results of DESPAC2, it is concluded that product purities can be produced on the smaller column.

4.2.3 Example 3

Shortcut Multicomponent Distillation (CERDA) & Sizing and Costing of the Calculated Column (COLCST)

This example problem is the same as example 2, but after calling RETREV and SYSTEM routines, number "9" from the menu is selected to employ shortcut multicomponent distillation method (CERDA) instead of SHTCUT. Hence the results of CERDA can be passed on COLCST routine which estimates the size and cost of the distillation column. Values of F, XF, LKEY, HKEY, FTL, FBH, T, P, Q, RFAC and COST must be supplied after selection of CERDA. If the value of COST is not equal to zero, CERDA calls the routine COLCST which requests column construction, column material, tray material, tray type, surface tension of liquid, tray spacing, active plate area, operating superficial velocity and current cost index. Symbol descriptions of parameters are explained in Appendix F.

Appendix H presents the particular values of the parameters (in the INPUT data file) and the computer output of DESPAC2 for this application.

TABLE 4.2 - Results of the Shortcut Multicomponent Distillation (SHTCUT)

	DESPAC2					Perry & Chilton [31]				
	FTL = 0.98		SMIN = 7.19	D = 49.15(kmol/h)		FLT = 0.98		SMIN = 7	D = 48.9(kmol/h)	
	FTR = 3.37		R = 2.5605	B = 50.85(kmol/h)		FTR = 5		R = 2.519	B = 51.1(kmol/h)	
	SD =10.31		RMIN = 0.877	F = 100 (kmol/h)		SD =11		RMIN = 0.9782	F = 100 (kmol/h)	
Component	XF(I)	XD(I)	XB(I)	AL(I)	XI(I)	XF(I)	XD(I)	XB(I)	AL(I)	XI(I)
1. propane	0.05	0.1017	0.0	6.3826	1.00	0.05	0.1004	0.0	4.98	n.a.
2. i-butane	0.15	0.3042	0.0009	2.8117	0.9969	0.15	0.2996	0.0017	2.61	n.a.
3. n-butane	0.25	0.4985	0.0098	2.1636	0.98	0.25	0.4852	0.0168	2.02	n.a.
4. i-pentane	0.20	0.0651	0.3304	1.00	0.16	0.20	0.070	0.3283	1.00	n.a.
5. n-pentane	0.35	0.0305	0.6589	0.81739	0.0427	0.35	0.448	0.6532	0.851	n.a.

Results of CERDA and COLCST routines are presented in Table 4.2.a and 4.2.b, respectively.

TABLE 4.2.a - Results of the Shortcut Multicomponent Distillation (CERDA)

NT =	0.8	T =	358.000	RFAC =	1.2000		
NB =	22.8	P =	8.270	RT =	1.2810	LT =	61.11
F =	100.00	Q =	1.000	RTMIN =	1.0675	VT =	108.81
D =	47.70	FTL =	0.9800	RB =	2.0804	LB =	161.11
B =	52.30	FBH =	0.8400	RBMIN =	1.8857	VB =	108.81

Component	XF(I)	XD(I)	XB(I)	AL(I)	K(I)
propane	0.05	0.1048	0.0000	6.383	3.926
i-butane	0.15	0.3145	0.0000	2.812	1.730
n-butane	0.25	0.5136	0.0096	2.164	1.331
i-pentane	0.20	0.0671	0.3212	1.000	0.6151
n-pentane	0.35	0.000	0.6692	0.8174	0.5028

TABLE 4.2.b - The Size and the Cost of the Distillation Column

GUTHRIE COLUMN COSTING

Liquid flowrate(g/s)	= 0.116×10^5	Liquid density(g/m^3)	= 0.5526×10^6
Vapor flowrate (g/s)	= 7836	Vapor density (g/m^3)	= 0.2001×10^5
Surface tension(N/m)	= 0.02	Column construction	= clad
Active area fraction	= 0.7	Column material	= carbon steel
Number of trays	= 24.62	Tray material	= carbon steel
Tray spacing (m)	= 0.3	Tray type	= Grid, Plate or sieve
Pressure (bar)	= 8.27	Cost index	= 350.0
Diameter (m)	= 1.955	Flooding velocity (m/s)	= 0.2331
Height (m)	= 13.09	Operating velocity (m/s)	= 0.1865
Pressure factor	= 1.064	Tray spacing factor	= 2.20
Material factor	= 1.000	Tray material factor	= 0.00
Matl-prs factor	= 1.064	Tray type factor	= 0.00
Module factor	= 4.230	Tray mat-spac factor	= 2.20

COSTS, 1000 $	INSTALLED	BASE COST, 1968
Column:	186.666	14.283
Trays :	12.519	1.870
Total :	199.186	

4.2.4 Example 4:

Multicomponent Liquid-Liquid Extraction (EXT)

Problem Statement:

First example for liquid-liquid extraction is obtained from Sen [37].

An equimolar mixture of acetone (1) and ethanol (2) is to be separated in a 15 stage extraction column. Feed rate is 0.2 kmol/h. Two solvents, chloroform (3) and water (4) are used, and their flow rates are 0.8 kmol/h and 1 kmol/h, respectively.

Hanson et al. [20] used the 3-suffix Morgules equation for the calculation of the activity coefficients, and gave the binary data as shown in Table 4.3.

TABLE 4.3 - 3-Suffix Margules Binary Interaction Parameters

	(1) - Acetone (2) - Ethanol		(3) - Chloroform (4) - Water			
Species i	*1*	*1*	*1*	*2*	*2*	*3*
Species j	*2*	*3*	*4*	*3*	*4*	*4*
Aij	*0.5446*	*-0.9417*	*1.8720*	*1.6100*	*1.4600*	*5.9100*
Aji	*0.5990*	*-0.6740*	*1.3380*	*0.5010*	*0.8770*	*4.760*

Initially routines RETREV and SYSTEM must be selected, and then number "22" is chosen to employ multicomponent liquid-liquid extraction (EXT). Routine EXT requires BALLPR, TIMINC, H1, H2, M, N, TOL, SREST, SNORM, SACTC, SWRIT, COMPS, COMPN, STARS, initially assumed profiles of X1, X2, F1 and F2, XF, FF and AVAL. In Appendix H, these particular values of the above parameters and the computer output of DESPAC2 are presented. Symbol descriptions are explained in Appendix F.

Table 4.4 tabulates the initially assumed profiles which are taken from Hanson et.al.[20]. The results of Sen [37] and that of DESPAC2 are given in Table 4.5 and Table 4.6, respectively.

Although the input data and the algorithm to solve this problem are the same, the results of DESPAC2 and Sen [37] are slightly different due to the round off criteria of computer systems; UNIVAC 1106 has eight-digit accuracy on the other hand CDC-Cyber 170/815 has 16-digit accuracy, i.e. the CDC's normal operation mode corresponds to the double precision mode of the UNIVAC 1106.

4.2.5 Example 5

Multicomponent Liquid-Liquid Extraction (EXT)

Problem Statement:

Second example for multicomponent liquid-liquid extraction is taken from Sen [37].

In order to separate a mixture of n-heptane (1), and cyclohexane (2), pure furfural (3) is used as the solvent. Flow rate of the mixture is 100 kmol/h and that of the solvent is 1210 kmol/h. Extraction column has 16 stages.

TABLE 4.4 - Initially-Assumed Profiles for Example 4

		Heavy Phase Component Mole Fractions					Light Phase Component Mole Fractions			
Stage No.	Overall Flow Rate (kmol/h)	Acetone	Ethanol	Chloroform	Water	Overall Flow Rate (kmol/h)	Acetone	Ethanol	Chloroform	Water
1	1.0	0.1080	0.0430	0.7940	0.0150	1.0	0.0089	0.0328	0.0024	0.9998
2	1.0	0.1170	0.0750	0.7960	0.0140	1.0	0.0096	0.0578	0.0024	0.9849
3	1.0	0.1190	0.0900	0.7960	0.0140	1.0	0.0098	0.0689	0.0024	0.9703
4	1.0	0.1210	0.0970	0.7960	0.0140	1.0	0.0099	0.0740	0.0024	0.9558
5	1.0	0.1220	0.1010	0.7960	0.0140	1.0	0.0100	0.0773	0.0024	0.9413
6	1.0	0.1240	0.1050	0.7960	0.0140	1.0	0.0102	0.0801	0.0024	0.9276
7	1.0	0.1260	0.1100	0.7960	0.0130	1.0	0.0104	0.0839	0.0024	0.9138
8	1.0	0.1290	0.1180	0.7960	0.0130	1.0	0.0106	0.0902	0.0024	0.9002
9	1.0	0.1310	0.1320	0.7960	0.0130	1.0	0.0108	0.1010	0.0024	0.8868
10	1.0	0.1340	0.1570	0.7960	0.0130	1.0	0.0110	0.1199	0.0024	0.8711
11	0.8	0.0460	0.1250	0.9950	0.0120	1.0	0.0038	0.0961	0.0030	0.8607
12	0.8	0.0320	0.1070	0.9970	0.0120	1.0	0.0027	0.0820	0.0030	0.8505
13	0.8	0.0250	0.0930	0.9970	0.0120	1.0	0.0021	0.0713	0.0030	0.8403
14	0.8	0.0170	0.0770	0.9980	0.0120	1.0	0.0014	0.0587	0.0030	0.8302
15	0.8	0.0090	0.0500	0.9990	0.0120	1.0	0.0008	0.0382	0.0030	0.8107

TABLE 4.5 - Results of the Multicomponent Liquid-Liquid Extraction by Sen [37]

		Heavy Phase Component Mole Fractions					Light Phase Component Mole Fractions			
Stage No.	Overall Flow Rate (kmol/h)	Acetone	Ethanol	Chloroform	Water	Overall Flow Rate (kmol/h)	Acetone	Ethanol	Chloroform	Water
1	0.951	0.10515	0.04389	0.83672	0.01423	1.062	0.00903	0.04276	0.00332	0.94490
2	1.013	0.10816	0.08601	0.78879	0.01704	1.115	0.01076	0.08110	0.00430	0.90384
3	1.066	0.10507	0.12399	0.75108	0.01987	1.163	0.01168	0.11303	0.00533	0.86997
4	1.114	0.10196	0.15549	0.71991	0.02264	1.202	0.01230	0.13659	0.00620	0.84491
5	1.153	0.09958	0.17863	0.69679	0.02501	1.228	0.01267	0.15162	0.00681	0.82891
6	1.179	0.09801	0.19334	0.68196	0.02669	1.244	0.01285	0.15995	0.00715	0.82004
7	1.194	0.09711	0.20148	0.67373	0.02768	1.251	0.01293	0.16411	0.00732	0.81564
8	1.202	0.09665	0.20553	0.66963	0.02819	1.255	0.01296	0.16607	0.00740	0.81357
9	1.206	0.09643	0.20743	0.66771	0.02843	1.256	0.01298	0.16696	0.00743	0.81262
10	1.207	0.09633	0.20830	0.66683	0.02854	1.235	0.01298	0.16738	0.00745	0.81218
11	0.986	0.01626	0.15055	0.81609	0.01710	1.193	0.00173	0.15197	0.00763	0.83867
12	0.944	0.00219	0.13033	0.85231	0.01517	1.168	0.00021	0.13696	0.00705	0.85578
13	0.919	0.00027	0.11065	0.87508	0.01400	1.139	0.00002	0.11799	0.00622	0.87577
14	0.890	0.00003	0.08554	0.90168	0.01274	1.104	0.00000	0.09226	0.00522	0.90252
15	0.855	0.00000	0.05096	0.93781	0.01123	1.049	0.00000	0.05557	0.00405	0.94039

TABLE 4.6 - Results of the Multicomponent Liquid-Liquid Extraction by DESPAC2

		Heavy Phase					Light Phase			
		Component Mole Fractions					Component Mole Fractions			
Stage No.	Overall Flow Rate (kmol/h)	Acetone	Ethanol	Chloroform	Water	Overall Flow Rate (kmol/h)	Acetone	Ethanol	Chloroform	Water
1	0.951	0.10510	0.04401	0.83665	0.01423	1.062	0.00903	0.04287	0.00332	0.04479
2	1.013	0.10810	0.08624	0.78868	0.01698	1.113	0.01078	0.08149	0.00431	0.90342
3	1.066	0.10503	0.12439	0.75084	0.01974	1.161	0.01172	0.11378	0.00533	0.86917
4	1.115	0.10192	0.15610	0.71948	0.0225	1.200	0.01235	0.13756	0.00622	0.84388
5	1.154	0.09952	0.17942	0.69616	0.02491	1.227	0.01272	0.15269	0.00683	0.82776
6	1.181	0.09793	0.19425	0.68116	0.02666	1.243	0.01290	0.16097	0.00719	0.81844
7	1.196	0.09703	0.20237	0.67288	0.02772	1.251	0.01297	0.16488	0.00736	0.81474
8	1.203	0.09658	0.20621	0.66895	0.02820	1.255	0.01299	0.16647	0.00742	0.81312
9	1.206	0.09639	0.20779	0.66734	0.02847	1.256	0.01298	0.16702	0.00743	0.81257
10	1.207	0.09632	0.20834	0.66680	0.02853	1.234	0.01298	0.16726	0.00744	0.81232
11	0.986	0.01625	0.15039	0.81631	0.01705	1.191	0.00173	0.15183	0.00761	0.83833
12	0.944	0.00218	0.13006	0.85264	0.01512	1.166	0.00021	0.13675	0.00702	0.85601
13	0.918	0.00027	0.11037	0.87542	0.01395	1.138	0.00002	0.11780	0.00620	0.87598
14	0.890	0.00003	0.08534	0.90192	0.01270	1.103	0.00000	0.09211	0.00520	0.90268
15	0.855	0.00000	0.05091	0.93782	0.01126	1.051	0.00000	0.05532	0.00402	0.94066

In this case to calculate the activity coefficients NRTL equation is used. NRTL binary data is obtained from Sen [37] and tabulated in Table 4.7.

TABLE 4.7 - NRTL Binary Interaction Parameters

(1) - n-heptane, (2) - Cyclohexane, (3) - Furfural
T = 30°C

Species i	*Species j*	α_{ij}	C_{ij} *(cal/mole)*	C_{ji} *(cal/mole)*
1	*2*	*0.30*	*-535*	*611*
1	*3*	*0.35*	*1401*	*1418*
2	*3*	*0.35*	*1443*	*992*

After employing RETREV, and SYSTEM routines, the user selects EXT routine and enters the particular values of this problem for the parameters required which are presented in the Example 4.

The computer output and the INPUT data file of this problem are given in Appendix H.

Table 4.8 tabulates the initially-assumed profiles. The results of Sen [37] and DESPAC2 are presented in Table 4.9 and Table 4.10 respectively. The results are slightly different due to the accuracy of UNIVAC 1106 and CDC Cyber 170/815 computer systems as discussed earlier in Example 4.

TABLE 4.8 - Initially-Assumed Profiles for Example 5

Stage No. (J)	Overall Flow Rate (kmol/h)	Heavy Phase Component Mole Fractions			Overall Flow Rate (kmol/h)	Light Phase Component Mole Fractions		
		n-heptane	Cyclohexane	Furfural		n-heptane	Cyclohexane	Furfural
$1 \leq j \leq 16$	1240	0.02	0.08	0.90	70	0.70	0.10	0.20

TABLE 4.9 - Results of the Multicomponent Liquid-Liquid Extraction by Sen [37]

Stage No.	Overall Flow Rate (kmol/h)	Heavy Phase Component Mole Fractions			Overall Flow Rate (kmol/h)	Light Phase Component Mole Fractions		
		n-heptane	Cyclohexane	Furfural		n-heptane	Cyclohexane	Furfural
1	1297.833	0.03853	0.03853	0.92295	48.846	0.57520	0.34949	0.07531
2	1246.488	0.02247	0.01365	0.96387	10.673	0.09234	0.04176	0.86590
3	1208.408	0.00073	0.00034	0.99893	12.812	0.00073	0.00034	0.99893
4	1210.296	0.00001	0.00000	0.99999	12.668	0.00001	0.00000	0.99999
5	1208.298	0.00000	0.00000	1.00000	12.892	0.00000	0.00000	1.00000
6	1208.813	0.00000	0.00000	1.00000	12.795	0.00000	0.00000	1.00000
7	1208.753	0.00000	0.00000	1.00000	12.150	0.00000	0.00000	1.00000
8	1208.048	0.00000	0.00000	1.00000	12.150	0.00000	0.00000	1.00000
9	1208.045	0.00000	0.00000	1.00000	12.150	0.00000	0.00000	1.00000
10	1208.050	0.00000	0.00000	1.00000	12.150	0.00000	0.00000	1.00000
11	1208.054	0.00000	0.00000	1.00000	12.150	0.00000	0.00000	1.00000
12	1208.059	0.00000	0.00000	1.00000	12.150	0.00000	0.00000	1.00000
13	1208.064	0.00000	0.00000	1.00000	12.150	0.00000	0.00000	1.00000
14	1208.068	0.00000	0.00000	1.00000	12.150	0.00000	0.00000	1.00000
15	1208.073	0.00000	0.00000	1.00000	12.150	0.00000	0.00000	1.00000
16	1208.077	0.00000	0.00000	1.00000	12.150	0.00000	0.00000	1.00000

TABLE 4.10 - Results of the Multicomponent Liquid-Liquid Extraction by DESPAC2

	Heavy Phase				Light Phase			
		Component Mole Fractions				Component Mole Fractions		
Stage No.	Overall Flow Rate (kmol/h)	n-heptane	Cyclohexane	Furfural	Overall Flow Rate (kmol/h)	n-heptane	Cyclohexane	Furfural
1	1297.786	0.03853	0.03852	0.92295	48.788	0.57520	0.34946	0.07534
2	1246.273	0.02241	0.01361	0.96398	11.051	0.07688	0.03596	0.88716
3	1208.737	0.00059	0.00029	0.00012	12.832	0.00059	0.00029	0.99912
4	1205.417	0.00001	0.0000	0.9999	12.679	0.00001	0.0000	0.9999
5	1205.640	0.0000	0.0000	1.0000	12.934	0.0000	0.0000	1.0000
6	1204.128	0.0000	0.0000	1.0000	12.150	0.0000	0.0000	1.0000
7	1204.196	0.0000	0.0000	1.0000	12.150	0.0000	0.0000	1.0000
8	1204.180	0.0000	0.0000	1.0000	12.150	0.0000	0.0000	1.0000
9	1204.174	0.0000	0.0000	1.0000	12.150	0.0000	0.0000	1.0000
10	1204.168	0.0000	0.0000	1.0000	12.150	0.0000	0.0000	1.0000
11	1204.162	0.0000	0.0000	1.0000	12.150	0.0000	0.0000	1.0000
12	1204.156	0.0000	0.0000	1.0000	12.150	0.0000	0.0000	1.0000
13	1204.150	0.0000	0.0000	1.0000	12.150	0.0000	0.0000	1.0000
14	1204.143	0.0000	0.0000	1.0000	12.150	0.0000	0.0000	1.0000
15	1204.137	0.0000	0.0000	1.0000	12.150	0.0000	0.0000	1.0000
16	1204.131	0.0000	0.0000	1.0000	12.150	0.0000	0.0000	1.0000

4.2.6 Example 6

Shell-and-Tube Heat Exchanger (HEX)

Problem Statement:

This example is taken from Kern [25].

175000 lb/hr (22.07 kg/s) of distilled water enters an exchanger at 93°F (307 K) and leaves at 85°F (302 K). The heat will be transformed to 280000 lb/hr (35.31 kg/s) of raw water coming from supply at 75°F (297 K) and leaving the exchanger at 80°F (300 K). Fouling factor is 0.0005 hr-ft^2-F/Btu for distilled water and 0.0015 hr-ft^2-F/Btu for raw water.

For this exchanger 18 B.W.G, 3/4 in (19 mm) OD tubes will be used. Standard tube length is 16'0" (4.88 m). Tubes will be laid out or 15/16 in (23.8 mm) triangular pitch. The bundle is arranged for two passes and baffles are spaced 12 in (305 mm) apart.

Inside and outside heat transfer coefficients are obtained from Table 3.1 of Backhurst and Harker [3] as initial guesses and their values are assumed as the same and are 1150 Btu/hr-ft^2-°F (6530 w/m^2-K).

The aim is to design a heat exchanger for the specified job.

After calling routines RETREV and SYSTEM, number "21" is selected from the table to employ the shell-and-tube heat exchanger calculation method (HEX). Subroutine HEX requires the values of TH1, TH2, TC1, TC2, N, HO, HDO, HDI, HI, DI, DO, SL, NTP, PT, B, Y, DE, MCOMP, KH, KC, VISH, VISC, TETA, FLAG, EPS, SWCH, SWCH1, SWCH2 and CPL to execute the method.

Explanations about the above abbreviations are given in Appendix F.

The computer output of DESPAC2 and the particular values of the above parameters are presented in Appendix H.

Results of DESPAC2 and that of Kern [25] are tabulated in Table 4.11.

TABLE 4.11 - Results of the Shell-and-Tube Heat Exchanger

	DESPAC2	Results of Kern [25]
UD (J/s-m^2-K)	1696.239	1470.602
A (m^2)	54.591	46.637
NT	188	160
DIS (mm)	389.989	387.35
HI (J/s-m^2-K)	7917.169	6558.090
HO (J/s-m^2-K)	6159.466	5734.78

The difference between the results listed above may be due to the fact that different procedures were employed for calculations. In computer results, correction factor F, (for true counterflow) and allowing a 10 percent heat overload are also taken under consideration, whereas Kern [25] ignores these facts. DESPAC2 calculates h_i and h_o from empirical equations, on the other hand Kern [25] employs figures to find the J_H factor which is used for the calculation of h_i and h_o values and this is the main cause of the differences in the results presented in Table 4.11.

4.3 PROCESS FLOWSHEET DEVELOPMENT

The capabilities of DESPAC2 for the solution of individual processing units have been shown in the preceding example, i.e. from example 1 to example 6, and the results obtained have been discussed in relation to the results obtained from related references.

Now, to demonstrate the capability and utility of DESPAC2 in process flowsheet development and synthesis calculations, a series of calculations are given. Firstly, a number of flowsheet alternatives are produced. After the elimination of some alternatives which do not seen to be feasible at the first glance the remaining ones are evaluated via DESPAC2 calculation.

In order to perform a particular application a processing system to separate a mixture containing hydrogen chloride, (HCl), 10 percent; benzene, (B), 40 percent and 50 percent monochlorobenzene, (MCB) will be designed to obtain minimum 99.7 percent benzene at the top product, and 99.9 percent MCB at the bottom product. To reach the desired output, numerous flowsheet configurations may be proposed.

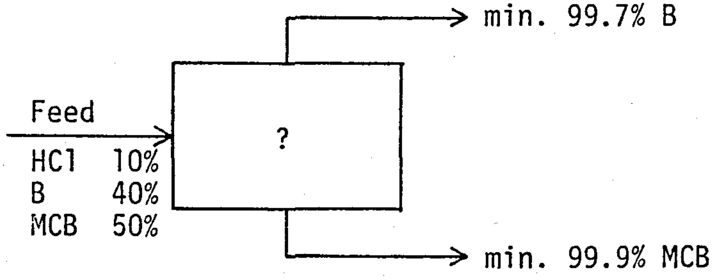


Figure 4.1 - Specifications of the separation problem.

As depicted in Figure 4.1 the black box may contain unit computations with various processing configurations.

As mentioned before DESPAC2 is capable of handling flash, distillation, absorption, liquid-liquid extraction and heat exchanger units. In order to check the applicability of the available units, firstly, some physical properties, which are of decisive importance such as boiling-point of the input species will be considered. Table 4.12, covers the boiling-point data of the input species.

TABLE 4.12 - Boiling - Point Data

Species	BP (°K at 1 atm)
HCl	188
B	353
MCB	405

Because of the substantial difference of the boiling-point of HCl and its corrosive character it seems logical to remove HCl at the beginning of the process. To take off HCl flash, distillation, absorption and extraction units may be proposed. Extraction may be performed using a polar solvent such as water which takes mainly HCl and some benzene and MCB from the mixture. Water forms an azeotropic mixture with HCl and also with benzene ([31], Table 13.11 and Table 13.10). Since loss of benzene and MCB is inevitable in extraction, this method is not probably economical and then it will be diminished from further consideration.

The boiling point of HCl is extremely low which rejects the distillation for separation, thus this method is also abandoned. On the other hand, the remaining alternatives flash and absorption may be applicable to remove HCl. Absorption uses a solvent to remove one of the species from a gas mixture. Flash prepares the required phase separation of the mixture. After the removal of HCl from the mixture, it is reasonable to use a distillation column to separate benzene and MCB.

Various proposed flowsheet configurations are depicted in Figure 4.2. These configurations will be studied in Section 4.3.1 and Section 4.3.2.

4.3.1 Discussion of the Proposed Flowsheet Configurations (c), (d) and (e)

Proposed flowsheets depicted in Figure 4.2 are studied starting from the most logical alternatives. Flowsheet (d) which is the improved version of flowsheet (c), and flowsheet (e) which is the modified version of (d) seem to be the most appropriate configurations to reach the desired product purity. Consequently, flowsheets (d) and (e) are studied and explained, in detail, below.

Firstly, the flowsheet (d) will be handled. Figure 4.3 is the detailed scheme of this flowsheet.

As shown in Figure 4.3, the feed is separated into two phases in the flash unit (F-1). The vapor from F-1 is sent to the absorber (A-1), and HCl is removed from the mixture using MCB as solvent.

Liquid products of (F-1) and (A-1) are mixed and sent to the distillation column (D-1) to separate benzene and MCB. Bottom product of (D-1) is passed through a heat-exchanger (H-1) so its temperature is reduced, then the required amount may be recycled to the absorber.

DESPAC2 contains various types of flash calculations. Because the flash temperature and pressure are specified, FLSHTP is appropriate. ABSEDM and HEX routines are suitable for absorption and heat exchanger calculations. For the binary distillation, MCCABE is selected. In Appendices A and B, detailed information about FLSHTP, ABSEDM, HEX and MCCABE routines are given.

Table 4.13 represents the available input data for the streams (i.e. S01, S05, S11) to and from the blocks, as shown in Figure 4.3.

TABLE 4.13 - Input Data for Figure 4.3

	S01 (kmol/h)	S05 (kmol/h)	S09 (kmol/h)	S10 (kmol/h)	S11 (kmol/h)
HCl	10	0	0		
B	40	0.067281	39.9561		
MCB	50	100.61	0.099722		
Total	100	100.68	40.056		
Degrees,K				425.9	321.88

The proposed process flow diagram will be tested at different flash temperatures, and these cases are explained in the following pages.

The input data required for this example are obtained from FLOWTRAN [12] and presented in Appendix I.

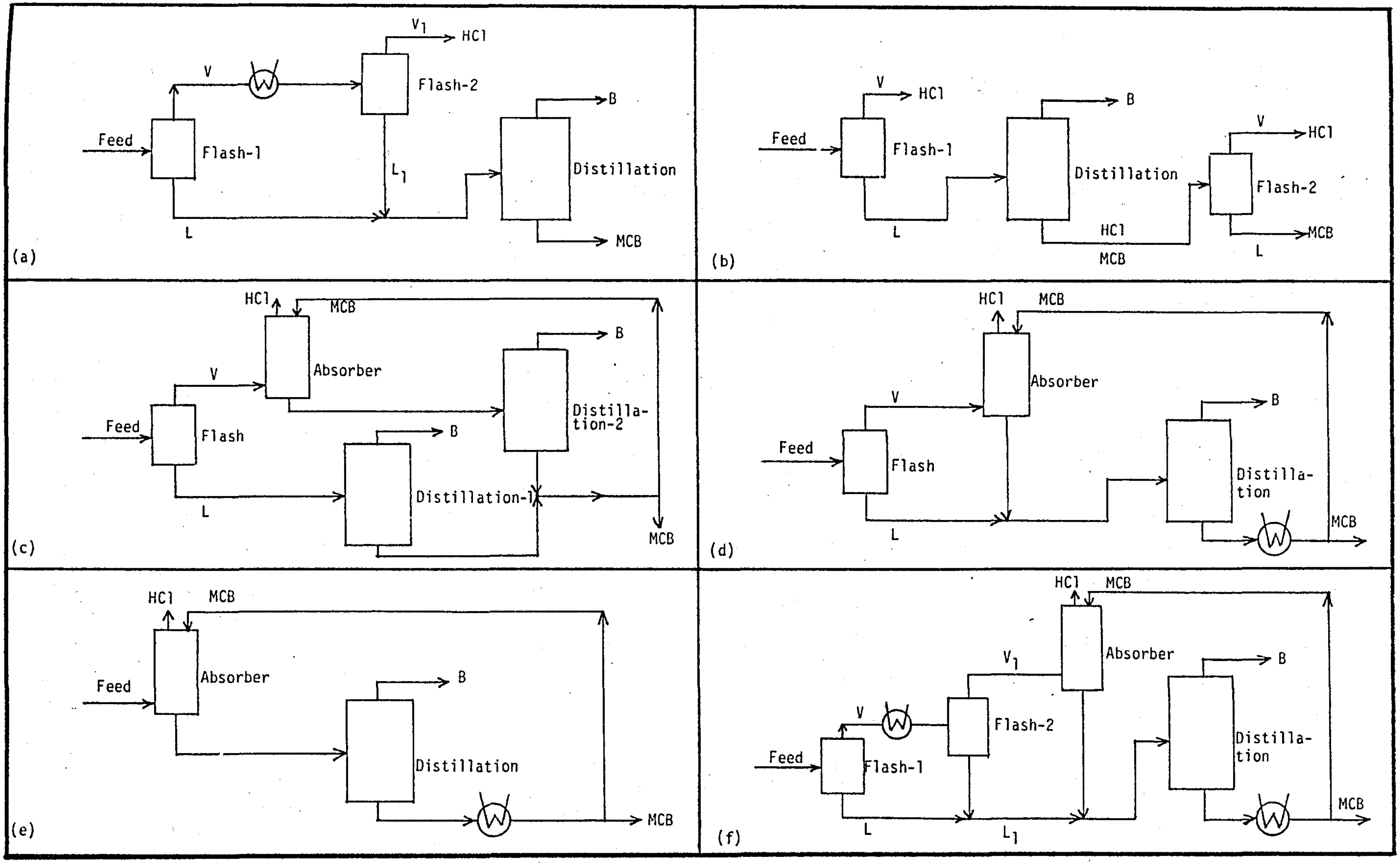


Figure 4.2 - Possible alternate flowsheet configurations.

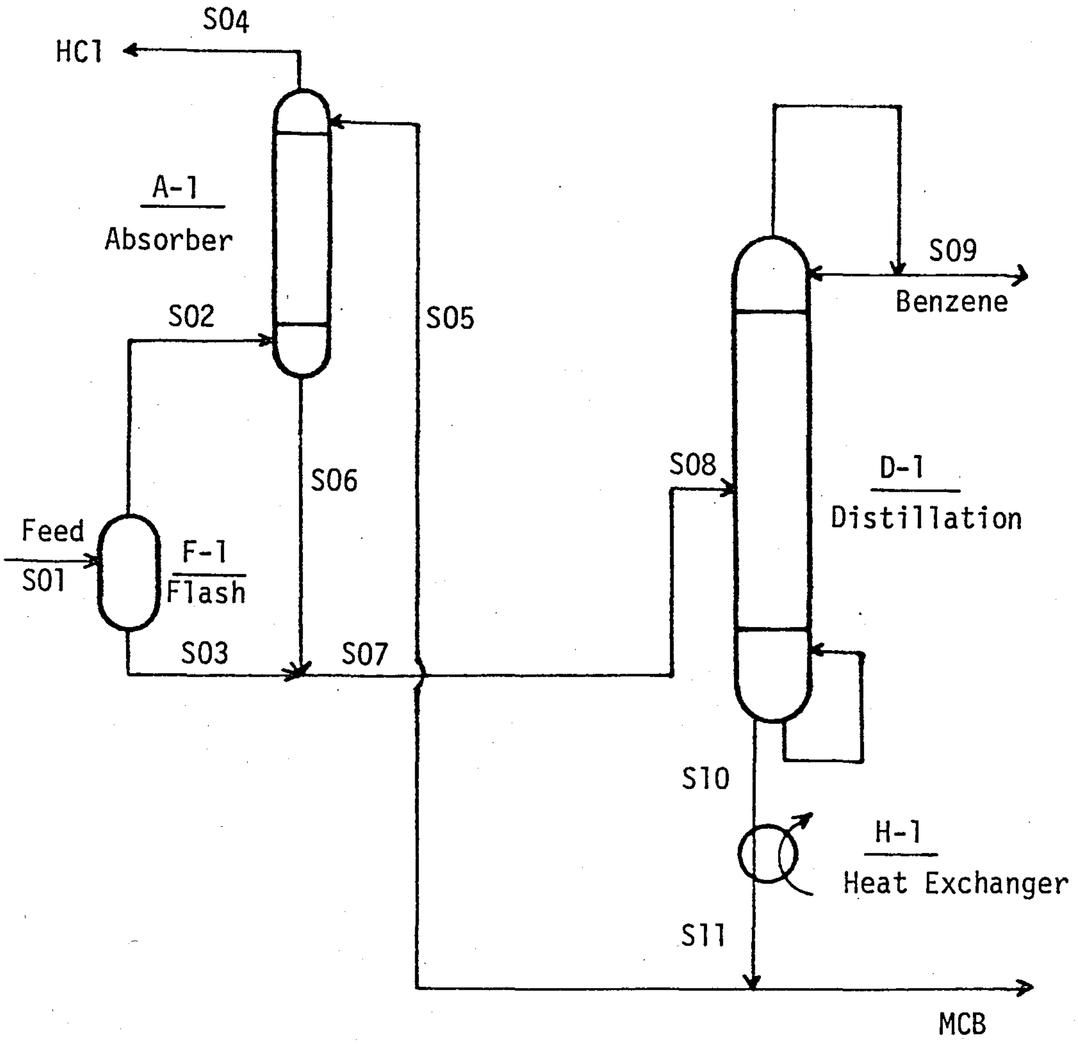


Figure 4.3 - Detailed scheme of the proposed flowsheet (d) of Figure 4.2.

CASE 1:

Feed temperature is assumed as 200°F (366.48°K). Specifications and the results of the flash, absorption, distillation and heat exchanger units may be observed in the computer output and the relevant data file in Appendix H. Input and output symbol descriptions of computer outputs are explained in Appendix F.

In DESPAC2, results of a unit computation can not be transferred to the other unit automatically. The user has to control the transfer of data between units. Necessary calculations and conversions must be done manually.

For this example, such calculations will be explained below and the procedure is the same for the others.

Feed is separated into two phases at T = 200°F (366.48°K). The input data for the flash unit are given below,

T = 366.48°K
P = 2.38 bar
Z = 10, 40, 50
HF = 26008 J/kmol

The results of the flash unit are depicted in Table 4.14.

The X(I), Y(I) and Z(I) values in Table 4.14 represent fractions of S03, S02 and S01 streams, respectively. XI(I) are the fractions of components entering in feed which leave in the vapor product.

TABLE 4.14 - Results of the Flash Unit

Component	X(I)	Y(I)	Z(I)	XI(I)	K(I)
HCl	0.0103	0.6594	0.10	0.9108	63.73
B	0.4216	0.2652	0.40	0.09157	0.629
MCB	0.5680	0.0754	0.50	0.02084	0.1328

The results of the flash unit are prepared as the input data for the absorber and the distillation column as follows:

Calculation of S02:

	Z(I) * XI(I)		S02 (kmol/h)
HCl	10 x 0.9108	=	9.108
B	40 x 0.0916	=	0.366
MCB	50 x 0.0208	=	1.04
Total		=	10.514

Calculation of S03:

S03 = S01 - S02

S03 = 89.486 kmol/h

	S03 * X(I)		S03 (kmol/h)
HCl	89.486 x 0.0103	=	0.921
B	89.486 x 0.4216	=	37.72
MCB	89.486 x 0.5680	=	50.83
Total		=	89.486

Y(I) values from the flash results are directly fed to the absorber. Recalling the total and the component flow rates of S05 stream from Table 4.13, LT and XT(I) values are obtained as the input to the absorber. In Table 4.15 the input data for the absorber are presented.

TABLE 4.15 - Input Data for the Absorber Unit

TT = 326.37 K

TB = 401.33 K

P = 2.17 bar

LT = 100.68 kmol/h, XT = 0., 0.0006683, 0.99

VB = 10.514 kmol/h, YB = 0.6594, 0.2652, 0.0754

N = 3

Results of the absorber are tabulated in Table 4.16.

TABLE 4.16 - Results of the Absorber Unit

VT = 6.3251 kmol/h
LB = 104.87 kmol/h

Component	XT(I)	XB(I)	YT(I)	YB(I)	XIT(I)	XIB(I)
HCl	0.0	0.0077	0.9683	0.6594	0.99285	0.11658
B	0.0007	0.0272	0.0002	0.2652	0.01362	0.99991
MCB	0.9993	0.9651	0.0315	0.0754	0.00198	1.00

VT and YT(I) values correspond to the S04 stream, LB and XB(I) values correspond to the S06 stream.

Preparation of the input data for the distillation column:

	LB * XB(I)		S06 (kmol/h)
HCl	104.87 x 0.0072	=	0.807
B	104.87 x 0.0272	=	2.852
MCB	104.87 x 0.9651	=	101.21
Total		=	104.87

Liquid products from the bottoms of the flash and absorber units are S03 and S06, respectively. These are mixed to obtain S07 stream as shown below:

	S03 (kmol/h)	S06 (kmol/h)	S07 (kmol/h)	$X(I)_{S07}$
HCl	0.921	0.807	1.728	0.00889
B	37.72	2.852	40.572	0.20877
MCB	50.83	101.21	152.04	0.78234
Total	89.486	104.87	194.34	

Even small amounts of HCl will affect the non-ideality of the system benzene and MCB considerably. However as can be concluded from the above results, the amount of HCl in the S07 stream is negligible for a rough initial calculation. Therefore, S07 stream is recalculated and named as S08, as shown below.

	S08 (kmol/h)	$X(I)_{S08}$
HCl	0.0	0.0
B	40.572	0.2106
MCB	152.04	0.7894
Total	192.61	

Consequently, binary distillation (MCCABE) can be employed.

Required parameters for the distillation unit are presented in Table 4.17. Feed is given to the column at $T = 259.91^{\circ}$F (from FLOWTRAN [12]). The distillate flow rate (D) and composition (XD) which correspond to the S09 column of Table 4.13, are input to the column. On the other hand S08 and $X(I)_{S08}$ values calculated above are entered as feed flow rate, F, and composition, XF, respectively. Reflux ratio is 1.3 which is obtained from Appendix F. The user has to refer to Appendix F, for the values of Q, Eta and Alpha.

TABLE 4.17 - Input Data for the Distillation Unit

Ratio = 1.3	XF = 0.2106
Alpha = 3.878	XD = 0.9975
Q = 1.	F = 192.61 kmol/h
Eta = 1.	D = 40.056 kmol/h

In Table 4.18, results of the distillation column are tabulated.

TABLE 4.18 - Results of the Distillation Unit

XW = 0.004	LB = 278.09
W = 152.56 kmol/h	VB = 125.53
L = 85.477	NT = 9
V = 125.53	NB = 8

Then, the amount and the composition of the bottom stream (S10) are obtained, as follows:

		S10 (kmol/h)	$X(I)_{S10}$
B	152.56 x 0.004 =	0.61024	0.004
MCB	152.56 x 0.996 =	151.949	0.996
Total	=	152.56	

Results of DESPAC2 and the desired fractions at the bottom product are given in Table 4.19 for comparison. The results of DESPAC2 for the proposed flowsheet (d) at T = 200°F is not appropriate because the amount of MCB does not fulfill the minimum requirement and the amount of benzene is more than allowed.

TABLE 4.19 - Results of CASE 1 for Figure 4.3.

	DESPAC2		Specified fractions at the bottom product	% Difference
	S10 (kmol/h)	$X(I)_{S10}$	$X(I)_{S10}$	
B	0.61024	0.0040	0.0010	75
MCB	151.949	0.9960	0.9990	0.4
Total	152.56			

Bottom product obtained from the distillation column is passed through a 1-2 shell-and-tube heat exchanger. The input data required are given in Appendix H, and symbol descriptions are presented in Appendix F.

The value of mcomp (1) is the flowrate of bottom product (kg/s) and mcomp (2) is the flow rate of water (kg/s).

Component 1 is the hot fluid (FLAG = 1), and hot fluid is in the shell side (SWCH = 0), Triangular pitch arrangement is selected (SWCH1 = 0), and tube wall correction is neglected (SWCH2 = 0).

Computer output and the corresponding INPUT data file are given in Appendix H.

CASE 2:

In order to obtain better results than that of CASE 1, feed temperature is increased to 250°F (394.1 K).

The computer output and the corresponding data file are presented in Appendix H.

The same procedure of CASE 1 is repeated to transfer data between the routines representing the processing units in the flowsheet.

Calculated values of DESPAC2 and the specifications required, and their relative differences are given in Table 4.20.

TABLE 4.20 - Results of CASE 2 for Figure 4.3.

	DESPAC2		Specified fractions at the bottom product	% Difference
	S10 (kmol/h)	$X(I)_{S10}$	$X(I)_{S10}$	
B	0.090174	0.0006	0.0010	40
MCB	150.199	0.9994	0.9990	0.04
Total	150.29			

Calculated results are acceptable in this case, since the amount of MCB fulfills the minimum amount requirement, and the amount of benzene is less than allowed.

CASE 3:

In this case temperature of the feed is raised to 270°F (405.2 K). The computer output and the data file are given in Appendix H. Table 4.21 depicts the results and their relative differences.

TABLE 4.21 - Results of CASE 3 for Figure 4.3.

	DESPAC2		Specified fractions at the bottom product	% Difference
	S10 (kmol/h)	$X(I)_{S10}$	$X(I)_{S10}$	
B	0.06009	0.0004	0.0010	60
MCB	150.1699	0.9996	0.9990	0.06
Total	150.23			

CASE 3 also meets the product requirements, therefore this case is also acceptable.

CASE 4:

Feed temperature is assumed as 280°F (410.77 K).

Computer output and the data file are presented in Appendix H.

Results are compared in Table 4.22.

TABLE 4.22 - Results of CASE 4 for Figure 4.3.

	DESPAC2		Specified fractions at the bottom product	% Difference
	S10 (kmol/h)	$X(I)_{S10}$	$X(I)_{S10}$	
B	0.06009	0.0004	0.0010	60
MCB	150.164	0.9996	0.9990	0.06
Total	150.26			

This case is also appropriate to fulfill the product requirements, since the amount of MCB is more than specified, and that of benzene is less than the required values.

CASE 5:

When feed temperature is raised to 300°F (421.88 K) it is observed from the computer output and the data file given in Appendix H that the feed is superheated vapor.

Another process flow diagram is proposed for this case, and presented in Figure 4.4 which is the same as the proposed flowsheet (e) of Figure 4.2. Feed is vapor and directly enters the absorber (A-1). Liquid product from the bottom of (A-1) is fed to the distillation column (D-1). Bottom product of (D-1) is passed through a heat exchanger (H-1).

CASE 6:

For this case the proposed flow diagram is shown in Figure 4.4.

Feed is directly sent to the absorber without using the flash unit.

Table 4.23 represents the input data for the streams in Figure 4.4.

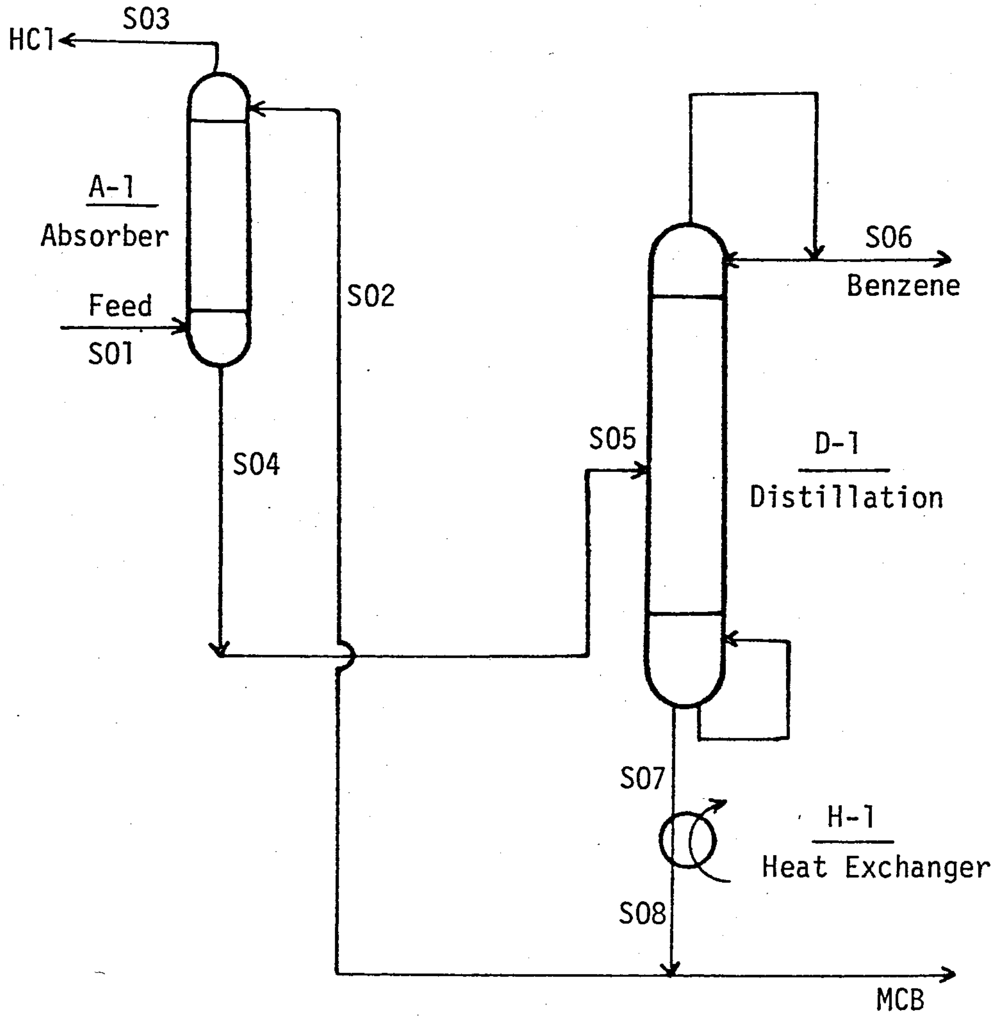


Figure 4.4 - Detailed scheme of the proposed flowsheet (e) of Figure 4.2.

TABLE 4.23 - Input Data for Figure 4.4.

	S01 (kmol/h)	S02 (kmol/h)	S06 (kmol/h)	S07 (kmol/h)	S08 (kmol/h)
HCl	10	0	0	0	0
B	40	0.067281	39.9561		
MCB	50	100.61	0.099722		
Total	100	100.68	40.056		
Degrees,K				425.9	321.88

The intermediate calculations are simpler for this case. In Appendix H, the computer output and the data file are presented. Results are given in Table 4.24.

TABLE 4.24 - Results of CASE 6 for Figure 4.4.

	DESPAC2		Specifed fractions at the bottom product	% Difference
	S07 (kmol/h)	$X(I)_{S07}$	$X(I)_{S07}$	
B	0.0	0.0	0.0010	100
MCB	150.14	1.00	0.9990	0.1
Total	150.14			

As observed in Table 4.24, the bottom product does not contain benzene. It may be concluded that some benzene is lost from the top of the absorber. In order to reduce this benzene loss;

- Number of stages in the absorber should be increased
- Flow rate of the solvent should be increased.

In the following pages, these cases will be studied.

CASE 7:

Number of theoretical stages are increased to six in the absorber.

The computer output and data file are given in Appendix H.

Results are tabulated in Table 4.25.

TABLE 4.25 - Results of CASE 7 for Figure 4.4.

	DESPAC2		Specified fractions at the bottom product	% Difference
	S07 (kmol/h)	$X(I)_{S07}$	$X(I)_{S07}$	
B	0.10517	0.0007	0.0010	30
MCB	150.144	0.9993	0.9990	0.03
Total	150.25			

Results of CASE 7 are also satisfactory, since the product requirements are fulfilled.

CASE 8:

Flow rate of solvent to the absorber is increased to 110.68 kmol/h.

The computer output and the data file are presented in Appendix H.

Results are given in Table 4.26.

TABLE 4.26 - Results of CASE 8 for Figure 4.4.

	DESPAC2		Specified fractions at the bottom product	% Difference
	S07 (kmol/h)	$X(I)_{S07}$	$X(I)_{S07}$	
B	0.0480	0.00030	0.0010	70
MCB	160.112	0.9997	0.9990	0.07
Total	160.16			

The required specifications are also met in this case.

4.3.1.1 Summary and Discussion of the Results of Flowsheets (d) and (e)

In order to separate a mixture of HCl, Benzene and MCB proposed flowsheets (d) and (e) of Figure 4.2 are studied at different processing conditions. Table 4.27 shows the results of these cases. For Figure 4.3 five cases are studied at different flash temperatures. Benzene percentage at the bottom is higher than the specified (0.001) at 200°F. On the other hand, benzene percentage is less than the specified, at a temperature range between 250 to 280°F. Hence, the proposed flowsheet Figure 4.3 is appropriate for this range. If the temperature is raised to the 300°F, the feed is superheated vapor and may be directly fed to the absorber as shown in Figure 4.4. In CASE 6 bottom product from the distillation column does not contain benzene, and this indicates some benzene is lost in the absorber, and it is observed that the number of stages of distillation tower is increased from 21 to 26.

TABLE 4.27 - Summary of the Results

	CASE 1	CASE 2	CASE 3	CASE 4	CASE 5	CASE 6	CASE 7	CASE 8
	FIGURE 4.3					FIGURE 4.4		
FLASH								
T (°F)	200	250	270	280	300	-	-	-
ABSORBER								
No. of stages	3	3	3	3	3	3	6	3
Flow rate of solvent(kmol/h)	100.68	100.68	100.68	100.68	100.68	100.68	100.68	110.68
DISTILLATION								
No. of stages	17	21	21	21	-	26	20	22
% Benzene at the bottom	0.40	0.06	0.04	0.04	-	0.0	0.07	0.03
% MCB at the bottom	99.6	99.94	99.96	99.96	-	100.0	99.93	99.97
Total flow rate of bottom (kmol/h)	152.56	150.29	150.23	150.26	-	150.14	150.25	160.16

In order to reduce the benzene loss, firstly the number of stages of the absorber is increased to 6 in CASE 7. For this case, benzene and MCB percentages fulfill the required specifications. Secondly, flow rate of solvent is increased to 110.68 kmol/h in CASE 8. It is observed that the benzene percentage is less than the specified, but the number of stages of the distillation column increases from 20 to 22. Furthermore, the total flow rate of bottoms is much higher than the other cases.

Either one of the two proposed flowsheets may be selected at the suitable conditions. First flowsheet (Fig. 4.3) contains a flash unit, second flowsheet (Fig. 4.4) is proposed to remove this flash unit, but in this case the feed must be heated up to a higher temperature and the number of stages in the distillation column increases. The appropriate process flowsheet may be chosen making a detailed analysis between the two processing schemes.

4.3.2 Discussion of the Proposed Flowsheet Configurations (a), (b) and (f)

Since the desired recovery of benzene and MCB is obtained either in flowsheet (d) or (e) it is unnecessary to test flowsheet (f) which requires more units than flowsheet (d).

Flowsheet (a) is also studied in order to observe the effect of the absence of an absorber unit. Detailed scheme of this flowsheet is given in Figure 4.5. In this configuration the feed is separated into two phases in flash unit (F-1). The vapor product

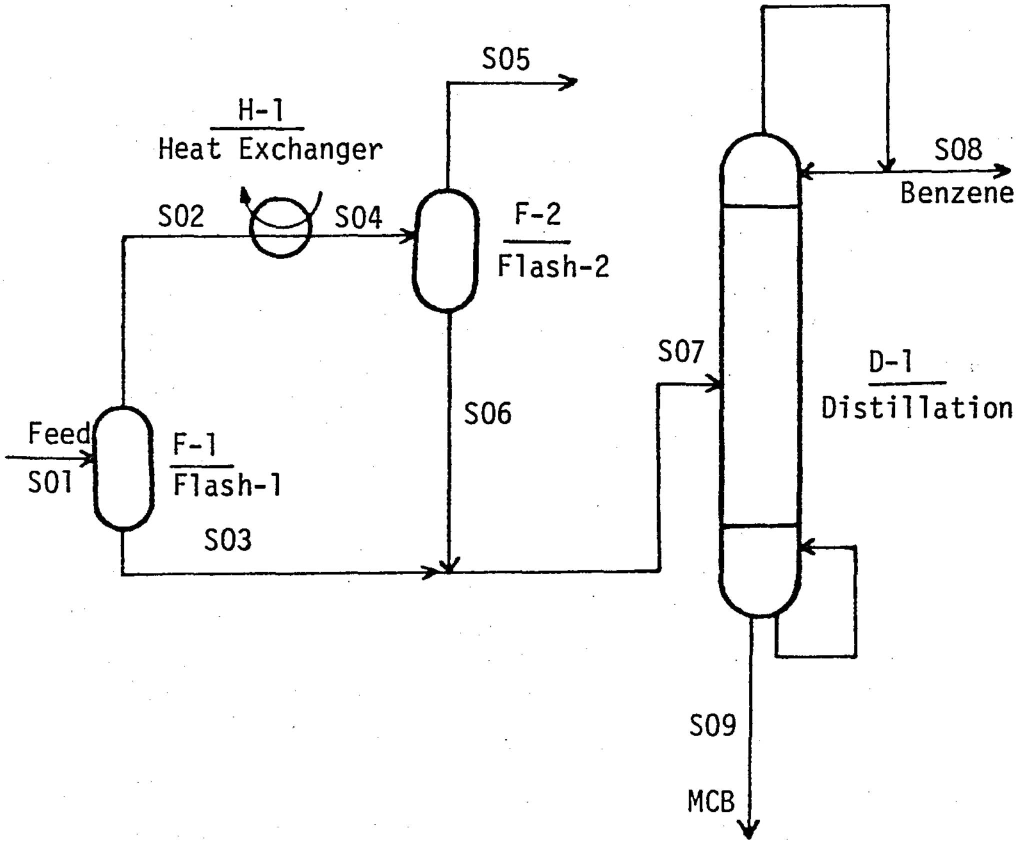


Figure 4.5 - Detailed scheme of the proposed flowsheet (a) of Figure 4.2.

is cooled and sent to the second flash unit (F-2). The liquid products of (F-1) and (F-2) are combined and fed to the distillation column (D-1).

The input data required are obtained from FLOWTRAN [12] and presented in Table 4.28.

TABLE 4.28 - Input Data for Figure 4.5.

	S01 (kmol/h)
HCl	10
B	40
MCB	50
Total	100
Degrees, °K	405.2
Bar	2.38

The results of the first flash unit are summarized in Table 4.29.

TABLE 4.29 - Results of the FLASH-1 Unit.

Component	X(I)	Y(I)	Z(I)	XI(I)	K(I)
HCl	0.0019	0.1995	0.10	0.9904	104.2
B	0.3006	0.5009	0.40	0.6215	1.666
MCB	0.6975	0.2996	0.50	0.2974	0.4295

The vapor product of the first flash unit is further cooled down to 250°F (394.1 K) and sent to the second flash unit. The input data required for this step are tabulated in Table 4.30.

TABLE 4.30 - Input Data for the FLASH-2 Unit.

	S04 (kmol/h)	$Z(I) = X(I)_{S04} = Y(I)$
HCl	9.904	0.1995
B	24.860	0.5009
MCB	14.870	0.2996
Total	49.634	
Degrees, °K	394.1	
Bar	2.38	

The results of the second flash unit are presented in Table 4.31.

TABLE 4.31 - Results of the FLASH-2 Unit.

Component	X(I)	Y(I)	Z(I)	XI(I)	K(I)
HCl	0.0031	0.2803	0.1998	0.9955	91.42
B	0.4163	0.5366	0.5016	0.7589	1.289
MCB	0.5806	0.1839	0.2986	0.4350	0.3153

Table 4.32 summarizes the values of the streams to and from the flash units.

TABLE 4.32 - Values of Streams for Figure 4.5

	S01 (kmol/h)	S02 (kmol/h)	S03 (kmol/h)	S04 (kmol/h)	S05 (kmol/h)	S06 (kmol/h)	S07 (kmol/h)
HCl	10	9.904	0.957	9.904	9.859	0.044	0.1397
B	40	24.86	15.14	24.86	18.86	6.014	21.154
MCB	50	14.87	35.13	14.87	6.47	8.387	43.517
Total	100	49.634	50.366	49.634	35.187	14.446	64.812
Degrees,K	405.2	405.2	405.2	394.1	394.1	394.1	394.1

Referring to Table 4.32, it is observed that after the second flash unit, almost the half of the benzene (18.86 kmol/h) is present in the vapor product (S05 stream) still mixed with HCl. Hence, because of the high rate of loss of benzene, it is not logical to continue such a process configuration.

The computer output and the data file are presented in Appendix H.

It is concluded that flowsheet (b) which contains only one flash unit is not applicable for this separation problem, since, even two flash units are not sufficient to separate HCl from benzene and MCB as explained in the previous flowsheet (a).

V. CONCLUSIONS AND RECOMMENDATIONS

A computer aided chemical process design package called DESPAC was originally developed to run on the DEC-20 system at Carnegie-Mellon University by Westerberg et.al [42]. DESPAC is modified to run on the Boğaziçi University's present CDC Cyber 170/815 system, since the compilers of the two systems differ from each other drastically. In addition to its capabilities are expanded.

DESPAC2, the modified and expanded version of DESPAC, can solve steady-state problems for single operation units and can be used to develop flowsheets for separation problems.

A major contribution of this study is believed to be in deciphering the structure of DESPAC which was provided with almost no structural information about the program. In this respect the procedures for the inclusion of new unit modules, i.e., calculational routines, have been explained in detail and examples for additions are given for routines EXT and HEX. Furthermore, procedures are outlined for the expansion of the thermophysical library file both for the addition of new properties for existing components in the library as well as for the addition of new components into the library.

DESPAC2 could be used with great ease and flexibility for flowsheet synthesis, development and design. Thus it could be used as a useful tool in Chemical Engineering education.

A package of these capabilities have to be able to deal with single operation units as well. To demonstrate this ability of DESPAC2, six examples covering various processing units have been included in the text. All examples are obtained from literature and the results of literature are compared with the results of DESPAC2. It is concluded that DESPAC2 can successfully be used for the calculation of the single operation units and yields results in a very short period of time.

Furthermore, to illustrate the utility of DESPAC2 for flowsheet synthesis, development and design, an example problem has been studied. Various flowsheet configurations are proposed to separate a mixture of HCl, benzene and monochlorobenzene. The proposed flowsheets are tested, and it is observed that the flowsheets which contain flash, absorption, and distillation units are appropriate for this separation problem. The proposed flowsheet (Fig. 4.3) which has a flash unit is studied at five different cases changing the flash temperature, and it is observed that above a certain temperature flash unit is not necessary. Then, removing the flash unit, another flowsheet (Fig. 4.4) is tested changing the number of stages of the absorber and the solvent flow rate to the absorber. Either one of the two flowsheets may be appropriate under different conditions. It is interesting to note that by changing the operation parameters it is possible to eliminate the flash unit. On the other hand, the result is increased number of stages in the distillation column and higher operation temperature. Cost of the required equipment may be the important factor for the final decision.

It is recommended to expand DESPAC2 to offer additional unit operations such as evaporation, filtration, reactor calculations and various types of heat exchangers. The thermophysical library file of DESPAC2 may also be enlarged by introducing new thermophysical properties and additional components.

Currently, the user has to supply the data required from one process unit routine to another one. Therefore, it seems reasonable to prepare an algorithm to carry the necessary data between processing units automatically. The user may test a processing unit changing the operation parameters and results of each run can be saved in a file. The most appropriate result(s) are selected by the user and these may be transferred to the next process unit with the aid of the program.

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APPENDIX A

PROPERTIES AND ORGANIZATION OF DESPAC2

DESPAC2

(Interactive Design Calculation Package)

1. PROPERTIES OF DESPAC2

The various routines are linked under the supervisory PROGRAM DESPAC which prompts the user for input parameters and reports output parameters to the user (Values for input parameters must be supplied by the user; values for output parameters are calculated by the computer). DESPAC2 also provides Auxiliary Routines to handle the manipulations of physical constants.

1.1 Parameters

A parameter, in this discussion, is a variable, such as temperature or pressure, whose value the user wishes to determine or define. Whenever DESPAC2 requires the value for some parameter, it prompts the user by typing a colon ":" and then waits for the user's response. When a parameter is computed by the program, it is named as an "OUTPUT PARAMETER". If a parameter is required by the program in order to complete a calculation, it is named as an "INPUT PARAMETER".

Parameters are entered to DESPAC2 using NAMELIST features. NAMELIST is applied to read the data instead of formatted read statements [30].

DESPAC2 requests values of parameters by typing the ":" in column 1. To assign values to these parameters, the user enters a list of parameters followed by a semicolon ";". Each element in this list is of the form

```
        <SCALAR SYMBOL> = <VALUE>
or      <VECTOR SYMBOL> = <VALUE1>, <VALUE2>,...,<VALUEN>
```

Element in the list are separated by commas. For example, the ENTRY

```
        T = 373, Z = 0.2,0.4,0.4;
```

Assign values to temperature T and mole fractions Z(1) through Z(3) for the PHASE routine.

Before requesting values of parameters, DESPAC2 types a prompting list of their symbols; the user may then assign values to any all or none of these parameters. Values of few parameters are defined by DESPAC2. The symbols for them are enclosed by square brackets in the prompting list.

1.2 Data Structures

DESPAC2 shuttles physical properties between three distinct locations:

1.2.1 Disk Files

Disk Files provide permanent storage for large sets of data. Properties stored on Disk Files are available between terminal sessions. Disk File containing some properties for 91 components is available to all users (in Appendix E the list of these components are presented).

1.2.2 Library

The "Library" stores, for a duration of a terminal session, physical properties for up to 25 components. The Library is lost when the STOP procedure is selected.

1.2.3 SYSTEM

The Auxiliary Routine SYSTEM copies properties, for a particular thermodynamic system of interest, from the Library to the "SYSTEM", the location accessed by the physical property routines. Properties in the SYSTEM are changed whenever a new SYSTEM is defined.

2. ORGANIZATION OF DESPAC2

PROGRAM DESPAC links design routines and prompts the user the following list to select the desired unit computation:

PROCEDURES:

1. KVALUE
2. ENTHALPY
3. PHASE
4. FLASH
5. ABSEDM
6. MCCABE
7. SHTCUT
8. COLUMN
9. CERDA
10. COLCST
21. HEX
22. EXT
11. RETREV
12. SYSTEM
13. DEFINE
14. STORE
15. ACTFIT
17. HELP
18. STOP
19. TIME & DATE

DESPAC2 contains Executive, Modelling, Auxiliary and Service routines. The detailed information about these routines are presented below.

2.1 Executive Routines

The Executive Routines provide the interface between the user and a model.

Executive Routines		Modelling Routines
XKVALU	←calls→	KVALUE
XNTH	⟷	HVAPOR, HLIQID
XPHASE	⟷	PHASET, PHASEP
XFLASH	⟷	FLSHPQ,FLSHTQ,FLSHQV,FLSHTV, FLSHPV,FLSHTP
XABSED	⟷	ABSEDM
XSHTCT	⟷	SHTCUT
XMCABE	⟷	MCCABE
XCERDA	⟷	CERDA
XCOLUM	⟷	COLUMN
XHEX	⟷	HEX
XEXT	⟷	EXT

2.2 Modelling Routines

They are the mathematical models of physical processes. Immediately after mentioning of each routine, the relevant references about that subject are quoted.

2.2.1 PHASE; Bubble Point and Dew Point Calculations

i. PHASET; performs flash calculation at a given pressure and vapor fraction.

ii. PHASEP; performs flash calculation at a given temperature and vapor fraction.

Reference: [26].

2.2.2 FLASH; Flash Calculations

User may choose any of the following seven alternatives:

i. FLSHPQ; P & Q are specified, T & V are computed.
ii. FLSHTQ; T & Q are specified, P & V are computed.
iii. FLSHQV; Q & V are specified, T & P are computed.
iv. FLSHTV; T & V are specified, P & Q are computed.
v. FLSHPV; P & V are specified, T & Q are computed.
vi. FLSHTP; T & P are specified, Q & V are computed.
vii. "ENTHALPY" Flash.

Version i and ii are called adiabatic flash, Version vi is called isothermal flash.

Version vii evaluates the enthalpy of the feed-stream, HF.

Reference: [5].

2.2.3 ABSEDM; Gas absorption by EDMISTER method.

Reference: [10].

2.2.4 MCCABE: Binary Distillation by MCCABE-THIELE method.

Reference: [29].

2.2.5 SHTCUT: Shortcut Multicomponent Distillation (Adjacent Keys) using the UNDERWOOD equation, FENSKE's equation and the GILLILAND correlation.

Key components must be adjacent in the list of components ranked by relative volatilities.

References: Maddox [27], Maddox [28], Mccabe and Smith [29], Treybol [41], Gilliland and Reid [17].

2.2.6 CERDA; Shortcut Multicomponent Distillation technique (Non-Adjacent Keys) developed by Jaime CERDA [6], [7].

2.2.7 COLUMN; Rigorous Multicomponent Distillation that simulates a multicomponent distillation column composed of ideal stages and with an arbitrary configuration of feeds, liquid and vapour side streams.

2.2.8 COLCST; Estimates size and cost of column. Results of the SHTCUT calculation can be passed to COLCST.

References: Fair [11], Guthrie [18], Perry and Chilton [31], Treybal [41].

2.2.9 HEX; Multipass Shell-and-Tube Heat Exchanger Calculation

References: Afgan and Schlunder [1], Backhurst and Harker [3], Blackwell [4], Fraas and Özışık [13], Frank [14], Kays and London [24], Kern [25], Peters and Timmerhaus [32], Reid et.al. [36].

2.2.10 EXT; Multicomponent, Multistage Liquid-Liquid Extraction Calculation

References: Hanson [20], Reid, et.al. [36], Sen [37].

Section 2.2.9 and 2.2.10 are explained in detail in Appendix B and C, respectively.

2.3 Models to Estimate the Thermodynamic Properties Required

Available Models to estimate the thermodynamic properties required for the above mentioned routines, are explained below.

2.3.1 KVALUE; It predicts Vapor-Liquid Equilibria for a variety of thermodynamic systems by employing one of the following methods:

i. Wilson Equation for subcritical components, Anderson Equation of Henry's Law constant for supercritical components, Truncated Virial equation for vapor fugacities.

ii. Prausnitz-Chueh Modification of the Redlich-Kwong Equation.

iii. Ideal Solutions; Perfect Gases; Antoine Equation.

References: Perry and Chilton [31], Prausnitz [33], Prausnitz, et.al. [34].

2.3.2 ENTHALPY; It predicts vapor and liquid enthalpies.

2.3.2.1 HVAPOR; estimates vapor enthalpies using one of the models below:

i. Ideal solution of Perfect Gases
ii. Residual Enthalpy from Virial Equation of State
iii. Residual Enthalpy from Redlich-Kwong Equation.

References: Perry and Chilton [31], Prausnitz [33], Reid, et.al. [36].

2.3.2.2 HLIQID; estimates Liquid enthalpies by one of the following models:

i. Ideal solution of saturated liquids
ii. Ideal solution with pressure correction
iii. Excess enthalpy from Wilson Equation
iv. Residual enthalpy from Redlich-Kwong Equation.

References: Prausnitz [33], Prausnitz, et.al. [34], Reid. et.al [36].

2.4 Auxiliary Routines

The Auxiliary Routines provide the interface between the user, the Modelling Routines and the computer system.

2.4.1 RETREV: Retrieves physical properties from disk files.

2.4.2 LOADLB: Copies data for a component from a file into the library.

2.4.3 SYSTEM: Defines a thermodynamic system by copying physical properties from/LIB*/ to /PHYS*/ and setting up whatever auxiliary information the thermodynamic property routines (KVALUE, HVAPOR, HLIQID) require.

2.4.4 CHKPHY (ERROR): Checks /PHYS*/ to ensure that a minimal set of data has been entered.

2.4.5 DEFINE: Allows user to enter values and new components into the library.

2.4.6 STORE: Writes data from Library /LIB*/ to a disk file named by the user.

2.4.7 SRCHLB: Searches the component name in the disk file.

2.4.8 ERASE: Erases all data in /LIB*/ for component I.

2.4.9 SELECT: Gets list of selected components from the user.

---

*Refer to Appendix D.

2.4.10 GSTPXY: Provides initial guesses for equilibrium values of X, Y and temperature, pressure, and vapor fraction.

2.4.11 ACTFIT: It fits Anderson and Wilson parameters of correlations for activity coefficients to experimental binary VLE data.

2.4.12 HALT: Stops the program.

2.5 Service Routines

The Service Routines are miscellaneous computing chores.

2.5.1 GETLST: Obtains from the user a list of distinct positive integers between 1 and max; Returns list and the number of such integers, N. If a read error occurs (perhaps the user requested help), N is set to -1.

2.5.2 SRCHFL: Performs sequential search of the disk file for named records.

2.5.3 READNL: Accepts lines of text from terminal and having delimited the text with "$NAME" and "$", writes the text to the scratch file USCR. The calling program may than use the NAMELIST features to read the lines from USCR, lines are read from the terminal until a semicolon (;) is encountered characters following the semicolon are ignored.

Figure A.1 shows the interrelationship among the Auxiliary, Service, Executive and Modelling Routines in DESPAC2.

Figure A.2 depicts the highly complex structure of the program for a selected Modelling Routine (FLSHPQ of FLASH) and its Executive Routine (XFLASH). Functions of subroutines which are observed in this figure, are explained in DESPAC2. Therefore, no information about them, are given in this text.

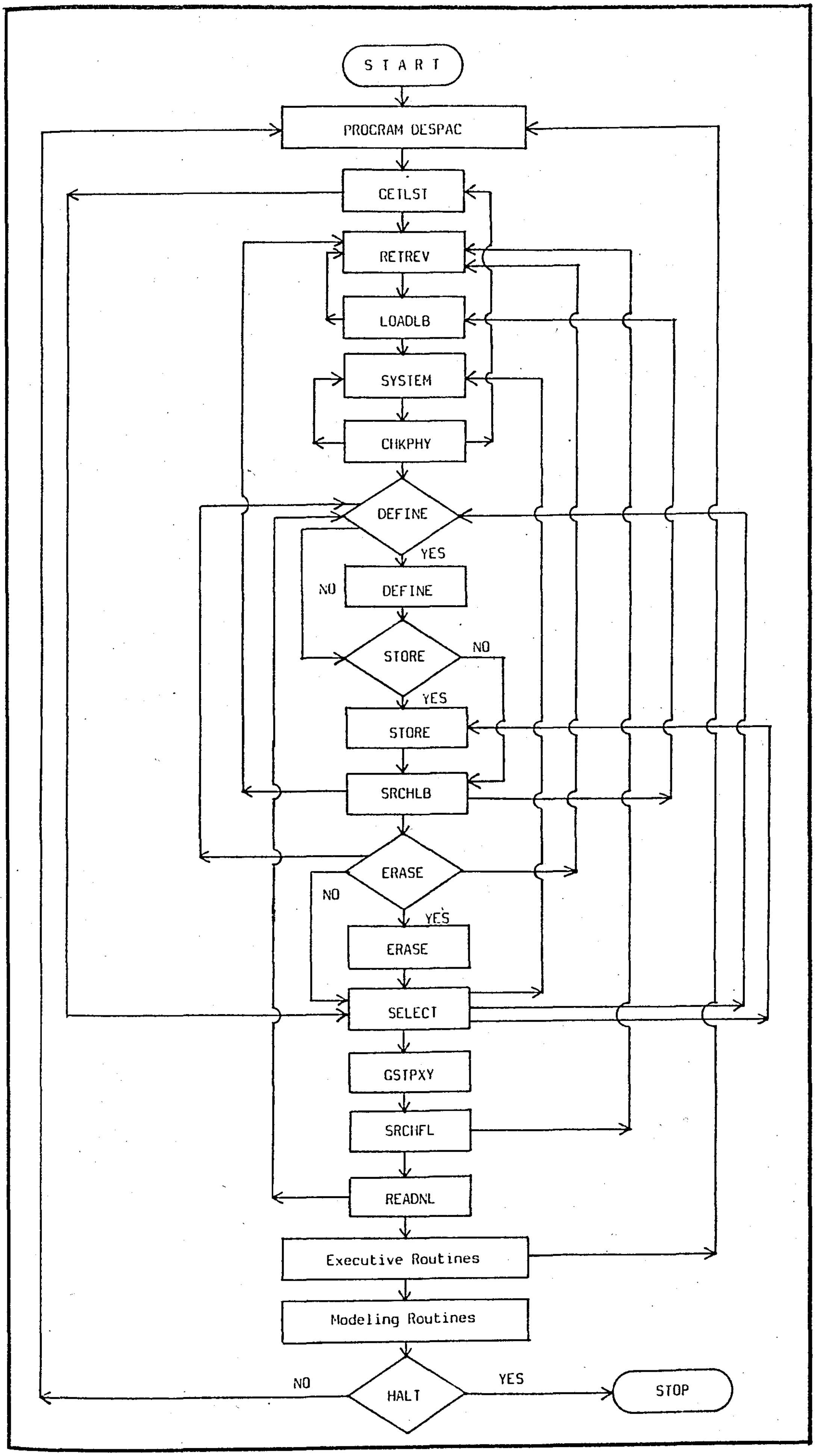
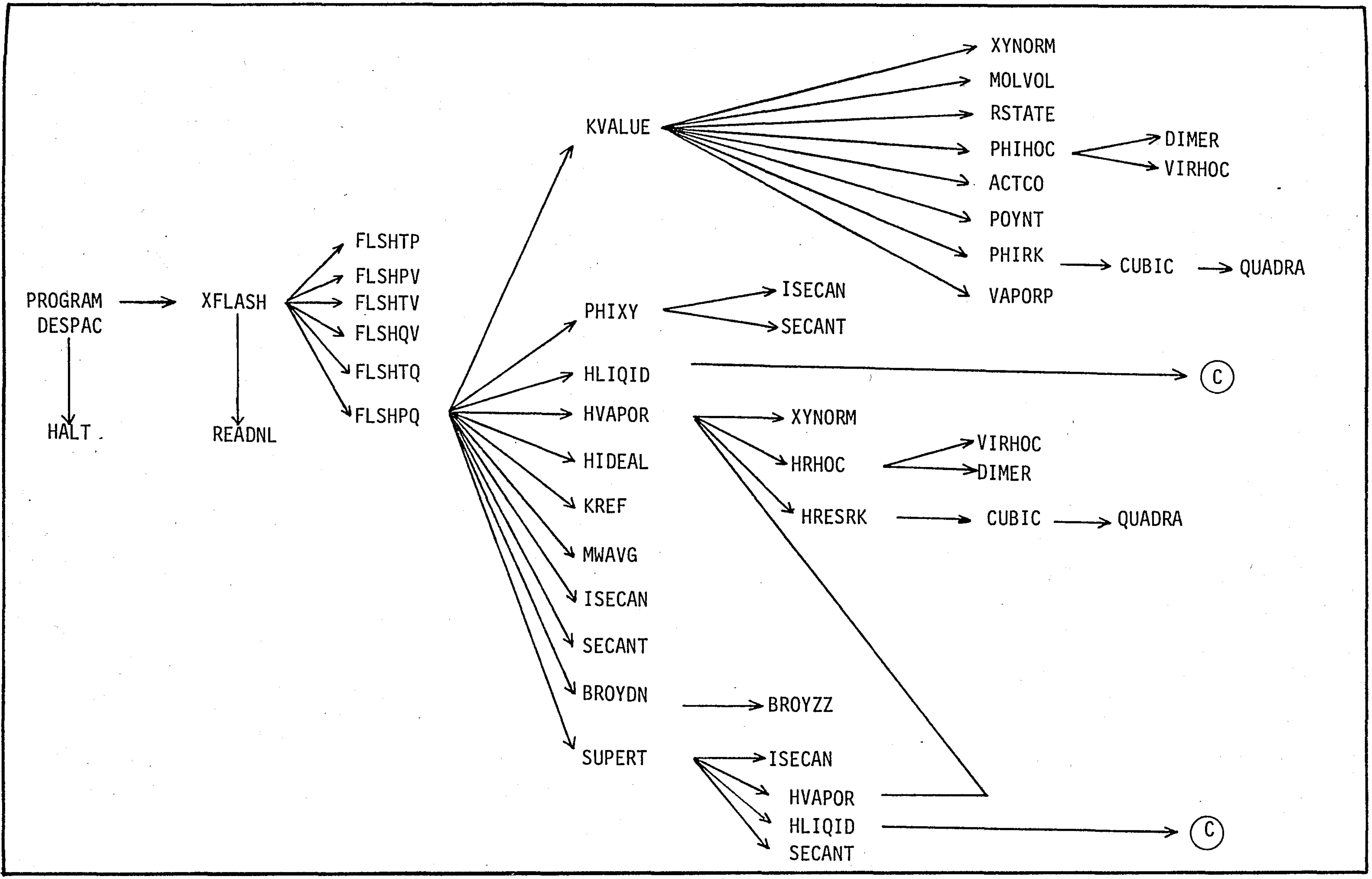


Figure A.1 - Flow diagram of Auxiliary, Service, Executive and Modelling Routines in DESPAC2.


XYNORM
MOLVOL
RSTATE
KVALUE
PHIHOC
DIMER
VIRHOC
ACTCO
POYNT
PHIRK
CUBIC
QUADRA
VAPORP
FLSHTP
FLSHPV
FLSHTV
FLSHQV
FLSHTQ
FLSHPQ
PROGRAM
DESPAC
XFLASH
HALT
READNL
PHIXY
ISECAN
SECANT
HLIQID
C
HVAPOR
XYNORM
HIDEAL
HRHOC
VIRHOC
DIMER
KREF
HRESRK
CUBIC
QUADRA
MWAVG
ISECAN
SECANT
BROYDN
BROYZZ
SUPERT
ISECAN
HVAPOR
HLIQID
SECANT
C

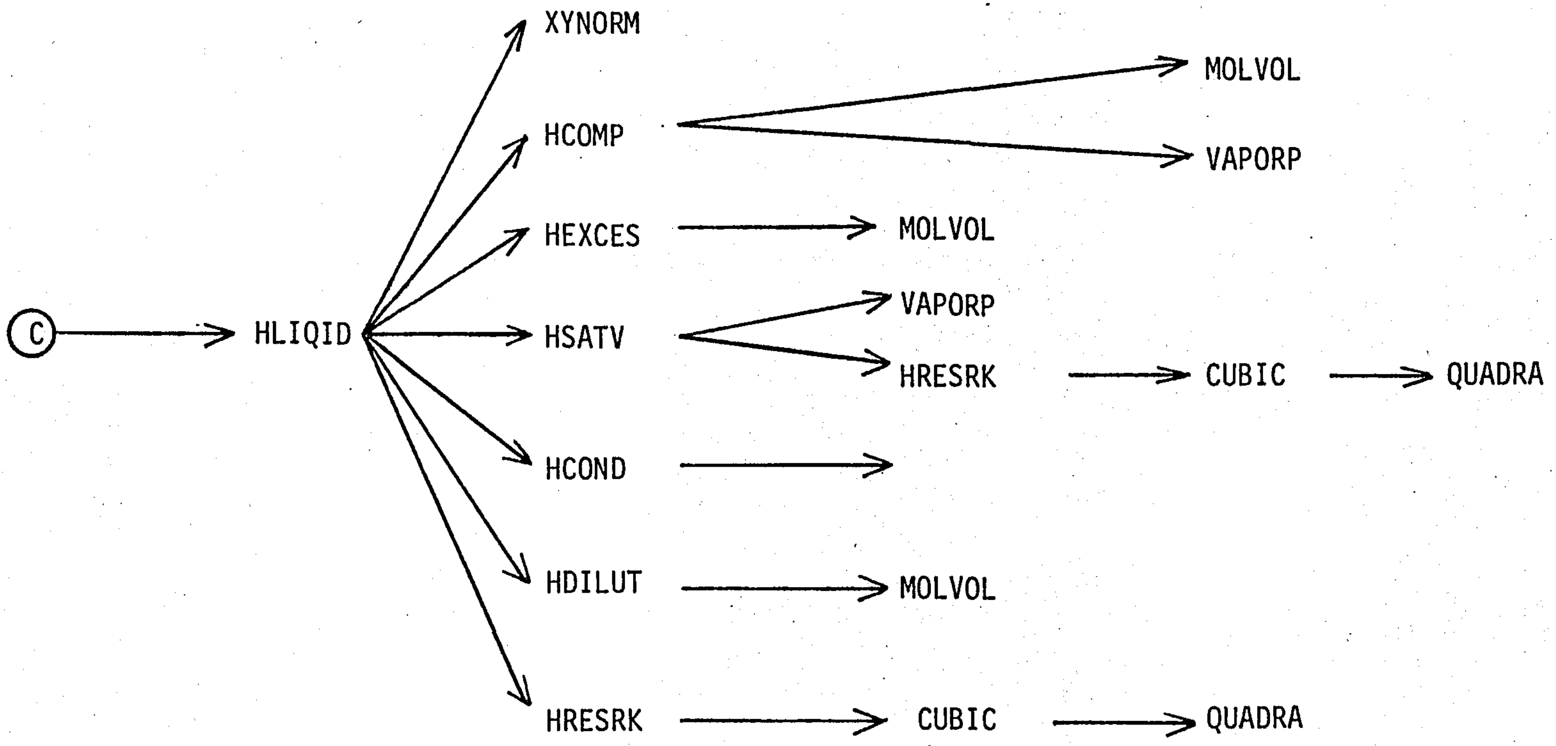


Figure A.2 - Flowchart of subroutine FLSHPQ.

APPENDIX B

DESIGN OF A SHELL-AND-TUBE HEAT EXCHANGER

APPENDIX B

Design of a Shell-and-Tube Heat Exchanger

The mathematical model of a multipass, counter-current shell-and-tube heat exchanger which is presented in Section 3.2.1.1, will be derived as follows:

The basic relationship for all calculations of heat transfer rates is

$$Q = U_D A \Delta t_m = m\ C_p \Delta T \tag{B.1}$$

Q = The amount of heat transferred per unit time (J/s)

U_D = The design value of the overall coefficient of heat transfer (J/s-m^2-K)

A = Heat transfer area (m^2)

Δt_m = Logarithmic mean temperature difference (°K)

m = Flow rate of fluid (kg/s)

C_p = Heat capacity of fluid (J/kg-°K)

ΔT = Temperature difference (°K)

Generally, a 10 percent overload is allowed.

The Logarithmic mean temperature difference (LMTD) is defined by the following equation:

$$\text{LMTD} = \frac{\Delta t_1 - \Delta t_2}{\ln(\Delta t_1/\Delta t_2)} \tag{B.2}$$

where for countercurrent flow

$\Delta t_1 = T_1 - t_2$, and

$\Delta t_2 = T_2 - t_1$.

For cocurrent flow,

$\Delta t_1 = T_1 - t_1$, and

$\Delta t_2 = T_2 - t_2$.

Temperatures:

T_1 = Hot-fluid inlet temperature, °K,

T_2 = Hot-fluid exit temperature, °K,

t_1 = Cold-fluid inlet temperature, °K,

t_2 = Cold-fluid exit temperature, °K.

In the majority of industrial operations, higher velocities, shorter tubes, and a more economical exchanger can be found using multipass design. In a multipass exchanger such as shown in Fig. B.1, the flow is partly countercurrent and partly cocurrent. As a result the mean temperature difference lies somewhere between the countercurrent and cocurrent LMTDs.

In this situation, a correction factor, F, is defined so that, when it is multiplied by the LMTD, the product is the corrected mean temperature-difference (CMTD) [4].

$$\text{CMTD} = F \times \text{LMTD} \qquad \text{(B.3)}$$

For pure countercurrent flow, F = 1. As more cocurrent flow is introduced, F is reduced and the efficiency of the exchanger drops. The lower limit of practical efficiency is F = 0.75 to 0.80.

When designing shell-and-tube heat exchangers in series, the lowest F value is for one shell. This value is raised as the number of shells increases, and the flow nearly resembles countercurrent flow. The optimum value of F is between 0.75 to 1.

The general equation to determine F factor is:

$$F = \left(\frac{\sqrt{R^2 + 1}}{R - 1}\right) \frac{\ln[(1 - P_x)/(1 - RP_x)]}{\ln\left[\dfrac{(2/P_x) - 1 - R + \sqrt{R^2 + 1}}{(2/P_x) - 1 - R - \sqrt{R^2 + 1}}\right]} \qquad \text{(B.4)}$$

where

$$P_x = \frac{1 - \left[\dfrac{RP - 1}{P - 1}\right]^{1/N}}{R - \left[\dfrac{RP - 1}{P - 1}\right]^{1/N}} \qquad \text{(B.5)}$$

and

$$P = (t_2 - t_1)/(T_1 - t_1) \qquad \text{(B.6)}$$

$$R = (T_1 - T_2)/(t_2 - t_1) \qquad \text{(B.7)}$$

N is the total number of shell passes, i.e., the product of shell passes per shell and the number of units in series.

If R = 1, the equation becomes

$$F = \frac{P_x\sqrt{R^2+1}\,/(1-P_x)}{\ln\left[\dfrac{(2/P_x)-1-R+\sqrt{R^2+1}}{(2/P_x)-1-R-\sqrt{R^2+1}}\right]} \qquad \text{(B.8)}$$

and

$$P_x = P/(N - NP + P) \qquad \text{(B.9)}$$

The equations presented are based on certain assumptions such as: the overall heat-transfer coefficient, U_D, is constant throughout the heat exchanger; the flow rate of each fluid is constant; the specific heat of each fluid is constant; there is no condensation of vapor or boiling of liquid in any part of the exchanger; heat losses are negligible; the heat-transfer surface in each pass is equal; the temperature of the shell-side fluid in any shell-side pass is uniform over any cross section.

This correction method is applicable only when the tube passes are even multiples of the shell passes as shown in Figure B.2.

After calculation of F factor and CMTD, U_D is assumed. In this method U_D is the main iteration criteria. For the initial guess of U_D, approximate values of h_o, h_i (Table 3.1 [3]) and h d_o, h d_i (Table 3.3 of Backhurst and Harker [3]) can be obtained and the U_D is calculated from the below equation:

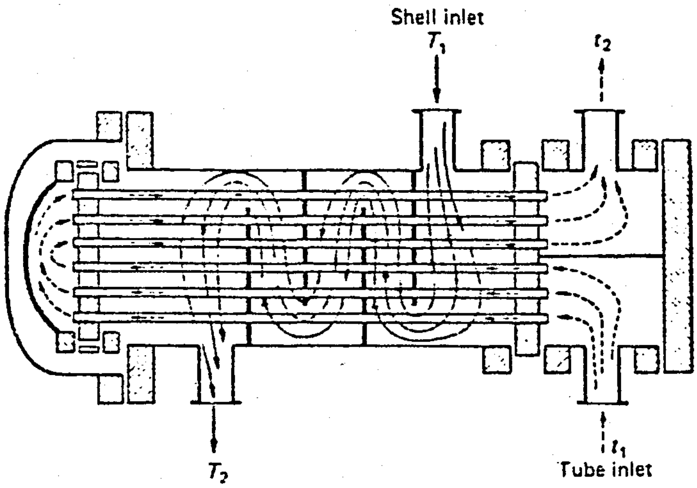
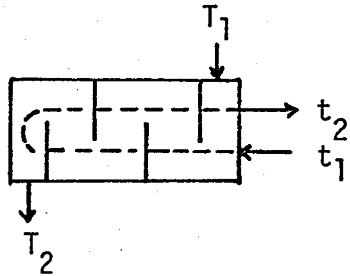
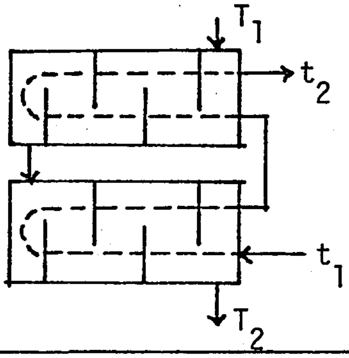


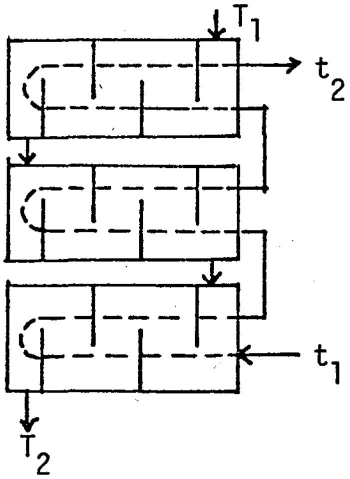
Figure B.1 - Flow patterns in a Multipass Heat Exchanger.



a) One shell pass, and two, four or any multiple tube passes.



b) Two shell passes, and four, eight or any multiple of tube passes.



c) Three shell passes, and six, twelve or any multiple of tube passes.

Figure B.2 - Flow configurations for Shell-and-Tube passes.

$$\frac{1}{U_D} = \frac{1}{h_o} + \frac{1}{h_{d_o}} + \frac{1}{h_i}\frac{D_i}{D_o} + \frac{1}{h_i}\frac{D_i}{D_o} \qquad (B.10)$$

Then heat transfer area is found from Eq. (B.1). The total length of tubes are computed, since

Area = (no.of tubes) x (tube length between inner faces of tube sheets) x (external surface area per unit length of tube)

Number of tubes is determined by dividing total tube length to the standard tube length.

For the tube side;

$$\text{Total Flow Area} = \frac{(\text{No. of tubes}) \times (\text{Cross-sectional Area of tubes})}{(\text{No. of tube passes})} \ (m^2) \qquad (B.11)$$

where,

$$\text{Cross-sectional Area of tubes} = \frac{\pi D_i^2}{4}$$

Then, mass flow rate of the fluid in the tube side can be calculated from

$$G_t = \frac{m_t}{\text{Total Flow Area}} \ (kg/s\text{-}m^2) \qquad (B.12)$$

where

m_t = Flow rate of fluid in the tube side (kg/s).

The exact form of the correlation for the film coefficient depends on the fluid flow regime of the system defined by the Reynolds Number, Re, where

$$Re = \frac{DG}{\mu} \tag{B.13}$$

where

D is the inside diameter of the tube (mm)

G is the mass flow rate of the fluid (kg/s-m²).

μ is the viscosity of the fluid at the temperature of the film (Ns/m²).

When $Re < 2100$ the flow is streamline and

when $Re > 10^4$ the flow is turbulent.

The following correlations may then be used for evaluating the film coefficient; Inside tubes for streamline flow, the Sieder and Tate relation may be used.

$$\frac{h_i D}{k} = 1.86\{(DG_t/\mu)(C_p\mu/k)(D/L)\}^{0.33}(\mu/\mu_w)^{0.14} \tag{B.14}$$

For turbulent flow,

$$\frac{h_i D}{k} = 0.027(DG_t/\mu)^{0.8}(C_p\mu/k)^{0.33}(\mu/\mu_w)^{0.14} \tag{B.15}$$

h_i is computed from one of the above equations, assuming the value of the $(\mu/\mu_w)^{0.14}$ as 1. Then, shell inner diameter (D_s) can be approximately calculated from the equation pairs below:

i) For square pitch arrangement

$$N_t = 0.75(Z/P_t)^2 \quad ; \quad D_s = Z + 38.1 \tag{B.16}$$

ii) For triangular pitch arrangement

$$N_t = 0.86(Z/P_t)^2 \quad ; \quad D_s = Z + 38.1 \qquad (B.17)$$

N_t is the number of tube,

Z is a constant (mm)

P_t is tube pitch (mm).

Next step is to evaluate fluid mass velocity on the shell side, as follows:

$$G_s = \frac{m_s}{a_s} \quad (kg/s\text{-}m^2) \qquad (B.18)$$

where

m_s = mass flow of fluid (kg/s)

a_s = cross area for flow (m^2).

The cross area for flow is defined as

$$a_s = [(D_s B y \times 10^{-6})/P_t] \quad (m^2) \qquad (B.19)$$

where

D_s = shell inner diameter (mm)

B = baffle spacing (mm)

y = clearance between tubes (mm)

P_t = tube pitch (mm).

In order to compute the shell side film coefficient below equation is selected.

$$\frac{h_o D_e}{k} = 0.36(D_e G_s/\mu)^{0.55}(C_p\mu/k)^{0.35}(\mu/\mu_w)^{0.14} \qquad (B.20)$$

Values of Equivalent diameter (D_e) for various tube layouts may be found in Table 3.4 of Backhurst and Harker [3]. Initially $(\mu/\mu_w)^{0.14}$ is set to 1 in the above equation.

Inside film coefficient based on the outside diameter (h_{io}) is obtained from:

$$h_{io} = \frac{h_i D_o}{D_i} \qquad (B.21)$$

The temperature of the tube wall (t_w) is calculated from the following equations:

For the hot fluid in the tubes

$$t_w = T_A - \left(\frac{h_o}{h_{io} + h_o}\right)(T_A - t_A) \qquad (B.22)$$

For the hot fluid in the shell

$$t_w = T_A - (h_{io}/(h_{io} + h_o))(T_A - t_A) \qquad (B.23)$$

where T_A and t_A are the arithmetic average fluid temperatures of the hot and cold streams, respectively.

Then, viscosity at wall temperature (μ_w) is evaluated from Thomas' Method [36].

$$\log \frac{8.569\mu^{\circ}}{(\rho_L)^{\frac{1}{2}}} = \theta\left(\frac{1}{T_r} - 1\right) \qquad (B.24)$$

where

$\mu°$ = viscosity (centipoise)

ρ_L = density (g/cm^3)

θ = viscosity constitutional constant calculated from atomic values from Table B.1

T_r = Reduced temperature.

TABLE B.1 - Structural Contributions to Calculate θ in Eq.(B.24)

C	-0.462	I	+0.335
H	+0.249	(=)	+0.478
O	+0.054	C_6H_5	+0.385
Cl	+0.340	S	+0.043
Br	+0.326	CO	+0.105
		CN	+0.381

Tube wall correction factor $(\mu/\mu_w)^{0.14}$ in Eqs. (B.14), (B.15) and (B.20) can be determined using the above equation. Tube side and Shell side film coefficients is calculated again including the tube wall correction factor. Finally h_{io} and U_D are obtained from Eq. (B.21) and Eq. (B.10), respectively and initial and final values of U_D are compared, if the difference is less than the stopping criteria the program terminates.

The logical flow diagram of the iteration cycle is given in Figure 3.1 in the main text.

APPENDIX C

MULTICOMPONENT LIQUID-LIQUID EXTRACTION TOWER SIMULATION FOR DESIGN

APPENDIX C

Multicomponent Liquid-Liquid Extraction Tower Simulation for Design

The algorithm to simulate multicomponent, multi-stage, equilibrium-stage liquid-liquid extraction column was originally prepared by Sen [37]. The original algorithms operates on the UNIVAC 1106 computer system. In order to increase the capabilities of DESPAC, the original algorithm is firstly modified to operate on the CDC Cyber 170/815 computer system, then structurally modified to fit into the DESPAC.

In the case of extraction simulation problem, number of theoretical stages, flow rates and compositions of feed streams, flow rates of side streams, and tower temperature and pressure are specified.

Compositions and overall stage flow rates of light and heavy phases constitute the iteration variables of the liquid-liquid extraction simulation problem.

Figure C.1 shows a general separation stage.

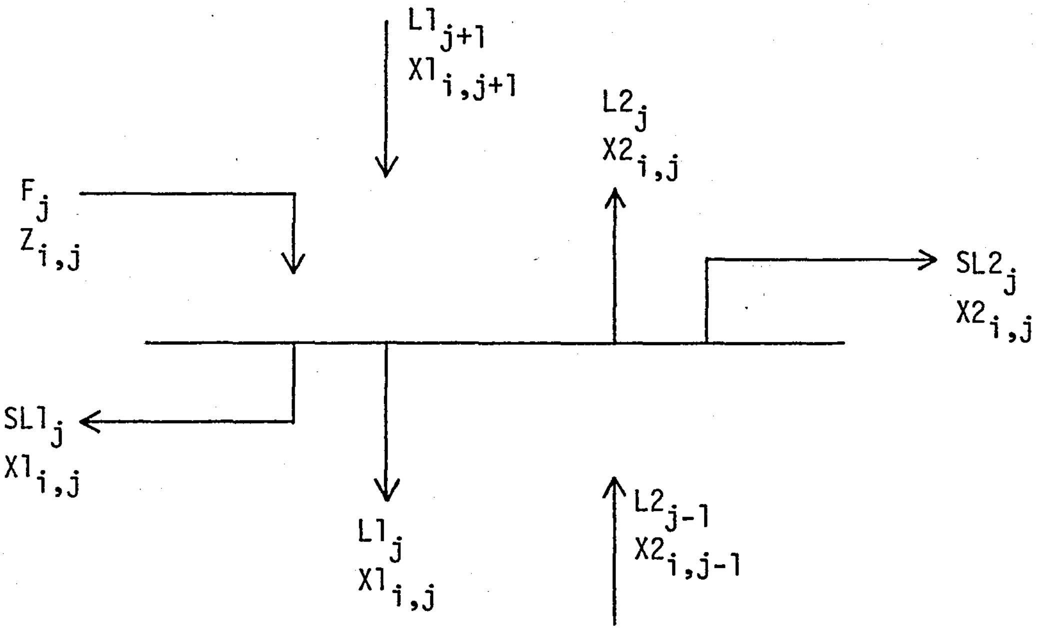


Figure C.1 - Schematic description of a general separation stage.

where,

F_j = overall flow rate of the feed stream to stage j,

$L2_j$ = overall flow rate of the light-phase stream leaving stage j,

$L1_j$ = overall flow rate of the heavy-phase stream leaving stage j,

$SL2_j$ = overall flow rate of the light-phase side-stream leaving stage j,

$SL1_j$ = overall flow rate of the heavy-phase side-stream leaving stage j,

i = component identification number,

j = stage identification number,

Z_j = component mole fraction in the feed,

$X2_j$ = component mole fraction in the heavy-phase,

$X1_j$ = component mole fraction in the light-phase.

The algorithm is based on the relaxation technique, i.e., it uses the transient model equations to reach the steady-state solution.

From Figure C.1, the transient component material balance equation for component i around stage j is given by

$$\frac{d}{d\tau}(H1_j X1_{i,j} + H2_j X2_{i,j}) = L1_{j+1} X1_{i,j+1} + L2_{j-1} X2_{i,j-1} + F_j Z_{i,j} - (L1_j + SL1_j) X1_{i,j} - (L2_j + SL2_j) X2_{i,j} \tag{C.1}$$

where H1 and H2 represent molar heavy and light-phase hold-ups respectively.

However, the liquid phase equilibrium relationship for component i at stage j is given by

$$X2_{i,j} = K_{i,j} X1_{i,j} \tag{C.2}$$

A summary discussion of the phase equilibrium relationships is explained below:

If two liquid phases are at equilibrium at a certain T and P the equilibrium relationship for any component i is given by

$$\hat{f}_i^{(1)} = \hat{f}_i^{(2)} \quad , \qquad 1 \leq i \leq N \tag{C.3}$$

where $\hat{f}_i^{(1)}$ and $\hat{f}_i^{(2)}$ refer to the fugacities of component i in the heavy and light phases respectively, and N is the number of components.

Fugacity of component i in a mixture of N components is expressed as

$$\hat{f}_i = \gamma_i x_i f_i \tag{C.4}$$

where

x_i = mole fraction of component i in the mixture

f_i = pure-component fugacity of component i at the same temperature and pressure as the mixture

γ_i = activity coefficient of component i in the mixture.

Thermodynamic functions of liquid phases are weakly-dependent upon pressure, but f_i and γ_i are dependent upon temperature. Therefore, different thermodynamic models used for calculation of the activity coefficients such as

- 3-suffix Margules,
- NRTL,
- UNIFAC equations.

If Eq. (C.4) is written for both heavy and light phases, and they are inserted into Eq. (C.3), the resulting equation is

$$X2_i = K_i X1_i \tag{C.5}$$

where K_i is called as the equilibrium ratio of component i, and defined as

$$K_i = \frac{\gamma_i^{(1)}}{\gamma_i^{(2)}} \tag{C.6}$$

The substitution of the phase equilibrium relationship Eq. (C.2) into the Eq. (C.1) results in

$$\frac{d}{d\tau}[(H1_j + H2_j K_{i,j})X1_{i,j}] = L2_{j-1}K_{i,j-1}X1_{i,j-1} - [L1_j + SL1_j$$
$$+ (L2_j + SL2_j)K_{i,j}]X1_{i,j}$$
$$+ L1_{j+1}X1_{i,j+1} + F_j Z_{i,j} \qquad (C.7)$$

Stage hold-ups of both of the phases are assumed to be constant and time independent aside from the very first stages of the transient operation. Moreover, the initially assumed profiles do not have to correspond to the profiles during the very first stages of the transient operation. If the time-dependence of the equilibrium ratios is neglected, the term $(H1_j + H2_j K_{i,j})$ may be taken out of the derivative operator, and Eq. (C.7) becomes

$$\frac{dX1_{i,j}}{d\tau} = \frac{1}{(H1_j + H2_j K_{i,j})}[L2_{j-1}K_{i,j-1}X1_{i,j-1} - [L1_j + SL1_j$$
$$+ (L2_j + SL2_j)K_{i,j}]X1_{i,j} + L1_{j+1}X1_{i,j+1} + F_j Z_{i,j}] \qquad (C.8)$$

Equation (C.8) may be written as

$$\frac{dX1_{i,j}}{d\tau} = A_{i,j}X1_{i,j-1} - B_{i,j}X1_{i,j} + C_{i,j}X1_{i,j+1} + E_{i,j} \qquad (C.9)$$

where

$$W_{i,j} = \frac{1}{H1_j + H2_j K_{i,j}} \qquad \text{C.10a)}$$

$$A_{i,j} = \begin{array}{l} L2_{j-1}/W_{i,j} \\ L2_{j-1}K_{i,j-1}/W_{i,j} \end{array} \qquad (C.10b)$$

$$B_{i,j} = \frac{L1_j + SL1_j + (L2_j + SL2_j)K_{i,j}}{W_{i,j}} \qquad (C.10c)$$

$$C_{i,j} = \frac{L1_{j+1}}{W_{i,j}} \qquad (C.10d)$$

$$E_{i,j} = \frac{F_j Z_{i,j}}{W_{i,j}} \qquad (C.10e)$$

Heavy-phase mole fractions are extrapolated by the Ball integration formula

$$X1^{\tau+1}_{i,j} = X1^{\tau}_{i,j} + \Delta t[\beta(dX1_{i,j}/d\tau)^{\tau+1} + (1 - \beta)(dX1_{i,j}/d\tau)^{\tau}]$$

$$\text{where} \quad 0 < \beta \leq 1 \,. \qquad C.11)$$

Applying Eq. (C.9) for times both τ and $\tau+1$, and inserting them into the Ball integration formula yields

$$-\beta\Delta\tau A^{\tau+1}_{i,j}\, X1^{\tau+1}_{i,j-1} + (1 + \beta\Delta\tau B^{\tau+1}_{i,j})X1^{\tau+1}_{i,j} - \beta\Delta\tau C^{\tau+1}_{i,j}\, X1^{\tau+1}_{i,j+1} =$$

$$X1^{\tau}_{i,j} + \Delta\tau[(1 - \beta)E^{\tau}_{i,j} + \beta E^{\tau+1}_{i,j}] + (1 - \beta)\Delta\tau(A^{\tau}_{i,j}\, X1^{\tau}_{i,j-1}$$

$$- B^{\tau}_{i,j}\, X1^{\tau}_{i,j} + C^{\tau}_{i,j}\, X1^{\tau}_{i,j+1} \qquad (C.12)$$

Equation (C .12) yields a nonlinear set of equations with respect to the iteration variables, i.e., compositions and overall stage flow rates of both of the phases. To be able to linearize, and to solve

Eq. (C.12) for the heavy-phase mole fractions, the following linearization approximations must be made:

$$L1_j^{\tau+1} = L1_j^{\tau} \tag{C.13a}$$

$$L2_j^{\tau+1} = L2_j^{\tau} \tag{C.13b}$$

$$K_{i,j}^{\tau+1} = K_{i,j}^{\tau} \tag{C.13c}$$

In this manner, values of the functions $A_{i,j}$, $B_{i,j}$, $C_{i,j}$, $E_{i,j}$ at time τ are used in Eq. (C.12), instead of their values at time τ+1.

The tridiagonal matrix algorithm used for the solution of the linearized form of Eq. (C.12).

The logical flow diagram of the iteration cycle is given in Figure 3.2 in the main text.

APPENDIX D

COMMON BLOCKS PRESENT IN DESPAC2

```
      BLOCK DATA
C
C     LISTED HERE ARE ALL LABELED COMMON BLOCKS, ALONG WITH
C     THE ROUTINES WHICH ACCESS EACH BLOCK.  BLANK (UNLABELED)
C     COMMON IS AVAILABLE TO THE EXECUTIVES AND AUXILIARIES ONLY.
C      ONLY ACTFIT USES BLANK COMMON IN THIS VERSION.
C
C     READ  ACCESS ALLOWS THE LISTED ROUTINES TO USE THE VALUES
C           OF VARIABLES IN THE BLOCK BUT NOT TO MODIFY THEM ;
C     WRITE ACCESS ALLOWS THE LISTED ROUTINES TO MODIFY THE VARIABLES.
C
C     AN ASTERISK FOLLOWING THE NAME OF A SUBROUTINE INDICATES THAT
C     ACCESS IS EXTENDED TO SUBROUTINES CALLED BY THAT SUBROUTINE.
C
C     IF A ROUTINE IS NOT LISTED, IT DOES NOT ACCESS THE BLOCK.
C     "GLOBAL" MEANS THAT MANY ROUTINES ARE PERMITTED THE INDICATED
C     TYPE OF ACCESS.
C
C---------------------------------------------------------------------
C
C ********  P A R A M  COMMON BLOCK   ***************
      INTEGER UFIL,USCR,O,DIMPHY,DIMLIB,DIMFSH
      PARAMETER(UFIL=1,USCR=2,UDF=-9999.,DIMLIB=25,DIMPHY=20)
      PARAMETER(IN=5,O=6)
C ******* N C O M P COMMON BLOCK      ****************
      COMMON /NCOMP/ NCOMP
C ******** I D E N T   COMMON BLOCK *****************
      CHARACTER*5 IDENT
      COMMON/IDENT/IDENT(5,DIMPHY)
C ******** P H Y S   COMMON  BLOCK    ***************
      INTEGER KMODEL,MODLHV,MODLHL
      INTEGER CON(DIMPHY),UCON(DIMPHY),NCON,NUCON
      LOGICAL NEWSYS, FHVAP,FHLIQ,FHID,FHRRK,FHDILU,FHEXCS,
     &  FVIRHO,FDIMER,CHMHOC
      REAL MOLWT
      DOUBLE PRECISION FUCON
      COMMON /PHYS/ KMODEL,MODLHV,MODLHL,CON,UCON,NCON,NUCON,
     &  NEWSYS, FHVAP,FHLIQ,FHID,FHRRK,FHDILU,FHEXCS,
     &  FVIRHO,FDIMER,CHMHOC,
     &  MOLWT(DIMPHY),TC(DIMPHY),PC(DIMPHY),VC(DIMPHY),OMEGA(DIMPHY),
     &  DELHF(DIMPHY),DELGF(DIMPHY),TREF(DIMPHY),PREF(DIMPHY),
     &  CPVAPA(DIMPHY),CPVAPB(DIMPHY),CPVAPC(DIMPHY),CPVAPD(DIMPHY),
     &  ANTA(DIMPHY),ANTB(DIMPHY),ANTC(DIMPHY),
     &  RDGYRA(DIMPHY),DIPOLE(DIMPHY),ETA(DIMPHY,DIMPHY),
     &  ZRA(DIMPHY), FUCON(DIMPHY,o), ACTPAR(DIMPHY,DIMPHY),
     &  RKCMGA(DIMPHY),RKOMGB(DIMPHY),RKPCK(DIMPHY,DIMPHY),
     &  DENS(DIMPHY)
C  ********* L I B   COMMON BLOCK *************
      REAL MW(DIMLIB),OM(DIMLIB),TTC(DIMLIB),PPC(DIMLIB),VVC(DIMLIB)
      REAL DH(DIMLIB),DG(DIMLIB),TRF(DIMLIB),PRF(DIMLIB)
      REAL CPA(DIMLIB),CPB(DIMLIB),CPC(DIMLIB),CPD(DIMLIB)
      REAL AA(DIMLIB),AB(DIMLIB),AC(DIMLIB)
      REAL RD(DIMLIB),DI(DIMLIB),ET(DIMLIB,DIMLIB),  ZR(DIMLIB)
      REAL LLAM(DIMLIB,DIMLIB),ACTA(DIMLIB,DIMLIB)
      REAL RKA(DIMLIB),RKB(DIMLIB),RKK(DIMLIB,DIMLIB)
      REAL  RHO(DIMLIB)
      DOUBLE PRECISION FU(6,DIMLIB)
C     INTEGER ID(5,DIMLIB),IDA(DIMLIB),NCLIB,LIBMAP(DIMLIB)
      INTEGER NCLIB,LIBMAP(DIMLIB)
      CHARACTER ID(5,DIMLIB)*5,IDA(DIMLIB)*5
      COMMON/LIBC/ID,IDA
      COMMON /LIB/ MW,OM, TTC,PPC,VVC, DH,DG,TRF,PRF,
     +              CPA,CPB,CPC,CPD, AA,AB,AC, RD,DI,ET, ZR,
     +              LLAM,ACTA, RKA,RKB,RKK, FU, NCLIB,LIBMAP
      COMMON/LIBHEX/ RHO
```

```
C
C   ******** C K V A L U   COMMON BLOCK ************
C
      COMMON /CKVALU/ VLIQ(DIMPHY),FREFER(DIMPHY),VLIQID,VVAPOR,
     +  PHIVAP(DIMPHY),PHILIQ(DIMPHY),GAMMA(DIMPHY),PCTRM(DIMPHY)
C  *************************************************************
C ********** F S H COMMON BLOCK **************
      PARAMETER(DIMFSH=23)
      REAL U,UHAT,USCALE,G, ALPHA,HID,DLNKDT,PI,K0, WORK
      REAL TLO,TUP, PLO,PUP
      COMMON /FSH/ U(DIMFSH),UHAT(DIMFSH),USCALE(DIMFSH),G(DIMFSH),
     +           ALPHA(DIMPHY),HID(DIMPHY),DLNKDT(DIMPHY),PI(DIMPHY),
     +            K0(DIMPHY), WORK(690),
     +            TLO,TUP, PLO,PUP

C *********************************************************
      COMMON/CSECAN/NSECAN(3),ITEST,MTONE,X,F,DX,XLO,XUP
      COMMON/CSECAN/KOUNT,MAXFUN,DXACC,EPS1,EPS2,ZERO,XM(4),FM(4)

C=================================================================
C  PARAMETERS (GLOBAL CONSTANTS)
C   DEFINITION OF VARIABLES
C     IN       LOGICAL DEVICE USED FOR INPUT FROM USER.
C     O        LOGICAL DEVICE USED FOR OUTPUT TO USER.
C     UFIL     NUMBER OF LOGICAL DEVICE USED FOR STORAGE AND RETRIEVAL
C              OF PHYSICAL PROPERTIES OR EXPERIMENTAL DATA.
C     USCR     LOGICAL DEVICE USED FOR SCRATCH FILE.
C     UDF      VALUE WHICH MEANS "UNDEFINED".
C     DIMLIB   DIMENSION OF /LIB/ ; THE MAXIMUM NUMBER OF COMPONENTS WHICH
C              CAN BE STORED IN THE LIBRARY.
C     DIMPHY   DIMENSION OF /PHYS/ ; THE MAXIMUM NUMBER OF COMPONENTS
C              IN A SYSTEM.
C
C=================================================================
C  /NCOMP/ - NUMBER OF COMPONENTS IN /PHYS/
C
C   ACCESS
C     READ     GLOBAL
C     WRITE    RETREV,SYSTEM,DEFINE,ACTFIT
C
C   DEFINITION OF VARIABLES
C     NCOMP    NUMBER OF COMPONENTS IN THE SYSTEM.
C              NCOMP=0  <=>  THE SYSTEM IS UNDEFINED.
C
      DATA NCOMP/100/
C
C=================================================================
C  /IDENT/ - ALPHANUMERIC NAMES OF COMPONENTS IN /PHYS/
C
C   ACCESS
C     READ     EXECUTIVES AND AUXILIARIES
C     WRITE    RETREV*,SYSTEM,DEFINE*
C
C   DEFINITION OF VARIABLES
C     IDENT    ARRAY OF 25-CHARACTER NAMES OF COMPONENTS IN SYSTEM.
C              NAMES ARE STORED IN 5-WORD COLUMNS, 5 CHARACTERS PER WORD.
C              IDENT(1,I) THRU (5,I) CONTAIN NAME OF COMPONENT I
C              IN /PHYS/.
C
```

```
C=========================================================================
C  /PHYS/ - PHYSICAL CONSTANTS FOR KVALUE
C
C   ACCESS
C     READ     KVALUE*,HVAPOR*,HLIQID*,GSTPXY
C     WRITE    SYSTEM,ACTOBJ
C
C   DEFINITION OF VARIABLES
C     NEWSYS   USED BY KVALUE TO SUPPRESS REPEATED COMPUTATION OF
C              QUANTITIES WHICH DEPEND ONLY ON THE IDENTITIES OF THE
C              COMPONENTS IN A SYSTEM AND WHICH ARE INDEPENDENT OF
C              TEMPERATURE, PRESSURE, AND COMPOSITION.
C              ANY ROUTINE WHICH MODIFIES /PHYS/ MUST SET NEWSYS=.TRUE. ;
C              KVALUE RESETS NEWSYS=.FALSE.
C     KMODEL   SELECTS THE MODEL USED BY KVALUE TO ESTIMATE K-VALUES.
C              =1 --> WILSON/VIRIAL MODEL.
C              =2 --> REDLICH-KWONG EQUATION OF STATE.
C              =3 --> ANTOINE EQUATION.
C     ------   THESE VARIABLES DEFINED ONLY WHEN KMODEL=1.  ------
C     CON      LIST OF "CONDENSABLE" COMPONENTS.
C     UCON     LIST OF "NON-CONDENSABLE" COMPONENTS.
C     NCON     NUMBER OF "CONDENSABLE" COMPONENTS.
C     NUCON    NUMBER OF "NON-CONDENSABLE" COMPONENTS.
C              ACTIVITY COEFFICIENTS FOR CONDENSABLES ARE COMPUTED FROM
C              THE WILSON EQUATION ; THE ANDERSON EQUATION (A CORRELATION
C              OF HENRY'S CONSTANTS) IS USED FOR NON-CONDENSABLES.
C     ------   ------
C     MOLWT    MOLECULAR WEIGHT.
C     TC       CRITICAL TEMPERATURE.
C     PC       CRITICAL PRESSURE.
C     VC       CRITICAL VOLUME.
C     OMEGA    PITZER'S ACENTRIC FACTOR.
C     ANTA,B,  ANTOINE COEFFICIENTS.
C     C
C     RDGYRA   RADIUS OF GYRATION.
C     DIPOLE   DIPOLE MOMENT.
C     ETA      ASSOCIATION PARAMETERS.
C     ZRA      CONSTANT IN RACKETT EQUATION FOR MOLAR VOLUMES.
C     FOCON    CONSTANTS IN EXPRESSION OF C.A.ECKERT FOR CORRELATION
C              OF ZERO-PRESSURE REFERENCE FUGACITIES.
C              6 PARAMETERS FOR EACH COMPONENT STORED BY ROW.
C     ACTPAR   ACTIVITY PARAMETERS.
C              IF BOTH I,J ARE "CONDENSABLE" (IE, APPEAR IN THE LIST
C              CON), THEN ACTPAR(I,J) IS A WILSON PARAMETER.
C              IF ONE OF I,J IS CONDENSABLE AND THE OTHER NON-CONDENSABLE
C              THEN ACTPAR(I,J) IS AN ANDERSON PARAMETER.
C     RKOMGA   "REDLICH-KWONG OMEGA A" ;  CORRELATING PARAMETER FOR
C              REDLICH-KWONG EQUATION AS MODIFIED BY PRAUSNITZ AND CHUEH.
C     RKOMGB   "REDLICH-KWONG OMEGA B".
C     RKPCK    "REDLICH-KWONG-PRAUSNITZ-CHUEH K".
C     DENS     DENSITY.
C
```

```
C=======================================================================
C  /LIB/ - LIBRARY OF PHYSICAL CONSTANTS
C
C   ACCESS
C     READ    AUXILIARIES
C     WRITE   RETREV*,DEFINE*,ACTFIT
C
C   DEFINITIONS OF VARIABLES
C     NOTE: SYSTEM COPIES VALUES FROM /LIB/ TO /IDENT/ AND /PHYS/.
C           RETREV LOADS /LIB/ WITH SELECTED COMPONENTS FROM DISK FILES.
C           DEFINE ALLOWS THE USER TO MANUALLY INSERT OR MODIFY VALUES
C           IN /LIB/.
C           NEARLY ALL VARIABLES IN /LIB/ HAVE DEFINITIONS CORRESPONDING
C           TO VARIABLES IN /IDENT/ OR /PHYS/.
C
C     MW      <--> MOLWT
C     OM      <--> OMEGA
C     TTC     <--> TC
C     PPC     <--> PC
C     VVC     <--> VC
C     DH      <--> DELHF
C     DG      <--> DELGF
C     TRF     <--> TREF
C     PRF     <--> PREF
C     CPA,B,  <--> CPVAPA,CPVAPB,CPVAPC,CPVAPD
C       C,D
C     AA,BB,CC<--> ANTA,ANTB,ANTC
C     RD      <--> RDGYRA
C     DI      <--> DIPOLE
C     ET      <--> ETA
C     ZR      <--> ZRA
C     LLAM    WILSON PARAMETER "LOWER-CASE LAMBDA".
C     ACTA    ANDERSON PARAMETER FOR CORRELATING ACTIVITY COEFFICIENTS
C             OF NON-CONDENSABLE COMPONENTS.
C             LN(GAMMAIJ) = ACTA(I,J) + ACTA(J,I)/T
C             WHERE GAMMAIJ IS ACTIVITY COEFFICIENT OF NON-CONDENSABLE I
C             IN CONDENSABLE J AT INFINITE DILUTION OF I AND
C             T IS TEMPERATURE.
C             LLAM AND ACTA ARE COPIED INTO ACTPAR IN /PHYS/.
C     RKA,B   <--> RKOMGA,RKOMGB
C     RKK     <--> RKPCK
C     RHO     <--> DENS
C     FO      <--> FOCON (PARAMETERS FO STORED BY COLUMN)
C     ID      <--> IDENT IN /IDENT/
C     IDA     ALIAS ;   5-CHARACTER ABBREVIATION FOR COMPONENT.
C     NCLIB   NUMBER OF COMPONENTS IN THE LIBRARY.
C     LIBMAP  LIST OF COMPONENTS WHICH HAVE BEEN COPIED ("CHECKED OUT")
C             FROM /LIB/ INTO /PHYS/.
C             IF II=LIBMAP(I), THEN THE I-TH COMPONENT IN /PHYS/ IS
C             A COPY OF THE II-TH COMPONENT IN /LIB/.
C
```

```
C=====================================================================
C   /CKVALU/ - THERMODYNAMIC QUANTITITES COMPUTED BY KVALUE.
C
C    ACCESS
C      READ     ACTOBJ,ACTEXP
C      WRITE    KVALUE
C
C    DEFINITIONS OF VARIABLES  --  SEE KVALUE*.
C
C=====================================================================
C   /FSH/ - WORKSPACE FOR THE FLASH MODELS
C
C    ACCESS
C      READ AND WRITE GRANTED ONLY TO XFLASH AND THE FLASH ROUTINES.
C
      DATA TLO,TUP/200.,800./, PLO,PUP/.001,50./
C
C=====================================================================
C   /CSECAN/ - INTERFACE WITH SECANT
C
C    ACCESS
C      READ AND WRITE ACCESS IS NECESSARY FOR ANY ROUTINE
C     .      WHICH USES SECANT.  SEE LISTING OF SECANT.
C
      END
```

APPENDIX E

EXPLANATIONS OF THE DESPAC2 LIBRARY FILE AND THERMOPHYSICAL PROPERTIES

```
C
C
C     COMPONENTS IN PUBDAT
C THESE 91 COMPONENTS ARE AVAILABLE TO ALL USERS.  THE FILE PUBDAT CONTAINS
C ONLY THE PURE-COMPONENT PROPERTIES FOR EACH COMPONENT ; NO BINARY PROPERT
C (E.G., WILSON PARAMETERS) ARE PROVIDED IN THE PUBLIC DATA FILE.
C     NAME                          ALIAS   FORMULA
C
C     ARGON                         AR      AR
C     NITROGEN                      N2      N2
C     OXYGEN                        02      02
C     SULFUR DIOXIDE                S02     02S
C     HYDROGEN CHLORIDE             HCL     HCL
C     HYDROGEN                      H2      H2
C     HYDROGEN SULFIDE              H2S     H2S
C     AMMONIA                       NH3     H3N
C     WATER                         H20     H20
C
C     CARBON TETRACHLORIDE          CCL4    CCL4
C     CARBON DISULFIDE              CS2     CS2
C     CARBON MONOXIDE               CO      CO
C     CARBON DIOXIDE                C02     C02
C     CHLOROFORM                    CCL3    CHCL3
C     DICHLOROMETHANE               CCL2    CH2CL2
C     FORMALDEHYDE                  C1AL    CH20
C     FORMIC ACID                   C1ç     CH202
C     NITROMETHANE                  C1N02   CH302N
C     METHANE                       C1      CH4
C     METHANOL                      MEOH    CH40
C
C     TRICHLORCETHYLENE             TCE     C2HCL3
C     ACETYLENE                     C2#     C2H2
C     METHYL FORMATE                C1F     C2H402
C     ACETONITRILE                  C2N     C2H3N
C     ETHYLENE                      C2=     C2H4
C     1,2-DICHLOROETHANE            12DCE   C2H4CL2
C     ACETALDEHYDE                  C2AL    C2H40
C     ACETIC ACID                   C2ç     C2H402
C     ETHYL IODIDE                  ETI     C2H5I
C     NITROETHANE                   C2NO    C2H502N
C     ETHANE                        C2      C2H6
C     ETHANOL                       ETOH    C2H60
C     ETHYLENE GLYCOL               EG      C2H602
C     DIMETHYLAMINE                 DMA     C2H7N
C
C     PROPYLENE                     C3=     C3H6
C     ACETONE                       ME2CO   C3H60
C     METHYL ACETATE                C1AC    C3H602
C     PROPIONIC ACID                C3ç     C3H602
C     1-NITROPROPANE                1C3NO   C3H702N
C     2-NITROPROPANE                2C3NO   C3H702N
C     PROPANE                       C3      C3H8
C     N-PROPANOL                    NC3OH   C3H80
C     I-PROPANOL                    IC3OH   C3H80
C     TRIMETHYLAMINE                TMA     C3H9N
C
```

```
C     1-BUTENE                      1C4=    C4H8
C     2-BUTANONE                    2C4=O   C4H8O
C     TETRAHYDROFURAN                       C4H8O
C     1,4-DIOXANE                   14DOX   C4H8O2
C     ETHYL ACETATE                 C2AC    C4H8O2
C     N-BUTANE                      NC4     C4H10
C     I-BUTANE                      IC4     C4H10
C     N-BUTANOL                     NC4OH   C4H10O
C     2-BUTANOL                     2C4OH   C4H10O
C     I-BUTANOL                     IC4OH   C4H10O
C     TERT-BUTANOL                  TC4OH   C4H10O
C     DIETHYL ETHER                 DEE     C4H10O
C     ETHYL CELLOSOLVE                      C4H10O2
C     DIETHYLAMINE                  DEA     C4H11N
C
C     FURFURALDEHYDE                FFAL    C5H4O2
C     PYRIDINE                      PYR     C5H5N
C     ISOPRENE                      IPREN   C5H8
C     CYCLOPENTANE                  OC5     C5H10
C     N-PENTANE                     NC5     C5H12
C     I-PENTANE                     IC5     C5H12
C
C     CHLOROBENZENE                 BZCL    C6H5CL
C     NITROBENZENE                  BZNO2   C6H5O2N
C     BENZENE                       BZ      C6H6
C     PHENOL                        BZOH    C6H6O
C     ANILINE                       BZNH2   C6H7N
C     CYCLOHEXANONE                         C6H10O
C     CYCLOHEXANE                   OC6     C6H12
C     1-HEXENE                      1C6=    C6H12
C     METHYLCYCLOPENTANE            MEOC5   C6H12
C     CYCLOHEXANOL                  OC6OH   C6H12O
C     2,2-DIMETHYLBUTANONE          22DMB   C6H12O
C     N-BUTYL ACETATE               NBAC    C6H12O2
C     N-HEXANE                      NC6     C6H14
C     2,3-DIMETHYLBUTANE            23DMB   C6H14
C     TRIETHYLAMINE                 TEA     C6H15N
C
C     TOLUENE                       TOL     C7H8
C     METHYLCYCLOHEXANE             MEOC6   C7H14
C     N-HEPTANE                     NC7     C7H16
C
C     STYRENE                       STYR    C8H8
C     O-XYLENE                      OXYL    C8H10
C     M-XYLENE                      MXYL    C8H10
C     P-XYLENE                      PXYL    C8H10
C     ETHYL BENZENE                 ETBZ    C8H10
C     N-OCTANE                      NC8     C8H18
C     2,2,4-TRIMETHYL PENTANE       224MP   C8H18
C
C     N-DECANE                      NC10    C10H22
C     N-HEXADECANE                  NC16    C16H34
C
```

```
PHYSICAL PROPERTIES FOR DESPAC

EXPLANATION
  EACH LINE IS OF THE FORM <PREFIX> SOURCE  DATA.

  PREFIX  DESCRIPTION OF DATA
     *      IDENTIFICATION.
     =      FUNDAMENTAL PROPERTIES OF PURE COMPONENT.
     0      STANDARD STATE RELATIVE TO PURE ELEMENTS.
     C      PERFECT GAS HEAT CAPACITIES.
     A      ANTOINE COEFFICIENTS.
     #      CONSTANTS USED BY VIRIAL AND MOLVOL.
     :      DIMENSIONLESS PARAMETERS FOR THE REDLICH-KWONG EQUATION.
    ()      CONSTANTS USED BY RSTATE.
     $      DENSITY
     E      BINARY ASSOCIATION PARAMETERS FOR VIRIAL.
     W      WILSON PARAMETERS.
     H      PARAMETERS FOR CORRELATION OF HENRY'S LAW DATA.
     K      INTERACTION PARAMETER IN PRAUSNITZ-CHUEH REDLICH-KWONG EQUATION.

DESCRIPTION OF VARIABLES

  * NAME I   25-CHARACTER NAME OF COMPONENT (FIRST IN BINARY SYSTEM).
  * ALIAS    5-CHARACTER ABBREVIATION.
  * FORMULA ATOMIC FORMULA (C H O N S F CL BR I ;   OTHERS ALPHABETICALLY).

  = MOLWT    MOLECULAR WEIGHT.
  = OMEGA    PITZER'S ACENTRIC FACTOR.
  = TC       CRITICAL TEMPERATURE (K).
  = PC       CRITICAL PRESSURE (BAR).
  = VC       CRITICAL VOLUME (ML/MOL).

  0 DELHF    ENTHALPY (J/MOL) OF FORMATION OF PURE COMPONENT IN THE
             PERFECT-GAS STATE AT TREF FROM PURE ELEMENTS IN THEIR MOST
             STABLE STATE AT 298 K AND 1 BAR.
  0 DELGF    GIBBS ENERGY (J/MOL) OF FORMATION OF PURE COMPONENT IN THE
             PERFECT GAS STATE AT TREF,PREF FROM PURE ELEMENTS IN THEIR
             MOST STABLE STATES AT 298 K AND 1 BAR.
  0 TREF     REFERENCE TEMPERATURE (K) FOR DELHF,DELGF.
  0 PREF     REFERENCE PRESSURE (BAR) FOR DELHF,DELGF.

  C CPVAPA   CONSTANTS IN THE PERFECT-GAS HEAT-CAPACITY EQUATION, WITH
  C CPVAPB   CP (J/MOL-K) = A + B*T + C*T**2 + D*T**3
  C CPVAPC   WHERE T IS TEMPERATURE (K).
  C CPVAPD
  C TMN,TMX INTERVAL OF TEMPERATURE (K) FOR WHICH A,B,C,D ARE VALID.

  A ANTA     CONSTANTS IN ANTOINE VAPOR-PRESSURE EQUATION, WITH
    ANTB     VAPOR PRESSURE VP (BAR) GIVEN AS FUNCTION OF T (K) BY
    ANTC     LN(VP) = ANTA - ANTB/(T + ANTC).
  A TMN,TMX DOMAIN OF TEMPERATURE (K) FOR ANTOINE EQUATION.

  # RDGYRA   RADIUS OF GYRATION (A).
  # DIPOLE   DIPOLE MOMENT (DEBYE).
  # ETA      CHEMICAL ASSOCIATION PARAMETER FOR PAIR I,I.
  # ZRA      CONSTANT IN THE RACKETT EQUATION.
  # VSTAR    CORRELATING PARAMETER (ML/MOL) ;  NOT USED BY KVALUE.

  : RKOMGA   CORRELATING PARAMETERS IN REDLICH-KWONG EQUATION.
  : RKOMGB

 (  FOCON    CONSTANTS IN ZERO-P REFERENCE FUGACITY CORRELATION OF C.A.ECKERT.
 (  TMN,TMX DOMAIN OF TEMPERATURE (K) OF DATA TO WHICH FOCON WERE FIT.
```

```
$ DENSITY AT 298 K (G/CM**3)

E NAME J  NAME OF SECOND COMPONENT IN BINARY SYSTEM.
E ETA     CHEMICAL ASSOCIATION PARAMETER FOR PAIR I,J.

W NAME J  NAME OF SECOND COMPONENT IN BINARY SYSTEM.
W LLAM    WILSON PARAMETERS (K).

H NAME J  NAME OF SECOND COMPONENT IN BINARY SYSTEM.
H ACTA    ANDERSON PARAMETERS FOR CORRELATING ACTIVITY COEFFICIENTS OF
          NON-CONDENSABLE COMPONENTS.
          LN(GAMMA12) = ACTA12 + ACTA21/T
          WHERE GAMMA12 IS ACTIVITY COEFFICIENT OF NON-CONDENSABLE 1
                        IN CONDENSABLE 2 AT INFINITE DILUTION OF 1.
                      T IS TEMPERATURE (K).

K NAME J  NAME OF SECOND COMPONENT IN BINARY SYSTEM.
K RKPCK   PRAUSNITZ-CHUEH INTERACTION PARAMETER FOR REDLICH-KWONG EQUATION.


FORMAT:
*   NAME I                   ALIAS  FORMULA
=          HOLHT        OMEGA          TC          PC          VC
0          DFLHF        DELGF        TREF        PREF
C         CPVAPA       CPVAPB      CPVAPC      CPVAPD        TMIN        TMAX
A           ANTA         ANTB        ANTC        TMIN        TMAX
#         RDGYRA       DIPOLE         ETA         ZRA       VSTAR
:         RKOMGA       RKOMGB
(         FOCON(1)             FOCON(2)             FOCON(3)    TMIN
)         FOCON(4)             FOCON(5)             FOCON(6)    TMAX
$         DENS
E   NAME J                          ETA(I,J)
W   NAME J                         LLAM(I,J)  LLAM(J,I)
H   NAME J                         ACTA(I,J)  ACTA(J,I)
K   NAME J                        RKPCK(I,J)
18.21.32.UCLP, BU, PU3     ,        0.136KLNS.
```

APPENDIX F

INPUT AND OUTPUT SYMBOL DESCRIPTION
FOR COMPUTER APPLICATION

```
C***********************************************************************
C
C     KVALUE - VLE PACKAGE
C
C***********************************************************************
C
C         KVALUE PARAMETERS
C
C INPUT PARAMETERS
C
C SYMBOL    DESCRIPTION
C
C
C
C T           TEMPERATURE (K).
C
C P           PRESSURE (BAR).
C
C X(I)        MOLE FRACTION OF COMPONENT I - LIQUID PHASE.
C
C Y(I)        MOLE FRACTION OF COMPONENT I - VAPOR PHASE.
C
C OUTPUT PARAMETERS
C
C SYMBOL    DESCRIPTION
C
C
C
C K(I)        EQUILIBRIUM CONSTANT (K-VALUE) OF COMPONENT I.
C
C NOTE:
C
C  - K(I) = Y(I)/X(I) ONLY WHEN THE LIQUID AND VAPOR PHASES ARE IN
C    EQUILIBRIUM ;   THUS, THE VALUE OF K(I) TESTS FOR BUT DOES NOT DICTATE
C    EQUILIBRIUM.
C
C
C
C***********************************************************************
C
C     PHASE - DEW POINT AND BUBBLE POINT CALCULATION
C
C***********************************************************************
C
C     PHASE PARAMETERS
C
C INPUT PARAMETERS
C
C SYMBOL    DESCRIPTION
C
C
C
C P           PRESSURE (BAR) FOR DEW/BUBBLE TEMPERATURES.
C
C T           TEMPERATURE (K) FOR DEW/BUBBLE PRESSURES.
C
C Z(I)        MOLE FRACTION OF I IN THE SYSTEM.
C
C TLO         LOWER BOUND ON DEW/BUBBLE TEMPERATURES (K).    100.0
C
C TUP         UPPER BOUND ON DEW/BUBBLE TEMPERATURES (K).    800.0
C
C PLO         LOWER BOUND ON DEW/BUBBLE PRESSURES (BAR).    0.0001
C
C PUP         UPPER BOUND ON DEW/BUBBLE PRESSURES (BAR).   100.0
```

```
C
C OUTPUT PARAMETERS
C
C SYMBOL      DESCRIPTION
C
C
C
C BT           BUBBLE TEMPERATURE (K) ;   TEMPERATURE OF SATURATED LIQUID OF
C          COMPOSITION Z AT P.
C
C DT           DEW TEMPERATURE (K) ;   TEMPERATURE OF SATURATED VAPOR OF COMPOSITION Z
C          AT P.
C
C BP           BUBBLE PRESSURE (BAR) ;   PRESSURE OF SATURATED LIQUID OF COMPOSITION Z
C          AT T.
C
C DP           DEW PRESSURE (BAR) ;   PRESSURE OF SATURATED VAPOR OF COMPOSITION Z AT
C          T.
C
C YBT(I)       MOLE FRACTION OF COMPONENT I IN VAPOR WHICH IS IN EQUILIBRIUM WITH
C          LIQUID OF COMPOSITION Z AT P,BT.
C
C XDT(I)       MOLE FRACTION OF COMPONENT I IN LIQUID WHICH IS IN EQUILIBRIUM WITH
C          VAPOR OF COMPOSITION Z AT P,DT.
C
C YBP(I)       MOLE FRACTION OF COMPONENT I IN VAPOR WHICH IS IN EQUILIBRIUM WITH
C          LIQUID OF COMPOSITION Z AT BP,T.
C
C XDP(I)       MOLE FRACTION OF COMPONENT I IN LIQUID WHICH IS IN EQUILIBRIUM WITH
C          VAPOR OF COMPOSITION Z AT DP,T.
C
C NOTES:
C
C  - DT AND BT ARE NEVER ALLOWED OUTSIDE THE CLOSED INTERVAL  TLO,TUP .
C
C  - DP AND BP ARE NEVER ALLOWED OUTSIDE THE CLOSED INTERVAL  PLO,PUP .
C
C  - THE INITIALIZED VALUES OF TLO, TUP, PLO, AND PUP ENCLOSE WIDE
C    INTERVALS WHICH USUALLY WORK WELL WITH THE WILSON/VIRIAL MODEL.  FOR
C    THE REDLICH-KWONG MODEL, IT MAY BE NECESSARY TO DEFINE MORE NARROW
C    INTERVALS APPROPRIATE TO THE SYSTEM OF INTEREST.
C-----------------
```

```
C
C*********************************************************************************
C
C     FLASH - FLASH CALCULATIONS
C
C*********************************************************************************
C FLASH PERFORMS TWO-PHASE VAPOR-LIQUID FLASH CALCULATIONS.  SIX VARIATIONS, OR
C "TYPES" OF FLASH, ARE AVAILABLE.  THEY INCLUDE THE ADIABATIC FLASHES (PQ,TQ),
C ISOTHERMAL FLASH (TP), AND DEW- AND BUBBLE-POINT CALCULATIONS (TV,PV).
C
C
C       FLASH PARAMETERS
C
C SYMBOL    DESCRIPTION
C
C
C
C T           TEMPERATURE (K) OF FLASH.
C
C P           PRESSURE (BAR) OF FLASH.
C
C Q           HEAT ADDED (J/MOL) TO FLASH PER MOLE OF FEED TO FLASH.
C
C V           FRACTION OF FEED WHICH IS VAPORIZED.  0 <= V <= 1.
C          V=0 ==> NO VAPOR PRODUCT FORMED.
C          V=1 ==> NO LIQUID PRODUCT FORMED.
C
C HF          ENTHALPY (J/MOL) OF FEED.
C
C HL          ENTHALPY (J/MOL) OF LIQUID PRODUCT.
C
C HV          ENTHALPY (J/MOL) OF VAPOR PRODUCT.
C
C K(I)        EQUILIBRIUM CONSTANT (K-VALUE) ; K(I) = Y(I)/X(I) WHEN TWO PHASES ARE
C          IN EQUILIBRIUM.
C
C XI(I)       SPLIT FRACTION ;  FRACTION OF I ENTERING IN FEED WHICH LEAVES IN THE
C          VAPOR PRODUCT.
C
C X(I)        MOLE FRACTION OF COMPONENT I IN LIQUID PRODUCT.
C
C Y(I)        MOLE FRACTION OF COMPONENT I IN VAPOR PRODUCT.
C
C Z(I)        MOLE FRACTION OF COMPONENT I IN FEED.
C
C TLO         LOWER BOUND ON T FOR PQ, PV FLASHES.
C
C TUP         UPPER BOUND ON T FOR PQ, PV FLASHES.
C
C PLO         LOWER BOUND ON P FOR TQ, TV FLASHES.
C
C PUP         UPPER BOUND ON P FOR TQ, TV FLASHES.
C          SEE THE DISCUSSION OF THESE PARAMETERS UNDER PHASE.
C
C GUESS       CONTROLS THE GUESSING OF OUTPUT VARIABLES T,P,X,Y,V.  THE FLASH
C          ALGORITHMS REQUIRE AN INITIAL GUESS FOR OUTPUT VARIABLES.  USUALLY AN
C          AUTOMATIC PROCEDURE PRODUCES GUESSES GOOD ENOUGH TO FIND THE CORRECT
C          SOLUTION, BUT OCCASIONALLY THIS GUESS IS TOO FAR FROM THE SOLUTION TO
C          ALLOW CONVERGENCE.  THIS IS OFTEN THE CASE WHEN EQUATIONS OF STATE
C          SUCH AS THE REDLICH-KWONG EQUATION ARE USED TO ESTIMATE K-VALUES.  IN
C          SUCH A CASE, THE USER MAY SUPPLY HIS OWN GUESSES (OR USE THE
C          CONVERGED RESULTS OF A PREVIOUS SOLUTION) FOR OUTPUT VARIABLES T, P,
C          X, Y, OR V.
C          GUESS = 0  -->   PROGRAM GUESSES OUTPUT VALUES.
C          GUESS = 1  -->   USER GUESSES OUTPUT VALUES.
```

```
C
C*******************************************************************************
C
C      ABSEDM - GAS ABSORPTION (EDMISTER METHOD)
C
C*******************************************************************************
C
C        ABSEDM PARAMETERS
C
C INPUT PARAMETERS
C
C SYMBOL    DESCRIPTION
C
C
C
C TT         TEMPERATURE (K) AT TOP OF COLUMN.
C
C TB         TEMPERATURE (K) AT BOTTOM OF COLUMN.
C
C P          AVERAGE PRESSURE (BAR) THROUGHOUT COLUMN.
C
C LT         MOLAR FLOWRATE OF LIQUID FEED INTO TOP OF COLUMN.
C
C VB         MOLAR FLOWRATE OF VAPOR FEED INTO BOTTOM OF COLUMN.
C
C N          NUMBER OF THEORETICAL EQUILIBRIUM STAGES.
C
C XT(I)      MOLE FRACTION OF COMPONENT I IN LIQUID FEED (TOP).
C
C YB(I)      MOLE FRACTION OF COMPONENT I IN VAPOR FEED (BOTTOM).
C
C OUTPUT PARAMETERS
C
C SYMBOL    DESCRIPTION
C
C
C
C VT         MOLAR FLOWRATE OF VAPOR PRODUCT FROM TOP OF COLUMN.
C
C LB         MOLAR FLOWRATE OF LIQUID PRODUCT FROM BOTTOM OF COLUMN.
C
C YT(I)      MOLE FRACTION OF COMPONENT I IN VAPOR PRODUCT (TOP).
C
C XB(I)      MOLE FRACTION OF COMPONENT I IN LIQUID PRODUCT (BOTTOM).
C
C XIT(I)     SPLIT FRACTION ;  FRACTION OF COMPONENT I ENTERING IN LT WHICH LEAVES
C          IN VT.
C
C XIB(I)     SPLIT FRACTION ;  FRACTION OF COMPONENT I ENTERING IN VB WHICH LEAVES
C          IN LB.
C
```

```
C
C***********************************************************************
C
C    MCCABE - MCCABE-THIELE BINARY DISTILLATION
C
C***********************************************************************
C
C     MCCABE PARAMETERS
C
C INPUT PARAMETERS
C
C SYMBOL    DESCRIPTION
C
C
C
C RATIO     USED TO CALCULATE THE ACTUAL REFLUX RATIO.  TYPICAL VALUE IS 1.3. THE
C         ACTUAL REFLUX RATIO WILL BE RATIO TIMES THE MINIMUM REFLUX RATIO.
C
C ALPHA     VOLATILITY OF COMPONENT 1 RELATIVE TO COMPONENT 2.
C         ALPHA MUST BE GREATER THAN 1.0.
C
C Q         QUALITY OF FEED.  SEE NOTE BELOW.
C         Q=0 -->  ALL FEED IS VAPOR AT DEW POINT.
C         Q=1 -->  ALL FEED IS LIQUID AT BUBBLE POINT.
C
C ETA       MURPHREE GAS-SIDE STAGE EFFICIENCY - USED TO STEP OFF STAGES. 1.0
C
C XF        MOLE FRACTION OF COMPONENT 1 IN FEED.
C
C XD        MOLE FRACTION OF COMPONENT 1 IN DISTILLATE.
C
C F         MOLAR FLOWRATE OF FEED.
C
C D         MOLAR FLOWRATE OF DISTILLATE.
C
C OUTPUT PARAMETERS
C
C SYMBOL    DESCRIPTION
C
C
C
C XW        MOLE FRACTION OF COMPONENT 1 IN BOTTOM PRODUCT.
C
C W         MOLAR FLOWRATE OF BOTTOM PRODUCT.
C
C L         INTERNAL MOLAR FLOWRATE OF LIQUID IN TOP OF COLUMN.
C
C V         INTERNAL MOLAR FLOWRATE OF VAPOR IN TOP OF COLUMN.
C
C LB        INTERNAL MOLAR FLOWRATE OF LIQUID IN BOTTOM OF COLUMN.
C
C VB        INTERNAL MOLAR FLOWRATE OF VAPOR IN BOTTOM OF COLUMN.
C
C NT        NUMBER OF STAGES IN TOP OF COLUMN (INCLUDES FEED TRAY).
C
C NB        NUMBER OF STAGES IN BOTTOM OF COLUMN.
C
C NOTE:
C
C  - DEFINITION OF FEED QUALITY, Q:
C
C                    HDP - HF
C               Q = --------
C                    HDP-HBPT
C
C               WHERE
C                       HDP  =  ENTHALPY OF VAPOR AT DEW POINT
C                       HF   =  ENTHALPY OF FEED
C                       HBPT =  ENTHALPY OF LIQUID AT BUBBLE POINT
C
```

```
C
C*********************************************************************
C
C     SHTCUT - SHORTCUT MULTICOMPONENT DISTILLATION
C
C*********************************************************************
C
C        SHTCUT PARAMETERS
C
C ENUMERATED PARAMETERS
C
C SYMBOL    DESCRIPTION
C
C
C
C NEW         TRUE FOR NEW COLUMN ;  FALSE FOR OLD COLUMN.
C          A NEW COLUMN IS DESIGNED BY SPECIFYING FTL ; AN OLD COLUMN (ONE WHICH
C          PHYSICALLY EXISTS) IS CHARACTERIZED BY SD, THE NUMBER OF THEORETICAL
C          STAGES.
C
C IK          SELECTS METHOD FOR FINDING REFLUX RATIO R.
C          IK=1 --> R IS CHOSEN SUCH THAT THE RATIO
C                   <INTERNAL MOLAR FLOWRATE OF VAPOR>
C                   ---------------------------------- = VFMAX.
C                         <MOLAR FLOWRATE OF FEED>
C          IK=2 --> R IS SPECIFIED A PRIORI.
C          IK=3 --> R IS A FUNCTION OF THE MINIMUM REFLUX RATIO ;
C                   IE, R = RFAC*RMIN.
C
C
C AUTO        TRUE IF VOLATILITTIES ARE TO BE COMPUTED AUTOMATICALLY BY FLSHTP ;
C          OTHERWISE FALSE.  THE VOLATILITY OF A COMPONENT I RELATIVE TO A
C          COMPONENT J IS GIVEN BY THE RATIO OF K-VALUES K(I)/K(J) ; THESE K-
C          VALUES ARE COMPUTED BY FLSHTP AT T, P AND Z=XF.
C
C INPUT PARAMETERS
C
C SYMBOL    DESCRIPTION
C
C
C
C LKEY        INDEX OF THE LIGHT KEY COMPONENT. THE HEAVY KEY IS THE COMPONENT
C          WHOSE RELATIVE VOLATILITY IS NEXT SMALLEST TO THAT OF THE LIGHT KEY.
C
C Q           QUALITY OF THE FEED.
C          Q=0 -->  FEED IS SATURATED VAPOR.
C          Q=1 -->  FEED IS SATURATED LIQUID.
C
C XF(I)        MOLE FRACTION OF COMPONENT I IN FEED.
C
C VFMAX       (REQUIRED WHEN IK=1)
C          THE MAXIMUM ALLOWABLE VALUE OF THE RATIO
C          <INTERNAL MOLAR FLOWRATE OF VAPOR>
C          ----------------------------------
C                <MOLAR FLOWRATE OF FEED>
C
```

```
C
C R           (REQUIRED WHEN IK=2) REFLUX RATIO.
C
C RFAC        (REQUIRED WHEN IK=3)
C          FACTOR BY WHICH RMIN IS MULTIPLIED TO GIVE R, THE ACTUAL REFLUX
C          RATIO.
C
C T,P         (REQUIRED WHEN AUTO IS TRUE)
C          TEMPERATURE (K) AND PRESSURE (BAR) AT WHICH FLSHTP COMPUTES RELATIVE
C          VOLATILITIES.
C
C AL(I)       (REQUIRED WHEN AUTO IS FALSE)
C          VOLATILITY OF COMPONENT I RELATIVE TO ANY OTHER COMPONENT ; ON OUTPUT,
C          ALL VOLATILITIES ARE SCALED RELATIVE TO THE HEAVY KEY.
C
C FTL         (REQUIRED WHEN NEW IS TRUE)
C          FRACTION OF LIGHT KEY RECOVERED AT TOP OF COLUMN.
C
C SD          (REQUIRED WHEN NEW IS FALSE)
C          THE NUMBER OF THEORETICAL STAGES IN AN EXISTING COLUMN.
C
C FBH         FRACTION OF HEAVY KEY RECOVERED AT BOTTOM OF COLUMN.
C
C OUTPUT PARAMETERS
C
C SYMBOL      DESCRIPTION
C
C
C
C FTL         (OUTPUT WHEN NEW IS FALSE)
C          FRACTION OF LIGHT KEY RECOVERABLE AT TOP OF COLUMN WITH A COLUMN OF
C          SD THEORETICAL STAGES.
C
C FTR         LOCATION OF FEED TRAY - THE NUMBER OF THEORETICAL STAGES FROM THE TOP
C          OF THE COLUMN.
C
C SD          (OUTPUT WHEN NEW IS TRUE)
C          NUMBER OF THEORETICAL STAGES NECESSARY TO EFFECT THE SEPARATION
C          SPECIFIED BY FTL.
C
C SMIN        MINIMUM NUMBER OF THEORETICAL STAGES. SD = SMIN WHEN R = INFINITY.
C
C R           (OUTPUT WHEN IK IS NOT 2) ACTUAL REFLUX RATIO.
C
C RMIN        MINIMUM REFLUX RATIO.
C
C XD(I)       MOLE FRACTION OF COMPONENT I IN DISTILLATE (TOP).
C
C XB(I)       MOLE FRACTION OF COMPONENT I IN BOTTOMS PRODUCT.
C
C AL(I)       (OUTPUT WHEN AUTO IS TRUE)
C          VOLATILITY OF COMPONENT I RELATIVE TO THE HEAVY KEY.
C
C REC(I)      RECOVERY OF I - FRACTION OF I ENTERING IN FEED WHICH LEAVES IN
C          DISTILLATE.
C
C R, AL, FTL, AND SD ARE EITHER INPUT OR OUTPUT, DEPENDING ON NEW, IK, AND
C AUTO.  DESPAC PROMPTS THE USER FOR ONLY THE REQUIRED NAMED PARAMETERS.
C
```

```
C
C
C*************************************************************************
C
C     COLUMN - RIGOROUS COLUMN CALCULATION
C
C*************************************************************************
C
C        COLUMN PARAMETERS
C
C INPUT PARAMETERS
C
C SYMBOL     DESCRIPTION
C
C
C
C NS         NUMBER OF STAGES.  NS >= 2.
C
C BETA       LIQUID FRACTION OF DISTILLATE PRODUCT.   1.0
C           BETA = 1 - V(NS)/D                 0 <= BETA <= 1
C           BETA = 1   ==>  TOTAL CONDENSER
C
C
C RT         REFLUX RATIO.
C
C RB         REBOIL RATIO.  RB = V(1)/L(1)
C
C PT         PRESSURE (BAR) IN CONDENSER.
C
C PB         PRESSURE (BAR) IN REBOILER.
C
C FEED
C
C
C
C K          INDEX OF FEED STAGE.  T,P
C           TEMPERATURE (K), PRESSURE (BAR) OF FEED TO STAGE K. Z(I)
C           MOLE FRACTION OF COMPONENT I IN FEED TO STAGE K. THE ENTHALPY HF(K)
C           OF THE FEED IS DETERMINED AT T,P,Z.  FK
C           MOLAR FLOWRATE OF FEED TO STAGE K.  100.0
C
C XI(I)     USER'S INITIAL GUESS OF THE SPLIT FRACTION.   0.5  THIS IS USED TO
C           GENERATE GUESSES FOR COMPOSITIONS, TEMPERATURES, AND FLOWRATES WITHIN
C           THE COLUMN.
C           XI(I) = 1 ==>   COMPONENT I IS VOLATILE ;
C                           100% RECOVERY IN DISTILLATE EXPECTED.
C           XI(I) = 0 ==>   COMPONENT I IS HEAVY ;
C                           100% RECOVERY IN BOTTOMS EXPECTED.
C
C
C SIDE
C
C
C
C SV(K)     FRACTION OF VAPOR LEAVING STAGE K WHICH IS WITHDRAWN AS A VAPOR
C           SIDESTREAM.  0 <= SV(K) < 1. SV(K) = 0  ==>  NO VAPOR SIDESTREAM FROM
C           STAGE K. SL(K)
C           FRACTION OF LIQUID LEAVING STAGE K WHICH IS WITHDRAWN AS A LIQUID
C           SIDESTREAM.  0 <= SL(K) < 1. SL(K) = 0  ==>  NO LIQUID SIDESTREAM
C           FROM STAGE K.
```

```
C OUTPUT PARAMETERS
C
C SYMBOL    DESCRIPTION
C
C
C
C QT          HEAT REMOVED (J/TIME) FROM CONDENSER.
C
C QB          HEAT ADDED (J/TIME) TO REBOILER.
C
C MOST OF THE RESULTS OF COLUMN ARE CONTAINED IN THE "PROFILE", A TABULATION OF
C SEVERAL VARIABLES BY STAGE INDEX.  THE FOLLOWING OUTPUT VARIABLES APPEAR IN THE
C PROFILE.  THE USER CHOOSES THE VARIABLES TO BE PROFILED FROM THIS LIST.
C
C PROFILE
C
C  SYMBOL    DESCRIPTION
C
C
C
C
C
C  1 L(K)    MOLAR FLOWRATE OF LIQUID LEAVING STAGE K.
C
C  2 V(K)    MOLAR FLOWRATE OF VAPOR LEAVING STAGE K.
C
C  3 F(K)    MOLAR FLOWRATE OF FEED ENTERING STAGE K.
C
C  4 L(I,K)
C          MOLAR FLOWRATE OF COMPONENT I LEAVING STAGE K IN LIQUID.
C
C  5 V(I,K)
C          MOLAR FLOWRATE OF COMPONENT I LEAVING STAGE K IN VAPOR.
C
C  6 F(I,K)
C          MOLAR FLOWRATE OF COMPONENT I ENTERING STAGE K IN FEED.
C
C  7 X(I,K)
C          MOLE FRACTION OF COMPONENT I IN LIQUID LEAVING STAGE K.
C
C  8 Y(I,K)
C          MOLE FRACTION OF COMPONENT I IN VAPOR LEAVING STAGE K.
C
C  9 Z(I,K)
C          MOLE FRACTION OF COMPONENT I IN FEED ENTERING STAGE K.
C
C 10 HL(K)  ENTHALPY (J/MOL) OF LIQUID LEAVING STAGE K.
C
C 11 HV(K)  ENTHALPY (J/MOL) OF VAPOR LEAVING STAGE K.
C
C 12 HF(K)  ENTHALPY (J/MOL) OF FEED ENTERING STAGE K.
C
C 13 L*HL(K)
C          ENTHALPY FLOWRATE (J/TIME) OF LIQUID LEAVING STAGE K.
C
C 14 V*HV(K)
C          ENTHALPY FLOWRATE (J/TIME) OF VAPOR LEAVING STAGE K.
C
C 15 F*HF(K)
C          ENTHALPY FLOWRATE (J/TIME) OF FEED ENTERING STAGE K.
C
C 16 K(I,K)
C          K-VALUE OF COMPONENT I ON STAGE K.
C
C 17 T(K)   TEMPERATURE (K) ON STAGE K.
C
C 19 LS(K)  MOLAR FLOWRATE OF LIQUID SIDESTREAM LEAVING STAGE K.
C          LS(K) = SL(K) * L(K)
C
C 20 VS(K)  MOLAR FLOWRATE OF VAPOR SIDESTREAM LEAVING STAGE K.
C          VS(K) = SV(K) * V(K)
C
C 21 SL(K)  FRACTION OF L(K) WITHDRAWN AS LIQUID SIDESTREAM.
C
C 22 SV(K)  FRACTION OF V(K) WITHDRAWN AS VAPOR SIDESTREAM.
C
C
```

```
C
C***********************************************************************
C
C     CERDA - SHORTCUT MULTICOMPONENT DISTILLATION (NON-ADJACENT KEYS)
C
C***********************************************************************
C CERDA USES THE SHORTCUT TECHNIQUES DEVELOPED BY CERDA AND WESTERBERG.
C RESULTS OF THE SHORTCUT CALCULATION CAN BE PASSED TO COLCST, WHICH ESTIMATES
C THE SIZE AND COST OF THE COLUMN.
C
C INPUT PARAMETERS
C
C SYMBOL    DESCRIPTION
C
C
C F           FLOWRATE OF FEED, MOL/TIME.   100
C          IF COST IS NON-ZERO, F SHOULD HAVE THE UNITS MOL/S.
C
C XF(I)    MOLE FRACTION OF COMPONENT I IN FEED.
C
C LKEY     NUMBER OF THE LIGHT KEY COMPONENT.  COMPONENTS MORE VOLATILE THAN THE
C          LIGHT KEY ARE ASSUMED TO EXIT IN THE DISTILLATE PRODUCT.
C
C HKEY     NUMBER OF THE HEAVY KEY COMPONENT.  COMPONENTS LESS VOLATILE THAN THE
C          HEAVY KEY ARE ASSUMED TO EXIT IN THE BOTTOM PRODUCT.
C
C          DISTRIBUTION OF COMPONENTS OF INTERMEDIATE VOLATILITY IS ESTIMATED
C          WITH HENGSTEBECK'S METHOD.
C
C FTL         FRACTION OF LIGHT KEY RECOVERED IN THE TOP PRODUCT.   .99
C
C FBH         FRACTION OF HEAVY KEY RECOVERED IN THE BOTTOM PRODUCT.   .99
C
C T           TEMPERATURE AT WHICH TO ESTIMATE RELATIVE VOLATILITY, K.  300
C
C P           PRESSURE AT WHICH TO ESTIMATE RELATIVE VOLATILITY, BAR.   1
C          AN ISOTHERMAL FLASH IS PERFORMED AT T, P, XF(I) TO DETERMINE K(I).
C          SEE ALSO COST.
C
C Q           QUALITY OF FEED.   1
C
C             Q=0 --> FEED IS SATURATED VAPOR.
C             Q=1 --> FEED IS SATURATED LIQUID.
C
C
C
C RFAC        FACTOR BY WHICH THE MINIMUM REFLUX RATIO RTMIN IS MULTIPLIED TO GIVE
C          THE ACTUAL REFLUX RATIO, RT.   1.2
C
C COST        IF NON-ZERO, RESULTS OF THE SHORTCUT CALCULATION ARE PASSED TO
C          COLCST.  0    SEE BELOW.
```

```
C
C OUTPUT PARAMETERS
C
C SYMBOL      DESCRIPTION
C
C
C
C NT          NUMBER OF TRAYS IN TOP OF COLUMN.
C
C NB          NUMBER OF TRAYS IN BOTTOM OF COLUMN.
C
C D           MOLAR FLOWRATE OF DISTILLATE PRODUCT, MOL/TIME.
C
C B           MOLAR FLOWRATE OF BOTTOM PRODUCT, MOL/TIME. F = D + B
C
C RT          REFLUX RATIO.  LT = RT*D
C
C RB          REBOIL RATIO.  VB = RB*B
C
C RTMIN       MINIMUM REFLUX RATIO.  RT = RFAC*RTMIN
C
C RBMIN       MINIMUM REBOIL RATIO.
C
C LT          INTERNAL LIQUID FLOWRATE IN TOP OF COLUMN, MOL/TIME.
C
C VT          INTERNAL VAPOR FLOWRATE IN TOP OF COLUMN, MOL/TIME.
C
C LB          INTERNAL LIQUID FLOWRATE IN BOTTOM OF COLUMN, MOL/TIME.
C
C VB          INTERNAL VAPOR FLOWRATE IN BOTTOM OF COLUMN, MOL/TIME.
C
C XD(I)       MOLE FRACTION OF COMPONENT I IN DISTILLATE PRODUCT.
C
C XB(I)       MOLE FRACTION OF COMPONENT I IN BOTTOM PRODUCT.
C
C XI(I)       SPLIT FRACTION ; FRACTION OF COMPONENT I RECOVERED IN DISTILLEDE
C             PRODUCT.
C
C               XI(LKEY) = FTL
C               XI(HKEY) = 1 - FBH
C
C
C
C AL(I)       VOLATILITY OF COMPONENT I RELATIVE TO THE HEAVY KEY.
C
C               AL(I) = K(I)/K(HKEY)
C
C
C
C K(I)        K-VALUE.  ESTIMATED BY ISOTHERMAL FLASH EVALUATED AT T, P, AND
C             COMPOSITION OF FEED XF.
C
```

```
C***********************************************************************
C
C       SIZING AND COSTING BY COLCST
C
C***********************************************************************
C WHEN COST IS SET NON-ZERO, CERDA ESTIMATES SEVERAL OF THE INPUT PARAMETERS
C FOR COLCST AND THEN CALLS THAT PROCEDURE.  COLCST WILL REQUEST THE REMAINING
C INPUTS AND THEN ESTIMATE THE SIZE AND COST OF THE DISTILLATION COLUMN.  THE
C FOLLOWING PARAMETERS ARE TRANSFERRED TO COLCST FROM CERDA:
C
C LIQUID FLOWRATE, VAPOR FLOWRATE
C               THE INTERNAL MOLAR FLOWRATES IN THE BOTTOM OF THE COLUMN, LB
C               AND VB, ARE USED TO ESTIMATE THESE PARAMETERS.  THE INPUT
C               PARAMETER F (MOLAR FLOWRATE OF THE FEED) IS ASSUMED TO HAVE THE
C               UNITS MOL/S.  BOTH STREAMS ARE ASSUMED TO HAVE THE COMPOSITION
C               OF THE BOTTOM PRODUCT, XB, IN ORDER TO ESTIMATE THE AVERAGE
C               MOLECULAR WEIGHTS.
C
C LIQUID DENSITY  IS EVALUATED AT THE TEMPERATURE, T, USED BY CERDA TO ESTIMATE
C               RELATIVE VOLATILITIES.  THE MOLE FRACTION AVERAGE OF THE PURE-
C               COMPONENT DENSITIES IS PASSED TO COLCST.  THE RACKETT EQUATION
C               IS USED TO ESTIMATE THE PURE-COMPONENT DENSITIES.
C
C VAPOR DENSITY   IS EVALUATED FROM THE PERFECT GAS LAW AT THE VALUES OF THE
C               PARAMETERS TEMPERATURE, T, AND PRESSURE, P, AND COMPOSITION XB.
C
C NUMBER OF TRAYS IS THE SUM OF THE OUTPUT PARAMETERS NT + NB.
C
C PRESSURE        IS THE INPUT PARAMETER P.
C
C
C***********************************************************************
C
C     COLCST - SIZE AND COST OF COLUMN
C
C***********************************************************************
C COLCST ESTIMATES SIZES AND COSTS FOR A VERTICAL SECTION OF A COLUMN WITH
C TRAYS.  THE SIZING IS BASED ON THE FLOODING CHARACTERISTICS OF THE COLUMN ;
C GUTHRIE'S MODULE METHOD IS USED TO ESTIMATE COSTS.
C
C FLOODING BEHAVIOR IS ESTIMATED FROM THE CORRELATION OF FAIR, AS REPORTED BY
C TREYBAL IN EQUATIONS 6.1 AND 6.2.  A GRAPH OF THIS EQUATION APPEARS IN PERRY'S,
C FIGURE 18-10, PAGE 18-6.  COLCST USES FAIR'S CORRELATION TO ESTIMATE THE
C DIAMETER OF THE COLUMN.  THE CORRELATION REQUIRES THE FOLLOWING INFORMATION:
C
C  - LIQUID FLOWRATE, G/S
C  - VAPOR FLOWRATE, G/S
C                         3
C  - LIQUID DENSITY, G/M
C                         3
C  - VAPOR DENSITY, G/M
C  - TRAY SPACING, M
C  - ACTIVE PLATE AREA AS FRACTION OF COLUMN CROSS-SECTION
C  - SURFACE TENSION OF LIQUID, N/M
C  - OPERATING SUPERFICIAL VELOCITY AS FRACTION OF FLOODING VELOCITY
C
C TABLE 18-3 IN PERRY'S HANDBOOK PROVIDES ESTIMATES FOR THE ACTIVE PLATE AREA
C FOR SEVERAL TYPES OF TRAY ;70% OF A TYPICAL TRAY IS AVAILABLE FOR VAPOR FLOW.
C
C GUTHRIE'S METHOD USES THE INFORMATION LISTED BELOW TO ESTIMATE COSTS.  A
C DISENGAGING SPACE OF 6 METERS IS ADDED TO THE HEIGHT OF THE TRAY STACK TO
C OBTAIN THE HEIGHT OF THE COLUMN.
C
C  - NUMBER OF TRAYS
C  - OPERATING PRESSURE, BAR
C  - COLUMN CONSTRUCTION
C  - COLUMN MATERIAL
C  - TRAY MATERIAL
C  - TRAY TYPE
C  - CHEMICAL ENGINEERING PLANT COST INDEX
C
```

```
C
C**********************************************************
C
C    HEX - SHELL-AND-TUBE HEAT EXCHANGER CALCULATIONN
C
C**********************************************************
C
C        HEX PARAMETERS
C
C INPUT PARAMETERS
C
C SYMBOL    DESCRIPTION
C
C
C TH1       HOT  STREAM INLET  TEMPERATURE, K
C
C TH2       HOT  STREAM OUTLET TEMPERATURE, K
C
C TC1       COLD STREAM INLET  TEMPERATURE, K
C
C TC2       COLD STREAM OUTLET TEMPERATURE, K
C
C N         NUMBER OF SHELL PASSES
C
C HO        OUTSIDE RESISTANCE, W / M**2-K
C
C HDO       OUTSIDE THERMAL RESISTANCE OF SCALE DEPOSITS, W / M**2-K
C
C HDI       INSIDE  THERMAL RESISTANCE OF SCALE DEPOSITS, W / M**2-K
C
C HI        INSIDE  RESISTANCE, W / M**2-K
C
C DI        TUBE INSIDE DIAMETER, MM
C
C DO        TUBE OUTSIDE DIAMETER, MM
C
C SL        STANDARD TUBE LENGHT, M
C
C NTR       NUMBER O TUBE PASSES
C
C PT        PITCH, MM
C
C B         BAFFLE SPACING, MM
C
C Y         CLEARANCE, MM
C
C DE        EQUIVALENT DIAMETER, MM
C
C MCOMP     MASS FLOW RATE OF FLUID, KG/S
C
C KH        THERMAL CONDUCTVITY OF HOT STREAM, W / M-K
C
C KC        THERMAL CONDUCTVITY OF COLD STREAM, W / M-K
C
C VISH      VISCOSITY OF HOT STREAM, CENTIPOISE
C
C VISC      VISCOSITY OF COLD STREAM, CENTIPOISE
C
C TETA      VISCOSITY CONSTITUTIONAL CONSTANT
```

```
C FLAG       DETERMINES THE HOT FLUID
C        FLAG=0--> COMPONENT 2 IS THE HOT FLUID
C        FLAG=1--> COMPONENT 1 IS THE HOT FLUID
C
C EPS        TOLERANCE
C
C SWCH       DETERMINES THE SHELL SIDE FLUID
C        SWCH=0--> HOT FLUID IN THE SHELL
C        SWCH=1--> HOT FLUID IN THE TUBE
C
C SWCH1      SELECTS PITCH ARRANGEMENT
C        SWCH1=0--> TRIANGULAR PITCH
C        SWCH1=1--> SQUARE PITCH
C
C SWCH2      DECIDES WHETHER TUBE CORRECTION IS NECESSARY
C
C        SWCH2=0--> TUBE WALL CORRECTION IS NOT REQUIRED
C        SWCH2=1--> TUBE WALL CORRECTION IS PERFORMED
C
C CPL        HEAT CAPACITY OF LIQUID, J / MOL-K
C
C
C OUTPUT PARAMETERS
C
C SYMBOL DESCRIPTION
C
C
C UD     OVERALL HEAT TRANSFER COEFFICIENT, W / M**2-K
C
C A      AVAILABLE AREA FOR HEAT TRANSFER, M**2
C
C L      TOTAL LENGHT OF TUBES, M
C
C NT     NUMBER OF TUBES
C
C HI     INSIDE  RESISTANCE, W / M**2-K
C
C HO     OUTSIDE RESISTANCE, W / M**2-K
C
C TW     TUBE WALL TEMPERATURE, K
C
C F      CORRECTION FACTOR
C
C CMTD   CORRECTED LOGARITHMIC MEAN TEMPERATURE, K
C
```

```
C
C*******************************************************************************
C
C     EXT - MULTICOMPONENT LIQUID-LIQUID EXTRACTION CALCULATION
C
C*******************************************************************************
C
C          EXT PARAMETERS
C
C INPUT AND OUTPUT PARAMETERS
C
C SYMBOL    DESCRIPTION
C
C
C
C BALLPR    PARAMETER OF THE BALL INTEGRATION FORMULA
C
C TIMINC    TIME INCRIMENT
C
C H1        HEAVY-PHASE HOLD-UP OF STAGES
C
C H2        LIGHT-PHASE HOLD-UP OF STAGES
C
C M         NUMBER OF THEORETICAL STAGES
C
C N         NUMBER OF COMPONENTS
C
C SREST     ITS VALUE IS ALWAYS ZERO
C
C SNORM     DETERMINES NORMALIZATION
C          SNORM=1--> NORMALIZATION IS PERFORMED
C          SNORM=0--> NORMALIZATION IS NOT REQUIRED
C
C SACTC     SELECTS METHODS TO CALCULATE ACTIVITY COEFFICIENT
C          SACTC=-1--> 3-SUFFIX MARGULES
C          SACTC= 0--> UNIFAC
C          SACTC= 1--> NRTL
C
C SWRIT     DECIDES TO PRINT ITERATIONS
C          SWRIT=1--> PRINTS ITERATIONS
C          SWRIT=0--> PRINTS RESULTS ONLY
C TOL       TOLERANCE
C
C COMPS     COMPONENT ABBRIVIATIONS
C
C COMPN     COMPONENT NAMES
C
C STARS     PRINTS STARS
C
```

```
C
C X1         COMPONENT MOLE FRACTION IN HEAVY-PHASE
C
C F1         HEAVY-PHASE FLOW RATE, KMOL/ H
C
C X2         COMPONENT MOLE FRACTION IN LIGHT-PHASE
C
C F2         LIGHT-PHASE FLOW RATE, KMOL/ H
C
C XF         COMPONENT MOLE FRACTION IN FEED
C
C FF         FEED FLOW RATE, KMOL/ H
C
C SF1        HEAVY-PHASE SIDE STREAM  FLOW RATE, KMOL/ H
C
C SF2        LIGHT-PHASE SIDE STREAM  FLOW RATE, KMOL/ H
C
C AVAL       3-SUFFIX MARGULES BINARY INTERACTION PARAMETERS
C
C TEMP       OPERATION TEMPERATURE, K
C
C SNRTL      IF SNRTL=1--> BINARY INTERACTION PARAMETERS  ARE
C            CALCULATED FOR THE STATED TEMPERATURE
C
C CC         NRTL BINARY INTERACTION PARAMETER
C
C CT         NRTL BINARY INTERACTION PARAMETER
C
C ALPC       NRTL BINARY INTERACTION PARAMETER
C
C ALPT       NRTL BINARY INTERACTION PARAMETER
C
C CG         NRTL BINARY INTERACTION PARAMETER
C
C ALP        NRTL BINARY INTERACTION PARAMETER

18.22.30.UCLP, BU, P03    ,      0.948KLNS.
```

APPENDIX G

OPERATION MANUAL FOR DESPAC2

APPENDIX G

Operation Manual for DESPAC2

Fulfilling the requirements of CDC Cyber 170/815 to execute DESPAC2, the following procedure must be followed:

a) The general command to execute the program is

```
/LGO, INPUT, OUTPUT, USCR, UFIL
```

b) Instead of UFIL, the library file that contains the thermophysical properties of components, (e.g. PUBDAT, VLE, etc.) must be written.

```
/LGO, INPUT, OUTPUT, USCR, PUBDAT
```

c) If the user would like to enter parameters interactively step (b) is sufficient.

d) Another method is to prepare an INPUT data file (e.g. ORNEK) as shown in the following pages. In this way the user prepares the INPUT data in their correct sequence, which simplifies the entry of the data.

```
/LGO, ORNEK, OUTPUT, USCR, PUBDAT
```

Step (d) offers the advantage of easy change of parameters. For repeated and enormous data requirement, this type of data file is beneficial.

e) To obtain a hard copy of results, the user has to give a certain name instead of OUTPUT (e.g. SONUC).

For step (b) type of operation, messages will not be seen on the screen: only question marks will be observed. Therefore, values that must be entered, have to be remembered in the correct sequence, and supplied after each question mark appears.

```
/LGO, INPUT, SONUC, USCR, PUBDAT
```

f) For step (d) type of running, it is very easy to obtain a hard copy. The user just writes

```
/LGO, ORNEK, SONUC, USCR, PUBDAT
```

Following commands are the same for (e) and (f) to print the results:

```
/RWF
/COPYSBF, SONUC, LL
/RWF
/ROUTE, LL, DC=PR
```

In the following pages computer output and the corresponding INPUT data file (ORNEK) are presented for ACTFIT routine in order to clarify the supply of the input data. For step (b) type of operation, the user has to enter the parameters interactively due to the sequence shown in ORNEK. For step (d) type of operation, ORNEK is directly supplied as explained before.

The user has to remember the followings to operate DESPAC2:

- Library file for ACTFIT routine is VLE.
- Library file for all other modelling routines is PUBDAT.

EXAMPLE RUN: ACTFIT Routine

```
 DESPAC 5.8 (6-APR-81)

 PROCEDURES:
  1.KVALUE        7.SHTCUT       11.RETREV       17.HELP
  2.ENTHALPY      8.COLUMN       12.SYSTEM       18.STOP
  3.PHASE         9.CERDA        13.DEFINE       19.TIME AND DATE
  4.FLASH        10.COLCST       14.STORE
  5.ABSEDM       21.HEX          15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:

 RETREV - RETRIEVE PHYSICAL CONSTANTS FROM DISK FILES

 ENTER NAME OF FILE (RETURN FOR PUBLIC DATA):
+DATA WILL BE RETRIEVED FROM FILE VLE
 RETRIEVE ALL COMPONENTS FROM FILE? (Y OR N):

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  1 IS ACETONE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  2 IS ETHANOL

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
 LIBRARY IS REDEFINED.  SYSTEM IS UNDEFINED.

 PROCEDURES:
  1.KVALUE        7.SHTCUT       11.RETREV       17.HELP
  2.ENTHALPY      8.COLUMN       12.SYSTEM       18.STOP
  3.PHASE         9.CERDA        13.DEFINE       19.TIME AND DATE
  4.FLASH        10.COLCST       14.STORE
  5.ABSEDM       21.HEX          15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:

 SYSTEM - DEFINE COMPONENTS IN SYSTEM

 MODELS FOR VAPOR ENTHALPY HV:
   1. IDEAL SOLUTION OF PERFECT GASES.
   2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
   3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR LIQUID ENTHALPY HL:
   1. IDEAL SOLUTION OF SATURATED LIQUIDS.
   2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
   3. EXCESS ENTHALPY FROM WILSON EQUATION.
   4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR VLE CALCULATIONS:
   1. LIQUID: WILSON ACTIVITY;VAPOR: VIRIAL EQN OF STATE.
   2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
   3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

 SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
 ENTER MINIMUM CRITICAL TEMPERATURE OF CONDENSABLES.BLANK THEN RETURN FOR 200 K:
 SELECT COMPONENTS (0 FOR HELP):

 SELECTED COMPONENTS:
   1. ACETONE
   2. ETHANOL
```

```
VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
K-VALUES: WILSON, ANDERSON, AND VIRIAL EQUATIONS.
  CONDENSABLES:    1  2
  PHYSICAL THEORY FOR VAPOR-PHASE NON-IDEALITY.

PROCEDURES:
 1.KVALUE         7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY       8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE          9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH         10.COLCST       14.STORE
 5.ABSEDM        21.HEX          15.ACTFIT
 6.MCCABE        22.EXT

SELECT PROCEDURE:

ACTFIT - FIT PARAMETERS FOR ESTIMATING ACTIVITIES TO BINARY VLE DATA

ONE MAY ESTIMATE ACTIVITY COEFFICIENTS FROM
 1. T-P-X DATA.
 2. T-P-X-Y DATA.
 3. HENRY'S CONSTANTS.
SELECT THE APPLICABLE CASE:
TOTAL PRESSURES OR PARTIAL PRESSURES? (T OR P):

ACTIVITY COEFFICIENTS WILL BE CORRELATED TO
T-P-X-Y DATA
+ FOR THE BINARY SYSTEM
 1. ACETONE
 2. ETHANOL

IDENTIFY THE KEY COMPONENT (1 OR 2):

*ENTRY OF EXPERIMENTAL DATA*
  X,Y ARE MOLE FRACTIONS OF COMPONENT 1.
  P IS TOTAL PRESSURE.

1.ENTER 2.READ 3.DELETE 4.SORT 5.REVIEW 6.STORE 7.DONE 8.HELP :
ENTER FIXED TEMPERATURE, PRESSURE, OR NEITHER (TO,PO ; )

+:
ENTER EXPERIMENTAL DATA.  (RETURN TO END)
   1.  T,X,Y:
   2.  T,X,Y:
   3.  T,X,Y:
   4.  T,X,Y:
   5.  T,X,Y:
   6.  T,X,Y:
   7.  T,X,Y:
   8.  T,X,Y:
   9.  T,X,Y:
  10.  T,X,Y:

1.ENTER 2.READ 3.DELETE 4.SORT 5.REVIEW 6.STORE 7.DONE 8.HELP :
   N      LLAM12           LLAM21        RMS ERROR
   1   0.               0.               .290584
   2     10.0000        0.               .279180
   3     10.0000         10.0000         .264553
   4     94.6680         118.763         .545387E-01
   5     210.594         44.2025         .526509E-01
   6     136.412         104.279         .498295E-01


ACTFIT RESULTS FOR THE BINARY SYSTEM
     1. ACETO
     2. ETHANOL
```

```
:::

   FITTED PARAMETERS:
      LLAM12 =   136.41
      LLAM21 =   104.28

   COMPARISON WITH EXPERIMENTAL DATA:

       --------------- E X P E R I M E N T A L --------------  --CALCULATED--
   K     T          P          X1      Y1    GAMMA1   GAMMA2 LNG1/G2  GAMMA1   GAMMA2
   1  348.1    1.013      .05800 .17300  1.7355   1.0003    .5510  1.7988   1.0030
   2  345.2    1.013      .12100 .29700  1.5409   1.0240    .4086  1.6379   1.0128
   3  343.1    1.013      .17500 .37600  1.4281   1.0560    .3018  1.5249   1.0260
   4  339.7    1.013      .27600 .49400  1.3089   1.1269    .1497  1.3611   1.0619
   5  338.2    1.013      .33900 .55500  1.2497   1.1592    .0752  1.2826   1.0911

   6  335.9    1.013      .44400 .63600  1.1698   1.2486   -.0652  1.1823   1.1514
   7  333.7    1.013      .58000 .72600  1.0917   1.3767   -.2319  1.0941   1.2510
   8  331.7    1.013      .73600 .82700  1.0417   1.5223   -.3794  1.0339   1.3972
   9  330.2    1.013      .87500 .91900  1.0204   1.6235   -.4644  1.0071   1.5599


  SAVE RESULTS IN LIBRARY? (Y OR N):
 +NOT SAVED. DEFINE MAY BE USED TO SAVE RESULTS MANUALLY.
  REPEAT ENTRY OF DATA? (Y OR N):

  PROCEDURES:
   1.KVALUE        7.SHTCUT       11.RETREV       17.HELP
   2.ENTHALPY      8.COLUMN       12.SYSTEM       18.STOP
   3.PHASE         9.CERDA        13.DEFINE       19.TIME AND DATE
   4.FLASH        10.COLCST       14.STORE
   5.ABSEDM       21.HEX          15.ACTFIT
   6.MCCABE       22.EXT

  SELECT PROCEDURE:
    PROGRAM IS STOPPED
```

```
11
VLE
N
ACETONE
ETHANOL

12
111

001002
15
2
T
1
1
PO=1.01325;
  348.1          .058        .173
  345.2          .121        .297
  343.1          .175        .376
  339.7          .276        .494
  338.2          .339        .555
  335.9          .444        .636
  333.7          .580        .726
  331.7          .736        .827
  330.2          .875        .919

7
N
N
18
22.23.20.UCLP, BU, P04      ,        0.235KLNS.
```

(INPUT Data file of ACTFIT for the batch run of the program) = ORNEK

APPENDIX H

COMPUTER OUTPUTS AND THE INPUT DATA FILES OF EXAMPLES SOLVED BY DESPAC2

COMPUTER OUTPUTS AND THE INPUT DATA FILES OF SINGLE OPERATION UNITS

```
 DESPAC 5.8 (6-APR-81)

 PROCEDURES:
  1.KVALUE         7.SHTCUT       11.RETREV        17.HELP
  2.ENTHALPY       8.COLUMN       12.SYSTEM        18.STOP
  3.PHASE          9.CERDA        13.DEFINE        19.TIME AND DATE
  4.FLASH         10.COLCST       14.STORE
  5.ABSEDM        21.HEX          15.ACTFIT
  6.MCCABE        22.EXT

 SELECT PROCEDURE:

 RETREV - RETRIEVE PHYSICAL CONSTANTS FROM DISK FILES

 ENTER NAME OF FILE (RETURN FOR PUBLIC DATA):
+DATA WILL BE RETRIEVED FROM FILE PUBDAT
 RETRIEVE ALL COMPONENTS FROM FILE? (Y OR N):

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  1 IS BENZENE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  2 IS TOLUENE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
 LIBRARY IS REDEFINED.  SYSTEM IS UNDEFINED.

 PROCEDURES:
  1.KVALUE         7.SHTCUT       11.RETREV        17.HELP
  2.ENTHALPY       8.COLUMN       12.SYSTEM        18.STOP
  3.PHASE          9.CERDA        13.DEFINE        19.TIME AND DATE
  4.FLASH         10.COLCST       14.STORE
  5.ABSEDM        21.HEX          15.ACTFIT
  6.MCCABE        22.EXT

 SELECT PROCEDURE:

 SYSTEM - DEFINE COMPONENTS IN SYSTEM

 MODELS FOR VAPOR ENTHALPY HV:
   1. IDEAL SOLUTION OF PERFECT GASES.
   2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
   3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR LIQUID ENTHALPY HL:
   1. IDEAL SOLUTION OF SATURATED LIQUIDS.
   2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
   3. EXCESS ENTHALPY FROM WILSON EQUATION.
   4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR VLE CALCULATIONS:
   1. LIQUID: WILSON ACTIVITY;VAPOR: VIRIAL EQN OF STATE.
   2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
   3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

 SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
 SELECT COMPONENTS (0 FOR HELP):

 SELECTED COMPONENTS:
   1. BENZENE
   2. TOLUENE

 VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
 LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
 K-VALUES: RAOULT'S LAW.
```

EXAMPLE 1 - Computer Output of McCabe-Thiele Binary Distillation (MCCABE).

```
PROCEDURES:
 1.KVALUE       7.SHTCUT      11.RETREV      17.HELP
 2.ENTHALPY     8.COLUMN      12.SYSTEM      18.STOP
 3.PHASE        9.CERDA       13.DEFINE      19.TIME AND DATE
 4.FLASH       10.COLCST      14.STORE
 5.ABSEDM      21.HEX         15.ACTFIT
 6.MCCABE      22.EXT

SELECT PROCEDURE:

MCCABE - MCCABE-THIELE BINARY DISTILLATION

ENTER INPUT PARAMETERS (RATIO/ALPHA/Q/ ETA /XF/XD/F/D ;  )

+:


MCCABE INPUT PARAMETERS
 RATIO = 3.50          XF =  .4400
 ALPHA = 2.250         XD =  .9740
     Q = 1.000          F =   350.00
   ETA = 1.000          D =   153.40


MCCABE RESULTS
    XW =  .0233        LB =   1255.9
     W =   196.60      VB =   1059.3
     L =   905.93      NT =    7
     V =   1059.3      NB =    5


REPEAT? (Y OR N):

PROCEDURES:
 1.KVALUE       7.SHTCUT      11.RETREV      17.HELP
 2.ENTHALPY     8.COLUMN      12.SYSTEM      18.STOP
 3.PHASE        9.CERDA       13.DEFINE      19.TIME AND DATE
 4.FLASH       10.COLCST      14.STORE
 5.ABSEDM      21.HEX         15.ACTFIT
 6.MCCABE      22.EXT

SELECT PROCEDURE:
  PROGRAM IS STOPPED
```

```
11
PUBDAT
N
BENZENE
TOLUENE

12
113
001002
6
RATIO=3.5,ALPHA=2.25,Q=1,ETA=1,XF=.44,XD=.974,F=350,D=153.4;
N
18
22.08.12.UCLP, BU, P04     ,       0.160KLNS.
```

Input Data File of EXAMPLE 1.

```
DESPAC 5.8 (6-APR-81)

 PROCEDURES:
  1.KVALUE        7.SHTCUT        11.RETREV        17.HELP
  2.ENTHALPY      8.COLUMN        12.SYSTEM        18.STOP
  3.PHASE         9.CERDA         13.DEFINE        19.TIME AND DATE
  4.FLASH        10.COLCST        14.STORE
  5.ABSEDM       21.HEX           15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:

 RETREV - RETRIEVE PHYSICAL CONSTANTS FROM DISK FILES

 ENTER NAME OF FILE (RETURN FOR PUBLIC DATA):
+DATA WILL BE RETRIEVED FROM FILE PUBDAT
 RETRIEVE ALL COMPONENTS FROM FILE? (Y OR N):

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  1 IS PROPANE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  2 IS I-BUTANE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  3 IS N-BUTANE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  4 IS I-PENTANE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  5 IS N-PENTANE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
 LIBRARY IS REDEFINED.  SYSTEM IS UNDEFINED.

 PROCEDURES:
  1.KVALUE        7.SHTCUT        11.RETREV        17.HELP
  2.ENTHALPY      8.COLUMN        12.SYSTEM        18.STOP
  3.PHASE         9.CERDA         13.DEFINE        19.TIME AND DATE
  4.FLASH        10.COLCST        14.STORE
  5.ABSEDM       21.HEX           15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:

 SYSTEM - DEFINE COMPONENTS IN SYSTEM

 MODELS FOR VAPOR ENTHALPY HV:
   1. IDEAL SOLUTION OF PERFECT GASES.
   2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
   3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR LIQUID ENTHALPY HL:
   1. IDEAL SOLUTION OF SATURATED LIQUIDS.
   2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
   3. EXCESS ENTHALPY FROM WILSON EQUATION.
   4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR VLE CALCULATIONS:
   1. LIQUID: WILSON ACTIVITY;VAPOR: VIRIAL EQN OF STATE.
   2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
   3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

 SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
```

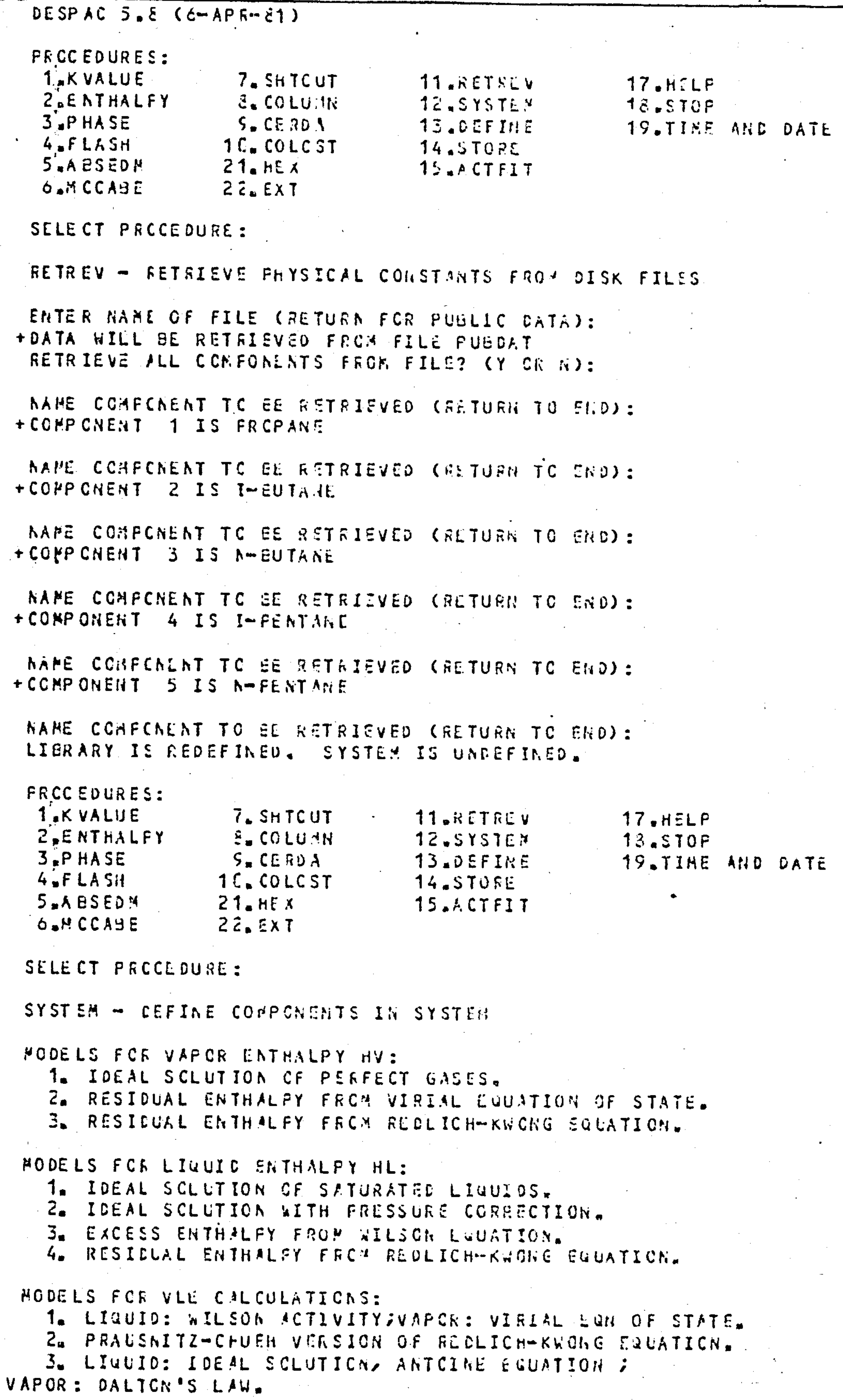
EXAMPLE 2 - Computer Output of Shortcut Multicomponent Distillation (SHTCUT)

```
SELECT COMPONENTS (0 FOR HELP):

SELECTED COMPONENTS:
  1. PROPANE
  2. I-BUTANE
  3. N-BUTANE
  4. I-PENTANE
  5. N-PENTANE

VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
K-VALUES: RAOULT'S LAW.

PROCEDURES:
 1.KVALUE        7.SHTCUT       11.RETREV       17.HELP
 2.ENTHALPY      8.COLUMN       12.SYSTEM       18.STOP
 3.PHASE         9.CERDA        13.DEFINE       19.TIME AND DATE
 4.FLASH        10.COLCST       14.STORE
 5.ABSEDM       21.HEX          15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

SHTCUT - SHORTCUT MULTICOMPONENT DISTILLATION

NEW COLUMN? (Y OR N):

METHODS FOR FINDING REFLUX RATIO
 1. FUNCTION OF VMAX
 2. SPECIFIED DIRECTLY
 3. FUNCTION OF RMIN
SELECT METHOD:

RELATIVE VOLATILITIES BY FLSHTP? (Y OR N):

ENTER INPUT PARAMETERS ( F ,LKEY,Q,XF,
+VFMAX,
+T,P,
+FTL,
+FBH ;  )

+:
+:
+:
+:
+:


SHTCUT INPUT PARAMETERS
  LKEY =  3 - N-BUTANE
     Q =    1.000
+VFMAX =   1.750
     T = 358.000       P =    8.271
   FTL =     .980
+  FBH =    .840


SHTCUT RESULTS
   FTL =    .9800   SMIN =     7.19      D =  49.150
   FTR =     3.37      R =  2.5605      B =  50.850
    SD =    10.31   RMIN =    .8770      F =  100.00

 I  COMPONENT           XF(I)   XD(I)   XB(I)    AL(I)       XI(I)
 1. PROPANE             .0500   .1017   .0000   6.3826      1.000
 2. I-BUTANE            .1500   .3042   .0009   2.8117      .9969
 3. N-BUTANE            .2500   .4985   .0098   2.1636      .9800
 4. I-PENTANE           .2000   .0651   .3304   1.0000      .1600
 5. N-PENTANE           .3500   .0305   .6589   .81739     .4276E-01
```

```
REPEAT? (Y OR N):

PROCEDURES:
 1.KVALUE        7.SHTCUT       11.RETREV       17.HELP
 2.ENTHALPY      8.COLUMN       12.SYSTEM       18.STOP
 3.PHASE         9.CERDA        13.DEFINE       19.TIME AND DATE
 4.FLASH        10.COLCST       14.STORE
 5.ABSEDM       21.HEX          15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:
  PROGRAM IS STOPPED
```

```
11
PUBDAT
N
PROPANE
I-BUTANE
N-BUTANE
I-PENTANE
N-PENTANE

12
113
00100200300400S
7
Y
1
Y
F=100,LKEY=3,Q=1,XF=0.05,0.15,0.25,0.20,0.35,
VFMAX=1.75,
T=358,P=8.271,
FTL=.98,
FBH=0.84;
N
18
22.08.54.UCLP, BU, P04     ,       0.208KLNS.
```

INPUT Data File of <u>EXAMPLE 2</u>.



```
DESPAC 5.8 (6-APR-81)

PROCEDURES:
 1.KVALUE        7.SHTCUT        11.RETREV        17.HELP
 2.ENTHALPY      8.COLUMN        12.SYSTEM        18.STOP
 3.PHASE         9.CERDA         13.DEFINE        19.TIME AND DATE
 4.FLASH        10.COLCST        14.STORE
 5.ABSEDM       21.HEX           15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

RETREV - RETRIEVE PHYSICAL CONSTANTS FROM DISK FILES

ENTER NAME OF FILE (RETURN FOR PUBLIC DATA):
+DATA WILL BE RETRIEVED FROM FILE PUBDAT
RETRIEVE ALL COMPONENTS FROM FILE? (Y OR N):

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  1 IS PROPANE

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  2 IS I-BUTANE

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  3 IS N-BUTANE

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  4 IS I-PENTANE

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  5 IS N-PENTANE

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
LIBRARY IS REDEFINED.  SYSTEM IS UNDEFINED.

PROCEDURES:
 1.KVALUE        7.SHTCUT        11.RETREV        17.HELP
 2.ENTHALPY      8.COLUMN        12.SYSTEM        18.STOP
 3.PHASE         9.CERDA         13.DEFINE        19.TIME AND DATE
 4.FLASH        10.COLCST        14.STORE
 5.ABSEDM       21.HEX           15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

SYSTEM - DEFINE COMPONENTS IN SYSTEM

MODELS FOR VAPOR ENTHALPY HV:
  1. IDEAL SOLUTION OF PERFECT GASES.
  2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
  3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR LIQUID ENTHALPY HL:
  1. IDEAL SOLUTION OF SATURATED LIQUIDS.
  2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
  3. EXCESS ENTHALPY FROM WILSON EQUATION.
  4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR VLE CALCULATIONS:
  1. LIQUID: WILSON ACTIVITY/VAPOR: VIRIAL EQN OF STATE.
  2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
  3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.
```

EXAMPLE 3 - Computer Output of Shortcut Multicomponent Distillation (CERDA) and the Cost and the Size Estimation Routine (COLCST).

```
SELECT MODELS FOR HV/HL/VLE (    BLANK THEN RETURN FOR 1 1 1):  _
SELECT COMPONENTS (0 FOR HELP):

SELECTED COMPONENTS:
  1. PROPANE
  2. I-BUTANE
  3. N-BUTANE
  4. I-PENTANE
  5. N-PENTANE

VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
K-VALUES: RAOULT'S LAW.

PROCEDURES:
 1.K VALUE        7.SHTCUT        11.RETREV         17.HELP
 2.ENTHALPY       8.COLUMN        12.SYSTEM         18.STOP
 3.PHASE          9.CERDA         13.DEFINE         19.TIME AND DATE
 4.FLASH         10.COLCST        14.STORE
 5.ABSEDM        21.HEX           15.ACTFIT
 6.MCCABE        22.EXT

SELECT PROCEDURE:

CERDA - J.CERDA SHORTCUT DISTILLATION

ENTER INPUT PARAMETERS (F,XF, LKEY,HKEY, FTL,FGH, T,P, Q, RFAC, COST ;  )

+:
+:
+:
+:
+:
+:
+:
+:
+:


CERDA RESULTS

 NT =      .8       T = 358.000          RFAC   =  1.2000
 NB =    22.8       P =   8.270          RT     =  1.2810       LT =   61.11
 F =   100.00       Q =   1.000          RTMIN  =  1.0675       VT =  108.81
 D =    47.70       FTL = .9800          RB     =  2.0804       LB =  161.11
 B =    52.30       FGH = .8400          RBMIN  =  1.8857       VB =  108.81

 I  COMPONENT            XF(I)   XD(I)   XB(I)    XI(I)    AL(I)  K(I)
 1  PROPANE              .0500   .1048   .0000   1.0000    6.383        3.926
 2  I-BUTANE             .1500   .3145   .0000   1.0000    2.812        1.730
 3* N-BUTANE             .2500   .5136   .0096    .9800    2.164        1.331
 4* I-PENTANE            .2000   .0671   .3212    .1600    1.000         .6151
 5  N-PENTANE            .3500   .0000   .6692    .0000     .8174        .5028
```

```
 COLCST


+COLUMN CONSTRUCTION (1.CLAD 2.SOLID):
+COLUMN MATERIAL (1.CARBON STEEL 2.STAINLESS 3.MONEL 4.TITANIUM):
+TRAY MATERIAL (1.CARBON STEEL 2.STAINLESS 3.MONEL):
+TRAY TYPE (1.GRID/PLATE/SIEVE 2.TROUGH/VALVE 3.BUBBLE-CAP 4.KOCH KASCADE):
+SURFACE TENSION OF LIQUID, N/M (WATER @ 298 K = .02):
+TRAY SPACING, M:
+ACTIVE PLATE AREAU)U  FRACTION OF TOTAL CROSS SECTION (TYPICAL: .7):
+OPERATING SUPERFICIAL VELOCITY ;   FRACTION OF FLOODING VELOCITY (TYPICAL: .8):
+CURRENT COST INDEX (115 @ JUNE 1968):


 GUTHRIE COLUMN COSTING
 =====================

 LIQUID FLOWRATE, G/S:  .1160E+05      LIQUID DENSITY, G/MU3:  .5526E+06
 VAPOR FLOWRATE, G/S:   7836.          VAPOR DENSITY, G/MU3:   .2001E+05
 SURFACE TENSION, N/M:  .0200          COLUMN CONSTRUCTION:       CLAD
 ACTIVE AREA FRACTION:  .7000          COLUMN MATERIAL: CARBON STEEL
 NUMBER OF TRAYS:  24.62                TRAY MATERIAL  : CARBON STEEL
 TRAY SPACING, M:  .3000               TRAY TYPE: GRID/PLATE, OR SIEVE
 PRESSURE, BAR:  8.270                 COST INDEX:  350.0
 DIAMETER, M:  1.955                   FLOODING VELOCITY, M/S:  .2331
 HEIGHT, M  :  13.09                   OPERATING VELOCITY  " :  .1265

 PRESSURE FACTOR:  1.064               TRAY SPACING FACTOR:   2.200
 MATERIAL FACTOR:  1.000               TRAY MATERIAL FACTOR:   .000
 MATL-PRS FACTOR:  1.064               TRAY TYPE FACTOR:       .000
 MODULE FACTOR:    4.230               TRAY MAT-SPAC FACTOR:  2.200

 COSTS, 1000 $      INSTALLED          BASE COST, 1968
       COLUMN:        186.666             14.283
       TRAYS :         12.519              1.370
       TOTAL :        199.186


 REPEAT COSTING? (Y OR N):


 REPEAT? (Y OR N):

 PROCEDURES:
  1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
  2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
  3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
  4.FLASH        10.COLCST       14.STORE
  5.ABSEDM       21.HEX          15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:
   PROGRAM IS STOPPED
```

```
11
PUBDAT
N
PROPANE
I-BUTANE
N-BUTANE
I-PENTANE
N-PENTANE

12
113.
001002003004005
9
F=100,XF=0.05,0.15,0.25,0.20,0.35,
LKEY=3,
HKEY=4,
FTL=.98,
FBH=0.84,
T=358,P=3.27,
Q=1,
RFAC=1.2,
COST=1;
1
1
1
1
.02
.3
.7
.8
350.
N
N
18
19.13.24.UCLP, BU, F04     ,        0.246KLNS.
```

INPUT Data File of <u>EXAMPLE 3</u>.

```
 DESPAC 5.8 (6-APR-81)

 PROCEDURES:
  1.KVALUE         7.SHTCUT        11.RETREV        17.HELP
  2.ENTHALPY       8.COLUMN        12.SYSTEM        18.STOP
  3.PHASE          9.CERDA         13.DEFINE        19.TIME AND DATE
  4.FLASH         10.COLCST        14.STORE
  5.ABSEDM        21.HEX           15.ACTFIT
  6.MCCABE        22.EXT

 SELECT PROCEDURE:

 RETREV - RETRIEVE PHYSICAL CONSTANTS FROM DISK FILES

 ENTER NAME OF FILE (RETURN FOR PUBLIC DATA):
+DATA WILL BE RETRIEVED FROM FILE PUBDAT
 RETRIEVE ALL COMPONENTS FROM FILE? (Y OR N):

 NAME COMPCNENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  1 IS ACETONE

 NAME COMPCNENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  2 IS ETHANOL

 NAME COMPCNENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  3 IS CHLOROFORM

 NAME COMPCNENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  4 IS WATER

 NAME COMPCNENT TO BE RETRIEVED (RETURN TO END):
 LIBRARY IS REDEFINED.  SYSTEM IS UNDEFINED.

 PROCEDURES:
  1.KVALUE         7.SHTCUT        11.RETREV        17.HELP
  2.ENTHALPY       8.COLUMN        12.SYSTEM        18.STOP
  3.PHASE          9.CERDA         13.DEFINE        19.TIME AND DATE
  4.FLASH         10.COLCST        14.STORE
  5.ABSEDM        21.HEX           15.ACTFIT
  6.MCCABE        22.EXT

 SELECT PROCEDURE:

 SYSTEM - DEFINE COMPONENTS IN SYSTEM

 MODELS FOR VAPOR ENTHALPY HV:
   1. IDEAL SOLUTION OF PERFECT GASES.
   2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
   3. RESIDUAL ENTHALPY FRCM REDLICH-KWONG EQUATION.

 MODELS FOR LIQUID ENTHALPY HL:
   1. IDEAL SOLUTION OF SATURATED LIQUIDS.
   2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
   3. EXCESS ENTHALPY FROM WILSON EQUATION.
   4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR VLE CALCULATIONS:
   1. LIQUID: WILSON ACTIVITY/VAPOR: VIRIAL EQN OF STATE.
   2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
   3. LIQUID: IDEAL SOLUTICN, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

 SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
 SELECT COMPONENTS (0 FOR HELP):

 SELECTED COMPONENTS:
```

EXAMPLE 4 - Computer Output of Multicomponent Liquid-Liquid Extraction (EXT).

```
      1. ACETONE
      2. ETHANOL
      3. CHLOROFORM
      4. WATER

   VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
   LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
   K-VALUES: RAOULT'S LAW.

   PROCEDURES:
    1.KVALUE         7.SHTCUT       11.RETREV        17.HELP
    2.ENTHALPY       8.COLUMN       12.SYSTEM        18.STOP
    3.PHASE          9.CERDA        13.DEFINE        19.TIME AND DATE
    4.FLASH         10.COLCST       14.STORE
    5.ABSEDM        21.HEX          15.ACTFIT
    6.MCCABE        22.EXT

   SELECT PROCEDURE:

  LIQUID-LIQUID EXTRACTION CALCULATION

  C  ENTER AVAL FOR MARGULES
  C  ENTER TEMP,SNRTL,CC,CT,ALPC,ALPT,CG,ALP FOR NRTL
  C  ENTER TEMP,NGMOL,NOGP,IDGP,NMG,NSG,QQ,RR,NKTAB
     PARAM FOR UNIFAC
  ENTER INPUT PARAMATERS
  +(BALLPR,TIMINC,H1,H2,M,N,SREST,SNORM,SACTC
    SWRIT,TOL,COMPS,COMPN,STARS,X1,F1,X2,F2,XF,FF,SF1
    SF2,AVAL,TEMP,SNRTL,CC,CT,ALPC,ALPT,CG,ALP,NGMOL
    NOGP,IDGP,NMG,NSG,QQ,RR,NKTAB,PARAM)

  +:
  +:
  +:
  +:
  +:
  +:
  +:
  +:
  +:
  +:
  +:
  +:
  +:
  +:
  +:
  +:
  +:
  +:
  +:
  +:
  +:
  +:
```

```
CONVERGED RESULTS



COMP-1=ACETO
COMP-2=ETHAN
COMP-3=CHLOR
COMP-4=WATER


FEEDS TO THE COLUMN

STAGE      FEED
  NO       FLOW      COMP-1     COMP-2     COMP-3     COMP-4
******   ********   *******    *******
  TOP        .800    .00000     .00000    1.00000     .00000
BOTTOM      1.000    .00000     .00000     .00000    1.00000
  10         .200    .50000     .50000     .00000     .00000

ERRORS IN THE COMPONENT MATERIAL BALANCE EQUATIONS. ERROR=1000(INPUT-OUTPUT)/INPUT


COMP-1     0.
COMP-2     0.
COMP-3     0.
COMP-4    -2.



ITERATION NO=10


1.STAGE FLOWS


STAGE     HEAVY      LIGHT
 NO       FHASE      PHASE
*****   ********   ********
  1         .951      1.062
  2        1.013      1.113
  3        1.066      1.161
  4        1.115      1.200
  5        1.154      1.227
  6        1.181      1.243
  7        1.196      1.251
  8        1.203      1.255
  9        1.206      1.256
 10        1.207      1.234
 11         .986      1.191
 12         .944      1.166
 13         .918      1.138
 14         .890      1.103
 15         .855      1.051
```

```
2.HEAVY-PHASE MOLE FRACTIONS

STAGE
 NO     COMP-1        C
*****   ******
  1     .10510     .04401     .83665     .01423
  2     .10810     .08624     .78868     .01698
  3     .10503     .12439     .75084     .01974
  4     .10192     .15610     .71948     .02250
  5     .09952     .17942     .69616     .02491
  6     .09793     .19425     .68116     .02666
  7     .09703     .20237     .67288     .02772
  8     .09658     .20621     .66895     .02826
  9     .09639     .20779     .66734     .02847
 10     .09632     .20834     .66680     .02853
 11     .01625     .15039     .81631     .01705
 12     .00218     .13006     .85264     .01512
 13     .00027     .11037     .87542     .01395
 14     .00003     .08534     .90192     .01270
 15     .00000     .05091     .93782     .01126



3.LIGHT PHASE MOLE FRACTIONS

STAGE
 NO     COMP-1        C
*****   ******
  1     .00503     .04287     .00332     .94479
  2     .01078     .08149     .00431     .90342
  3     .01172     .11378     .00533     .86917
  4     .01235     .13756     .00622     .84388
  5     .01272     .15269     .00683     .82776
  6     .01290     .16097     .00719     .81894
  7     .01297     .16488     .00736     .81479
  8     .01299     .16647     .00742     .81312
  9     .01298     .16702     .00743     .81257
 10     .01298     .16726     .00744     .81232
 11     .00173     .15183     .00761     .83883
 12     .00021     .13675     .00702     .85601
 13     .00002     .11780     .00620     .87598
 14     .00000     .09211     .00520     .90268
 15     .00000     .05532     .00402     .94066

REPEAT ? (Y OR N) :
? SYSTEM IS UNDEFINED

 PROCEDURES:
  1.KVALUE       7.SHTCUT       11.RETREV       17.HELP
  2.ENTHALPY     8.COLUMN       12.SYSTEM       18.STOP
  3.PHASE        9.CERDA        13.DEFINE       19.TIME AND DATE
  4.FLASH       10.COLCST       14.STORE
  5.ABSEDM      21.HEX          15.ACTFIT
  6.MCCABE      22.EXT

 SELECT PROCEDURE:
   PROGRAM IS STOPPED
```

```
11
PUBDAT
N
ACETONE
ETHANOL
CHLOROFORM
WATER

12
113
001002003004
22
BALLPR=0.75,TIMINC=10.,M1=1.,H2=0.,M=15,N=4,TOL=0.001,
SREST=0.,SNORM=1.,SACTC=-1.,SWRIT=0.,COMPS(1)='COMP-1',
COMPS(2)='COMP-2',COMPS(3)='COMP-3',COMPS(4)='COMP-4',
COMPN(1)='ACETONE',COMPN(2)='ETHANOL',COMPN(3)='CHLOROFORM',
COMPN(4)='WATER',
STARS(1)='******',STARS(2)='********',STARS(3)='**********',
STARS(4)='************',
X1(1,2)=.108,.043,0.794,0.015,0.,0.117,0.075,0.796,0.014,0.,0.119,0.09,0.796,
        .014,0.,.121,.097,0.796,0.014,0.,0.122,0.101,0.796,0.014,0.,0.124,0.105,
       .796,0.014,0.,.126,0.110,0.796,0.013,0.,0.129,0.118,0.796,0.013,0.,0.131,
      0.132,0.796,0.013,0.,.134,0.157,0.796,0.013,0.,0.046,0.125,0.995,0.012,
      0.,0.032,0.107,0.997,.012,0.,0.025,0.093,0.997,0.012,0.,0.017,0.077,0.998,
        0.012,0.,0.009,0.050,0.999,0.012,0.,2*0.0,1.,
X2(4,1)=1.,0.,.0089,.0328,.0024,.9998,0.,.0096,.0578,0.0024,0.9849,0.,0.0098,
        .0689,.0024,0.9703,0.,0.0099,0.074,0.0024,.9558,0.,0.010,0.0773,0.0024,
        .9416,0.,.0102,.0801,.0024,.9276,0.,.0104,.0839,.0024,.9138,0.,
  .0106,.0902,.0024,.9002,0.,0.0108,0.101,0.0024,0.8868,0.,0.011,0.1199,0.0024,
        .8711,0.,0.0038,.0961,0.0030,0.8607,0.,0.0027,0.0820,0.003,0.8505,0.0,
  .0021,0.0713,.003,.8403,0.,0.0014,0.0587,0.003,0.8302,0.,0.0008,0.0382,0.003,
        0.8107,
F1(2)=10*1.0,6*0.8,  F2(1)=16*1.0,   XF(1,11)=2*0.5,     FF(11)=0.2,
AVAL(2,1)=.599,-0.674,1.338,0.,0.5446,0.,0.501,0.877,0.,-0.9417,1.61,0.,
             4.76,0.,1.872,1.46,5.91;
N
18
22.21.08.UCLP, BU, P04    ,      0.326KLNS.
```

INPUT Data File of EXAMPLE 4.

```
DESPAC 5.8 (6-APR-81)

PROCEDURES:
 1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH        10.COLCST       14.STORE
 5.ABSEDM       21.HEX          15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

RETREV - RETRIEVE PHYSICAL CONSTANTS FROM DISK FILES

ENTER NAME OF FILE (RETURN FOR PUBLIC DATA):
+DATA WILL BE RETRIEVED FROM FILE PUBDAT
RETRIEVE ALL COMPONENTS FROM FILE? (Y OR N):

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  1 IS N-HEPTANE

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  2 IS CYCLOHEXANE

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  3 IS FURFURALDEHYDE

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
LIBRARY IS REDEFINED.  SYSTEM IS UNDEFINED.

PROCEDURES:
 1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH        10.COLCST       14.STORE
 5.ABSEDM       21.HEX          15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

SYSTEM - DEFINE COMPONENTS IN SYSTEM

MODELS FOR VAPOR ENTHALPY HV:
  1. IDEAL SOLUTION OF PERFECT GASES.
  2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
  3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR LIQUID ENTHALPY HL:
  1. IDEAL SOLUTION OF SATURATED LIQUIDS.
  2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
  3. EXCESS ENTHALPY FROM WILSON EQUATION.
  4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR VLE CALCULATIONS:
  1. LIQUID: WILSON ACTIVITY;VAPOR: VIRIAL EQN OF STATE.
  2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
  3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
SELECT COMPONENTS (0 FOR HELP):

SELECTED COMPONENTS:
  1. N-HEPTANE
  2. CYCLOHEXANE
  3. FURFURALDEHYDE
```

EXAMPLE 5 - Computer Output of Multicomponent Liquid-Liquid Extraction (EXT).

```
 VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
 LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
 K-VALUES: RAOULT'S LAW.

 PROCEDURES:
  1.KVALUE        7.SHTCUT       11.RETREV       17.HELP
  2.ENTHALPY      8.COLUMN       12.SYSTEM       18.STOP
  3.PHASE         9.CERDA        13.DEFINE       19.TIME AND DATE
  4.FLASH        10.COLCST       14.STORE
  5.ABSEDM       21.HEX          15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PRCCEDURE:

LIQUID-LIQUID EXTRACTION CALCULATION

C  ENTER AVAL FOR MARGULES
C  ENTER TEMP,SNRTL,CC,CT,ALPC,ALPT,CG,ALP FOR NRTL
C  ENTER TEMP,NGMOL,NOGP,IDGP,NMG,NSG,QQ,RR,NKTAB
   PARAM FCR UNIFAC
ENTER INPUT PARAMATERS
+(BALLPR,TIMINC,H1,H2,M,N,SREST,SNORM,SACTC
  SWRIT,TOL,COMPS,CCMPN,STARS,X1,F1,X2,F2,XF,FF,SF1
  SF2,AVAL,TEMP,SNRTL,CC,CT,ALPC,ALPT,CG,ALP,NGMOL
  NOGP,IDGP,NMG,NSG,QQ,RR,NKTAB,PARAM)

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```

```
+:
+:

CONVERGED RESULTS



COMP-1=N-HEP
COMP-2=CYCLO
COMP-3=FURFU


FEEDS TO THE COLUMN

STAGE       FEED
  NO        FLOW      COMP-1     COMP-2     COMP-3
******    ********   *******    ******
  TOP     1210.000    .00000     .00000    1.00000
BOTTOM     100.000    .50000     .50000     .00000

ERRORS IN THE COMPONENT MATERIAL BALANCE EQUATIONS. ERROR=1000(INPUT-OUTPUT)/INF


COMP-1      0.
COMP-2      0.
COMP-3      0.



ITERATION NO= 7


1.STAGE FLOWS


STAGE     HEAVY       LIGHT
 NO       PHASE       PHASE
*****   ********    ********
   1    1297.786      48.788
   2    1246.273      11.051
   3    1208.737      12.832
   4    1205.417      12.679
   5    1204.640      12.934
   6    1205.128      12.150
   7    1204.196      12.150
   8    1204.180      12.150
   9    1204.174      12.150
  10    1204.168      12.150
  11    1204.162      12.150
  12    1204.156      12.150
  13    1204.150      12.150
  14    1204.143      12.150
  15    1204.137      12.150
  16    1204.131      12.150
```

```
2.HEAVY-PHASE MOLE FRACTICNS


STAGE
 NO      CCMP-1          C
*****    ******
  1       .03853     .03852     .92295
  2       .02241     .01361     .96398
  3       .00059     .00029     .99912
  4       .00001     .00000     .99999
  5       .00000     .00000    1.00000
  6       .00000     .00000    1.00000
  7       .00000     .00000    1.00000
  8       .00000     .00000    1.00000
  9       .00000     .00000    1.00000
 10       .00000     .00000    1.00000
 11       .00000     .00000    1.00000
 12       .00000     .00000    1.00000
 13       .00000     .00000    1.00000
 14       .00000     .00000    1.00000
 15       .00000     .00000    1.00000
 16       .00000     .00000    1.00000




3.LIGHT PHASE MOLE FRACTICNS


STAGE
 NO      COMP-1          C
*****    ******
  1       .57520     .34946     .07534
  2       .07688     .03596     .88716
  3       .00059     .00029     .99912
  4       .00001     .00000     .99999
  5       .00000     .00000    1.00000
  6       .00000     .00000    1.00000
  7       .00000     .00000    1.00000
  8       .00000     .00000    1.00000
  9       .00000     .00000    1.00000
 10       .00000     .00000    1.00000
 11       .00000     .00000    1.00000
 12       .00000     .00000    1.00000
 13       .00000     .00000    1.00000
 14       .00000     .00000    1.00000
 15       .00000     .00000    1.00000
 16       .00000     .00000    1.00000
```

```
REPEAT ? (Y OR N) :
? SYSTEM IS UNDEFINED

 PROCEDURES:
  1.KVALUE         7.SHTCUT        11.RETREV         17.HELP
  2.ENTHALPY       8.COLUMN        12.SYSTEM         18.STOP
  3.PHASE          9.CERDA         13.DEFINE         19.TIME AND DATE
  4.FLASH         10.COLCST        14.STORE
  5.ABSEDM        21.HEX           15.ACTFIT
  6.MCCABE        22.EXT

 SELECT PROCEDURE:
   PROGRAM IS STOPPED
```

```
11
PUBDAT
N
N-HEPTANE
CYCLOHEXANE
FURFURALDEHYDE

12
113
0010002003
22
BALLPR=0.80,TIMINC=10.,H1=1.,H2=0.,M=16,N=3,TOL=0.001,
SREST=0.,SNORM=1.,SACTC=1.,SWRIT=0.,COMPS(1)='COMP-1',
COMPS(2)='COMP-2',COMPS(3)='COMP-3',
COMPN(1)='N-HEPTANE',COMPN(2)='CYCLOHEXANE',
COMPN(4)='FURFURALDEHYDE',
STARS(1)='*******',STARS(2)='**********',STARS(3)='************',
X1(1,2)=.02,.08,0.90,0.,0.,
         .02,.08,0.90,0.,0.,
         .02,.08,0.90,0.,0.,
         .02,.08,0.90,0.,0.,
         .02,.08,0.90,0.,0.,
         .02,.08,0.90,0.,0.,
         .02,.08,0.90,0.,0.,
         .02,.08,0.90,0.,0.,
         .02,.08,0.90,0.,0.,
         .02,.08,0.90,0.,0.,
         .02,.08,0.90,0.,0.,
         .02,.08,0.90,0.,0.,
         .02,.08,0.90,0.,0.,
         .02,.08,0.90,0.,0.,
         .02,.08,0.90,0.,0.,
         0.,0.,1.,0.,0.,
X2(1,1)=.50,.50,.0,0.,0.,
         .70,.10,0.20,0.,0.,
         .70,.10,0.20,0.,0.,
         .70,.10,0.20,0.,0.,
         .70,.10,0.20,0.,0.,
         .70,.10,0.20,0.,0.,
         .70,.10,0.20,0.,0.,
         .70,.10,0.20,0.,0.,
         .70,.10,0.20,0.,0.,
         .70,.10,0.20,0.,0.,
         .70,.10,0.20,0.,0.,
         .70,.10,0.20,0.,0.,
         .70,.10,0.20,0.,0.,
         .70,.10,0.20,0.,0.,
         .70,.10,0.20,0.,0.,
         .70,.10,0.20,0.,0.,
         .70,.10,0.20,0.,0.,
F1(2)=16*1240.,1210.,
F2(1)=100.,16*70.,
AVAL(5,5)=0.,
CC(5,5)=0.,
CT(5,5)=0.,
ALPC(5,5)=0.,
ALPT(5,5)=0.,
TEMP=303.15,  SNRTL=0.,
CG(1,1)=0.,611.,1418.,0.,0.,-535.,0.,992.,0.,0.,
        1401.,1443.,0.,0.,0.,
ALP(1,1)=1.,0.3,0.35,0.,0.,0.3,1.,0.35,0.,0.,
          0.35,.35,1.,0.,0.,0.,0.,0.,1.,0.,
          0.,0.,0.,0.,1.;
N
18
```

INPUT Data File of <u>EXAMPLE 5</u>.

```
DESPAC 5.8 (6-APR-81)

PROCEDURES:
 1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH        10.COLCST       14.STORE
 5.ABSEDM       21.HEX          15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

RETREV - RETRIEVE PHYSICAL CONSTANTS FROM DISK FILES

ENTER NAME OF FILE (RETURN FOR PUBLIC DATA):
+DATA WILL BE RETRIEVED FROM FILE PUBDAT
RETRIEVE ALL COMPONENTS FROM FILE? (Y OR N):

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  1 IS WATER

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  2 IS WATER1

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
LIBRARY IS REDEFINED.  SYSTEM IS UNDEFINED.

PROCEDURES:
 1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH        10.COLCST       14.STORE
 5.ABSEDM       21.HEX          15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

SYSTEM - DEFINE COMPONENTS IN SYSTEM

MODELS FOR VAPOR ENTHALPY HV:
  1. IDEAL SOLUTION OF PERFECT GASES.
  2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
  3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR LIQUID ENTHALPY HL:
  1. IDEAL SOLUTION OF SATURATED LIQUIDS.
  2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
  3. EXCESS ENTHALPY FROM WILSON EQUATION.
  4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR VLE CALCULATIONS:
  1. LIQUID: WILSON ACTIVITY;VAPOR: VIRIAL EQN OF STATE.
  2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
  3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
SELECT COMPONENTS (0 FOR HELP):

SELECTED COMPONENTS:
  1. WATER
  2. WATER1

VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
K-VALUES: RAOULT'S LAW.
```

EXAMPLE 6 - Computer Output of Shell-and-Tube Heat Exchanger (HEX).

```
 PROCEDURES:
  1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
  2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
  3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
  4.FLASH        10.COLCST       14.STORE
  5.ABSEDM       21.HEX          15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:

HEAT EXCHANGER CALCULATION

ENTER INPUT PARAMETERS
+(TH1,TH2,TC1,TC2,N,HO,HDO,HDI,HI,DI,DO
  SL,NTP,PT,B,Y,DE,MCOMP,KH,KC,VISH,VISC
  TETA,FLAG,EPS,SWCH,SWCH1,SWCH2,CPL)

+:
+:
+:
+:
+:


HEAT EXCHANGER RESULTS



     UD=     1696.2397 J/(S*M**2*K)

     A=       54.5917M**2

     L=      914.5837 M

     NT=        188.0

     DIS=     389.9898MM

     HI=    7917.1696 J/(S*M**2*K)

     HO=    6159.4662 J/(S*M**2*K)

     TW=      300.9450KELVIN

     F=          .9242

     CMTD=        5.4937 KELVIN

REPEAT? ( Y OR N ):
? SYSTEM IS UNDEFINED

 PROCEDURES:
  1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
  2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
  3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
  4.FLASH        10.COLCST       14.STORE
  5.ABSEDM       21.HEX          15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:
   PROGRAM IS STOPPED
```

```
11
PUBDAT
N
WATER
WATER1

12
113
001002
21
TH1=307,TH2=302,TC1=297,TC2=300,N=1,HO=6530,HDO=11356,
HDI=3785,HI=6530,DI=16.5,DC=19,SL=4.88,NTP=2,PT=23.8,
B=305,Y=4.76,DE=14,MCOMP=22.07,35.31,KH=.623,KC=.609,
VISH=.81,VISC=.92,TETA=.552,.552,
FLAG=1,EPS=.01,SWCH=0,SWCH1=0,SWCH2=1,CPL=75.5,75.5;
N
18
22.16.49.UCLP, BU, P04     ,       0.185KLNS.
```

INPUT Data File of <u>EXAMPLE 6.</u>

COMPUTER OUTPUTS AND THE INPUT DATA FILES FOR THE PROCESS FLOWSHEET DEVELOPMENT EXAMPLE

```
 DESPAC 5.8 (6-APR-81)

 PROCEDURES:
  1.KVALUE         7.SHTCUT        11.RETREV        17.HELP
  2.ENTHALPY       8.COLUMN        12.SYSTEM        18.STOP
  3.PHASE          9.CERDA         13.DEFINE        19.TIME AND DATE
  4.FLASH         10.COLCST        14.STORE
  5.ABSEDM        21.HEX           15.ACTFIT
  6.MCCABE        22.EXT

 SELECT PROCEDURE:

 RETREV - RETRIEVE PHYSICAL CONSTANTS FROM DISK FILES

 ENTER NAME OF FILE (RETURN FOR PUBLIC DATA):
+DATA WILL BE RETRIEVED FROM FILE PUBDAT
 RETRIEVE ALL COMPONENTS FROM FILE? (Y OR N):

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  1 IS HYDROGEN CHLORIDE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  2 IS BENZENE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  3 IS CHLOROBENZENE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  4 IS WATER

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
 LIBRARY IS REDEFINED.  SYSTEM IS UNDEFINED.

 PROCEDURES:
  1.KVALUE         7.SHTCUT        11.RETREV        17.HELP
  2.ENTHALPY       8.COLUMN        12.SYSTEM        18.STOP
  3.PHASE          9.CERDA         13.DEFINE        19.TIME AND DATE
  4.FLASH         10.COLCST        14.STORE
  5.ABSEDM        21.HEX           15.ACTFIT
  6.MCCABE        22.EXT

 SELECT PROCEDURE:

 SYSTEM - DEFINE COMPONENTS IN SYSTEM

 MODELS FOR VAPOR ENTHALPY HV:
   1. IDEAL SOLUTION OF PERFECT GASES.
   2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
   3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR LIQUID ENTHALPY HL:
   1. IDEAL SOLUTION OF SATURATED LIQUIDS.
   2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
   3. EXCESS ENTHALPY FROM WILSON EQUATION.
   4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR VLE CALCULATIONS:
   1. LIQUID: WILSON ACTIVITY;VAPOR: VIRIAL EQN OF STATE.
   2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
   3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

 SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
 SELECT COMPONENTS (0 FOR HELP):
```

CASE 1 - Computer Output of the Flowsheet (d) of Figure 4.2.
(Flash Temperature = 200°F = 366.48°K).

```
SELECTED COMPONENTS:
  1. HYDROGEN CHLORIDE
  2. BENZENE
  3. CHLOROBENZENE

VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
K-VALUES: RAOULT'S LAW.

PROCEDURES:
 1.KVALUE        7.SHTCUT        11.RETREV        17.HELP
 2.ENTHALPY      8.COLUMN        12.SYSTEM        18.STOP
 3.PHASE         9.CERDA         13.DEFINE        19.TIME AND DATE
 4.FLASH        10.COLCST        14.STORE
 5.ABSEDM       21.HEX           15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

FLASH CALCULATIONS

SELECT TYPE OF FLASH:

+1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :
 ENTER INPUT PARAMETERS
+(T,P,Z,(GUESS,X,Y,V) ;   )

+:


 FLASH RESULTS
  HF =  2.6008E+04       T = 366.480
  HL =  3.5209E+04       P =    2.380
  HV = -3.1400E+04       V =    .1331

  I  COMPONENT            X(I)    Y(I)    Z(I)    XI(I)         K(I)
  1. HYDROGEN CHLORI     .0103   .6594   .1000   .9108         63.73
  2. BENZENE             .4216   .2652   .4000   .9157E-01     .6290
  3. CHLOROBENZENE       .5680   .0754   .5000   .2084E-01     .1328


 REPEAT? (Y OR N):
+1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :
 ENTER INPUT PARAMETERS
+(T,P,Z,HF,(GUESS,X,Y,V) ;   )

+:


 FLASH RESULTS
  HF =  2.6008E+04       T = 366.480
  HL =  3.5209E+04       P =    2.380
  HV = -3.1400E+04       V =    .1331
   Q =  1.4478E-01

  I  COMPONENT            X(I)    Y(I)    Z(I)    XI(I)         K(I)
  1. HYDROGEN CHLORI     .0103   .6594   .1000   .9108         63.73
  2. BENZENE             .4216   .2652   .4000   .9157E-01     .6290
  3. CHLOROBENZENE       .5680   .0754   .5000   .2084E-01     .1328


 REPEAT? (Y OR N):
+1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :
```

```
PROCEDURES:
 1.KVALUE          7.SHTCUT        11.RETREV         17.HELP
 2.ENTHALPY        8.COLUMN        12.SYSTEM         18.STOP
 3.PHASE           9.CERDA         13.DEFINE         19.TIME AND DATE
 4.FLASH          10.COLCST        14.STORE
 5.ABSEDM         21.HEX           15.ACTFIT
 6.MCCABE         22.EXT

SELECT PROCEDURE:

ABSEDM - GAS ABSORPTION (EDMISTER METHOD)

ENTER INPUT PARAMETERS (TT/TB/P/LT/VB/N/XT/YB ;  )

+:
+:


ABSEDM RESULTS
 TT = 326.370      LT =  100.68     VT =  6.3251
 TB = 401.330      VB =  10.514     LB =  104.87
  P =   2.170
  N =   3

  I  COMPONENT              XT(I)    XB(I)     YT(I)   YB(I)     XIT(I)   XIB(I)
  1. HYDROGEN CHLORI        .0000    .0077     .9683   .6594     .99285   .11658
  2. BENZENE                .0007    .0272     .0002   .2652     .01362   .99991
  3. CHLOROBENZENE          .9993    .9651     .0315   .0754     .00198  1.00000


REPEAT? (Y OR N):

PROCEDURES:
 1.KVALUE          7.SHTCUT        11.RETREV         17.HELP
 2.ENTHALPY        8.COLUMN        12.SYSTEM         18.STOP
 3.PHASE           9.CERDA         13.DEFINE         19.TIME AND DATE
 4.FLASH          10.COLCST        14.STORE
 5.ABSEDM         21.HEX           15.ACTFIT
 6.MCCABE         22.EXT

SELECT PROCEDURE:

MCCABE - MCCABE-THIELE BINARY DISTILLATION

ENTER INPUT PARAMETERS (RATIO/ALPHA/Q/ ETA /XF/XD/F/D ;  )

+:
+:


MCCABE INPUT PARAMETERS
 RATIO = 1.30          XF =  .2106
 ALPHA = 3.878         XD =  .9975
     Q = 1.000          F =   192.61
   ETA = 1.000          D =   40.056


MCCABE RESULTS
    XW =   .0040       LB =   278.09
     W =    152.56     VB =   125.53
     L =    85.477     NT =    9
     V =    125.53     NB =    8
```

```
 REPEAT? (Y OR N):

 PROCEDURES:
  1.KVALUE       7.SHTCUT       11.RETREV        17.HELP
  2.ENTHALPY     8.COLUMN       12.SYSTEM        18.STOP
  3.PHASE        9.CERDA        13.DEFINE        19.TIME AND DATE
  4.FLASH       10.COLCST       14.STORE
  5.ABSEDM      21.HEX          15.ACTFIT
  6.MCCABE      22.EXT

 SELECT PROCEDURE:

 SYSTEM - DEFINE COMPONENTS IN SYSTEM

 MODELS FOR VAPOR ENTHALPY HV:
   1. IDEAL SOLUTION OF PERFECT GASES.
   2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
   3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR LIQUID ENTHALPY HL:
   1. IDEAL SOLUTION OF SATURATED LIQUIDS.
   2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
   3. EXCESS ENTHALPY FROM WILSON EQUATION.
   4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR VLE CALCULATIONS:
   1. LIQUID: WILSON ACTIVITY/VAPOR: VIRIAL EQN OF STATE.
   2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
   3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

 SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
 SELECT COMPONENTS (0 FOR HELP):

 SELECTED COMPONENTS:
   1. CHLOROBENZENE
   2. WATER

 VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
 LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
 K-VALUES: RAOULT'S LAW.

 PROCEDURES:
  1.KVALUE       7.SHTCUT       11.RETREV        17.HELP
  2.ENTHALPY     8.COLUMN       12.SYSTEM        18.STOP
  3.PHASE        9.CERDA        13.DEFINE        19.TIME AND DATE
  4.FLASH       10.COLCST       14.STORE
  5.ABSEDM      21.HEX          15.ACTFIT
  6.MCCABE      22.EXT

 SELECT PROCEDURE:

HEAT EXCHANGER CALCULATION

ENTER INPUT PARAMETERS
+(TH1,TH2,TC1,TC2,N,HO,HDO,HDI,HI,DI,DO
  SL,NTP,PT,B,Y,DE,MCOMP,KH,KC,VISH,VISC
  TETA,FLAG,EPS,SWCH,SWCH1,SWCH2,CPL)

+:
+:
+:
+:
+:
```

```
HEAT EXCHANGER RESULTS



       UD=       505.1768 J/(S*M**2*K)

       A=        30.5008M**2

       L=      510.9857 M

       NT=          105.0

       DIS=      301.0798MM

       HI=    6158.3505 J/(S*M**2*K)

       HO=     895.0426 J/(S*M**2*K)

       TW=       310.4119KELVIN

       F=           .9660

       CMTD=        56.2678 KELVIN


REPEAT? ( Y OR N ):
? SYSTEM IS UNDEFINED

 PROCEDURES:
  1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
  2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
  3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
  4.FLASH        10.COLCST       14.STORE
  5.ABSEDM       21.HEX          15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:
   PROGRAM IS STOPPED
```

```
11
PUBDAT
N
HYDROGEN CHLORIDE
BENZENE
CHLOROBENZENE
WATER

12
113
00100 2003
4
7
T=366.48,P=2.38,Z=10,40,50;
N
6
T=366.48,P=2.38,Z=10,40,50,HF=26008;
N
8
5
TT=326.37,TB=401.33,P=2.17,LT=100.68,VB=10.514,N=3,
XT=0.,0.0006683,0.99,YB=0.6594,0.2652,0.0754;
N
6
RATIO=1.3,ALPHA=3.878,Q=1,ETA=1,XF=0.2106,XD=0.9975,
F=192.613,D=40.056;
N
12
113
003004
21
TH1=425.9,TH2=321.88,TC1=299.6,TC2=305.2,N=1,HO=1570,HDO=5000,
HDI=1666,HI=6550,DI=16.5,DC=19,SL=4.88,NTP=2,PT=23.8,
B=305,Y=4.76,DE=14,MCOMP=4.77,15.145,KH=.1308,KC=.616,
VISH=.32,VISC=.85,TETA=0.,C.,
FLAG=1,EPS=.01,SWCH=0,SWCH1=0,SWCH2=0,CPL=179.8,75.5;
N
18
20.31.17.UCLP, BU, P04     ,       0.374KLNS.
```

INPUT Data File of CASE 1.

```
 DESPAC 5.8 (6-APR-81)

 PROCEDURES:
  1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
  2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
  3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
  4.FLASH        10.COLCST       14.STORE
  5.ABSEDM       21.HEX          15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:

 RETREV - RETRIEVE PHYSICAL CONSTANTS FROM DISK FILES

 ENTER NAME OF FILE (RETURN FOR PUBLIC DATA):
+DATA WILL BE RETRIEVED FROM FILE PUBDAT
 RETRIEVE ALL COMPONENTS FROM FILE? (Y OR N):

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  1 IS HYDROGEN CHLORIDE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  2 IS BENZENE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  3 IS CHLOROBENZENE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  4 IS WATER

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
 LIBRARY IS REDEFINED.  SYSTEM IS UNDEFINED.

 PROCEDURES:
  1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
  2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
  3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
  4.FLASH        10.COLCST       14.STORE
  5.ABSEDM       21.HEX          15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:

 SYSTEM - DEFINE COMPONENTS IN SYSTEM

 MODELS FOR VAPOR ENTHALPY HV:
   1. IDEAL SOLUTION OF PERFECT GASES.
   2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
   3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR LIQUID ENTHALPY HL:
   1. IDEAL SOLUTION OF SATURATED LIQUIDS.
   2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
   3. EXCESS ENTHALPY FROM WILSON EQUATION.
   4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR VLE CALCULATIONS:
   1. LIQUID: WILSON ACTIVITY;VAPOR: VIRIAL EQN OF STATE.
   2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
   3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

 SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
 SELECT COMPONENTS (0 FOR HELP):
```

CASE 2 - Computer Output of the Flowsheet (d) of Figure 4.2.
(Flash Temperature = 250°F = 394.1°K).

```
SELECTED COMPONENTS:
  1. HYDROGEN CHLORIDE
  2. BENZENE
  3. CHLOROBENZENE

VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
K-VALUES: RAOULT'S LAW.

PROCEDURES:
 1.K VALUE       7.SHTCUT       11.RETREV       17.HELP
 2.ENTHALPY      8.COLUMN       12.SYSTEM       18.STOP
 3.PHASE         9.CERDA        13.DEFINE       19.TIME AND DATE
 4.FLASH        10.COLCST       14.STORE
 5.ABSEDM       21.HEX          15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:.

FLASH CALCULATIONS

SELECT TYPE OF FLASH:

+1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :
 ENTER INPUT PARAMETERS
+(T,P,Z,(GUESS,X,Y,V) ;  )

+:


 FLASH RESULTS
  HF =  3.4851E+04      T  = 394.100
  HL =  3.8223E+04      P  =   2.380
  HV =  2.6903E+04      V  =    .2979

  I  COMPONENT            X(I)     Y(I)     Z(I)     XI(I)       K(I)
  1. HYDROGEN CHLORI     .0036    .3272    .1000    .9749       91.42
  2. BENZENE             .3683    .4747    .4000    .3536       1.289
  3. CHLOROBENZENE       .6281    .1981    .5000    .1180       .3153


 REPEAT? (Y OR N):
+1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :
 ENTER INPUT PARAMETERS
+(T,P,Z,HF,(GUESS,X,Y,V) ;   )

+:


 FLASH RESULTS
  HF =  3.4851E+04      T  = 394.100
  HL =  3.8223E+04      P  =   2.380
  HV =  2.6903E+04      V  =    .2979
   Q = -3.8826E-01

  I  COMPONENT            X(I)     Y(I)     Z(I)     XI(I)       K(I)
  1. HYDROGEN CHLORI     .0036    .3272    .1000    .9749       91.42
  2. BENZENE             .3683    .4747    .4000    .3536       1.289
  3. CHLOROBENZENE       .6281    .1981    .5000    .1180       .3153


 REPEAT? (Y OR N):
+1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :
```

```
PROCEDURES:
 1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH        10.COLCST       14.STORE
 5.ABSEDM       21.HEX          15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

ABSEDM - GAS ABSORPTION (EDMISTER METHOD)

ENTER INPUT PARAMETERS (TT,TB,P,LT,VB,N,XT,YB ;  )

+:
+:


ABSEDM RESULTS
 TT = 326.370      LT =   100.68     VT =   9.6370
 TB = 401.330      VB =   29.793     LB =   120.84
  P =    2.170
  N =    3

  I  COMPONENT           XT(I)    XB(I)    YT(I)    YB(I)    XIT(I)    XIB(I)
  1. HYDROGEN CHLORI     .0000    .0037    .9655    .3272    .99895    .04548
  2. BENZENE             .0007    .1175    .0011    .4747    .02482    .99935
  3. CHLOROBENZENE       .9993    .8788    .0333    .1981    .00319    .99999


REPEAT? (Y OR N):

PROCEDURES:
 1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH        10.COLCST       14.STORE
 5.ABSEDM       21.HEX          15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

MCCABE - MCCABE-THIELE BINARY DISTILLATION

ENTER INPUT PARAMETERS (RATIO,ALPHA,Q, ETA ,XF,XD,F,D ;  )

+:
+:


MCCABE INPUT PARAMETERS
 RATIO = 1.30            XF =  .2104
 ALPHA = 3.378           XD =  .9975
     Q = 1.000            F =   190.35
   ETA = 1.000            D =   40.056


MCCABE RESULTS
     XW =  .0006         LB =   275.91
      W =   150.29       VB =   125.61
      L =   85.558       NT =   10
      V =   125.61       NB =   11
```

```
 REPEAT? (Y OR N):

 PROCEDURES:
  1.KVALUE         7.SHTCUT         11.RETREV          17.HELP
  2.ENTHALPY       8.COLUMN         12.SYSTEM          18.STOP
  3.PHASE          9.CERDA          13.DEFINE          19.TIME AND DATE
  4.FLASH         10.COLCST         14.STORE
  5.ABSEDM        21.HEX            15.ACTFIT
  6.MCCABE        22.EXT

 SELECT PROCEDURE:

 SYSTEM - DEFINE COMPONENTS IN SYSTEM

 MODELS FOR VAPOR ENTHALPY HV:
   1. IDEAL SOLUTION OF PERFECT GASES.
   2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
   3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR LIQUID ENTHALPY HL:
   1. IDEAL SOLUTION OF SATURATED LIQUIDS.
   2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
   3. EXCESS ENTHALPY FROM WILSON EQUATION.
   4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR VLE CALCULATIONS:
   1. LIQUID: WILSON ACTIVITY;VAPOR: VIRIAL EQN OF STATE.
   2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
   3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

 SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
 SELECT COMPONENTS (0 FOR HELP):

 SELECTED COMPONENTS:
   1. CHLOROBENZENE
   2. WATER

 VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
 LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
 K-VALUES: RAOULT'S LAW.

 PROCEDURES:
  1.KVALUE         7.SHTCUT         11.RETREV          17.HELP
  2.ENTHALPY       8.COLUMN         12.SYSTEM          18.STOP
  3.PHASE          9.CERDA          13.DEFINE          19.TIME AND DATE
  4.FLASH         10.COLCST         14.STORE
  5.ABSEDM        21.HEX            15.ACTFIT
  6.MCCABE        22.EXT

 SELECT PROCEDURE:

HEAT EXCHANGER CALCULATION

ENTER INPUT PARAMETERS
+(TH1,TH2,TC1,TC2,N,HO,HDO,HDI,HI,DI,DO
  SL,NTP,PT,B,Y,DE,MCOMP,KH,KC,VISH,VISC
  TETA,FLAG,EPS,SWCH,SWCH1,SWCH2,CPL)

+:
+:
+:
+:
+:
```

```
    HEAT EXCHANGER RESULTS



         UD=       511.4111 J/(S*M**2*K)

         A=        29.6806M**2

         L=       497.2434 M

         NT=          102.0

         DIS=      297.2957MM

         HI=     6302.8316 J/(S*M**2*K)

         HO=      912.1111 J/(S*M**2*K)

         TW=       310.3813KELVIN

         F=          .9660

         CHTD=        56.2678 KELVIN

    REPEAT? ( Y OR N ):
    ? SYSTEM IS UNDEFINED

     PROCEDURES:
      1.KVALUE          7.SHTCUT         11.RETREV          17.HELP
      2.ENTHALPY        8.COLUMN         12.SYSTEM          18.STOP
      3.PHASE           9.CERDA          13.DEFINE          19.TIME AND DATE
      4.FLASH          10.COLCST         14.STORE
      5.ABSEDM         21.HEX            15.ACTFIT
      6.MCCABE         22.EXT

     SELECT PROCEDURE:
       PROGRAM IS STOPPED
```

```
11
PUBDAT
N
HYDROGEN CHLORIDE
BENZENE
CHLOROBENZENE
WATER

12
113
001002003
4
7
T=394.1,P=2.38,Z=10,40,50;
N
6
T=394.1,P=2.38,Z=10,40,50,HF=34851;
N
8
5
TT=326.37,TB=401.33,P=2.17,LT=100.08,VB=29.793,N=3,
XT=0.,0.0006683,0.99,YB=0.3272,0.4747,0.1981;
N
6
RATIO=1.3,ALPHA=3.878,Q=1,ETA=1,XF=0.2104,XD=0.9975,
F=190.35,D=40.056;
N
12
113
003004
21
TH1=425.9,TH2=321.88,TC1=299.6,TC2=305.2,N=1,HO=1570,HDO=5000,
HDI=1666,HI=6550,DI=16.5,DO=19,SL=4.88,NTP=2,PT=23.8,
B=305,Y=4.76,DE=14,MCOMP=4.699,15.145,KH=.1348,KC=.616,
VISH=.32,VISC=.85,TETA=0.,0.,
FLAG=1,EPS=.01,SWCH=0,SWCH1=0,SWCH2=0,CPL=178.8,75.5;
N
18
20.34.30.UCLP, BU, PU4    ,      0.374KLNS.
```

INPUT Data File of <u>CASE 2.</u>

```
 DESPAC 5.8 (6-APR-81)

 PROCEDURES:
  1.KVALUE          7.SHTCUT        11.RETREV         17.HELP
  2.ENTHALPY        8.COLUMN        12.SYSTEM         18.STOP
  3.PHASE           9.CERDA         13.DEFINE         19.TIME AND DATE
  4.FLASH          10.COLCST        14.STORE
  5.ABSEDM         21.HEX           15.ACTFIT
  6.MCCABE         22.EXT

 SELECT PROCEDURE:

 RETREV - RETRIEVE PHYSICAL CONSTANTS FROM DISK FILES

 ENTER NAME OF FILE (RETURN FOR PUBLIC DATA):
+DATA WILL BE RETRIEVED FROM FILE PUBDAT
 RETRIEVE ALL COMPONENTS FROM FILE? (Y OR N):

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  1 IS HYDROGEN CHLORIDE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  2 IS BENZENE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  3 IS CHLOROBENZENE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  4 IS WATER

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
 LIBRARY IS REDEFINED.  SYSTEM IS UNDEFINED.

 PROCEDURES:
  1.KVALUE          7.SHTCUT        11.RETREV         17.HELP
  2.ENTHALPY        8.COLUMN        12.SYSTEM         18.STOP
  3.PHASE           9.CERDA         13.DEFINE         19.TIME AND DATE
  4.FLASH          10.COLCST        14.STORE
  5.ABSEDM         21.HEX           15.ACTFIT
  6.MCCABE         22.EXT

 SELECT PROCEDURE:

 SYSTEM - DEFINE COMPONENTS IN SYSTEM

 MODELS FOR VAPOR ENTHALPY HV:
   1. IDEAL SOLUTION OF PERFECT GASES.
   2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
   3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR LIQUID ENTHALPY HL:
   1. IDEAL SOLUTION OF SATURATED LIQUIDS.
   2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
   3. EXCESS ENTHALPY FROM WILSON EQUATION.
   4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR VLE CALCULATIONS:
   1. LIQUID: WILSON ACTIVITY/VAPOR: VIRIAL EQN OF STATE.
   2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
   3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

 SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
 SELECT COMPONENTS (0 FOR HELP):
```

CASE 3 - Computer Output of the Flowsheet (d) of Figure 4.2
(Flash Temperature = 270°F = 405.2°K).

```
SELECTED COMPONENTS:
  1. HYDROGEN CHLORIDE
  2. BENZENE
  3. CHLOROBENZENE

VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
K-VALUES: RAOULT'S LAW.

PROCEDURES:
 1.KVALUE        7.SHTCUT        11.RETREV        17.HELP
 2.ENTHALPY      8.COLUMN        12.SYSTEM        18.STOP
 3.PHASE         9.CERDA         13.DEFINE        19.TIME AND DATE
 4.FLASH        10.COLCST        14.STORE
 5.ABSEDM       21.HEX           15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

FLASH CALCULATIONS

SELECT TYPE OF FLASH:

+1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :
 ENTER INPUT PARAMETERS
+(T,P,Z,(GUESS,X,Y,V) ;   )

+:


 FLASH RESULTS
  HF =   4.2918E+04       T  = 405.200
  HL =   3.7698E+04       P  =    2.380
  HV =   4.8216E+04       V  =    .4963

  I  COMPONENT              X(I)     Y(I)     Z(I)      XI(I)        K(I)
  1. HYDROGEN CHLORI       .0019    .1995    .1000     .9904        104.2
  2. BENZENE               .3006    .5009    .4000     .6215        1.666
  3. CHLOROBENZENE         .6975    .2996    .5000     .2974        .4295


 REPEAT? (Y OR N):
+1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :
 ENTER INPUT PARAMETERS
+(T,P,Z,HF,(GUESS,X,Y,V) ;   )

+:


 FLASH RESULTS
  HF =   4.2918E+04       T  = 405.200
  HL =   3.7698E+04       P  =    2.380
  HV =   4.8216E+04       V  =    .4963
   Q =   9.6915E-02

  I  COMPONENT              X(I)     Y(I)     Z(I)      XI(I)        K(I)
  1. HYDROGEN CHLORI       .0019    .1995    .1000     .9904        104.2
  2. BENZENE               .3006    .5009    .4000     .6215        1.666
  3. CHLOROBENZENE         .6975    .2996    .5000     .2974        .4295


 REPEAT? (Y OR N):
+1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :
```

```
PROCEDURES:
 1.KVALUE         7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY       8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE          9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH         10.COLCST       14.STORE
 5.ABSEDM        21.HEX          15.ACTFIT
 6.MCCABE        22.EXT

SELECT PROCEDURE:

ABSEDM - GAS ABSORPTION (EDMISTER METHOD)

ENTER INPUT PARAMETERS (TT,TB,P,LT,VB,N,XT,YB ;  )

+:
+:


ABSEDM RESULTS
 TT = 326.370      LT =   100.68     VT =    9.9631
 TB = 401.330      VB =   49.634     LB =   140.35
  P =   2.170
  N =    3

  I  COMPONENT            XT(I)   XB(I)    YT(I)   YB(I)    XIT(I)   XIB(I)
  1.  HYDROGEN CHLORI     .0000   .0023    .9622   .1995    .99941   .03189
  2.  BENZENE             .0007   .1774    .0031   .5009    .02880   .99883
  3.  CHLOROBENZENE       .9993   .8203    .0347   .2996    .00344   .99999


REPEAT? (Y OR N):

PROCEDURES:
 1.KVALUE         7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY       8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE          9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH         10.COLCST       14.STORE
 5.ABSEDM        21.HEX          15.ACTFIT
 6.MCCABE        22.EXT

SELECT PROCEDURE:

MCCABE -- MCCABE-THIELE BINARY DISTILLATION

ENTER INPUT PARAMETERS (RATIO,ALPHA,Q, ETA ,XF,XD,F,D ;  )

+:
+:


MCCABE INPUT PARAMETERS
 RATIO = 1.30          XF =   .2103
 ALPHA = 3.878         XD =   .9975
     Q = 1.000          F =    190.29
   ETA = 1.000          D =    40.056


MCCABE RESULTS
    XW =   .0004       LB =    275.89
     W =    150.23     VB =    125.65
     L =    85.599     NT =     9
     V =    125.65     NB =    12
```

```
 REPEAT? (Y OR N):

 PROCEDURES:
  1.KVALUE        7.SHTCUT       11.RETREV       17.HELP
  2.ENTHALPY      8.COLUMN       12.SYSTEM       18.STOP
  3.PHASE         9.CERDA        13.DEFINE       19.TIME AND DATE
  4.FLASH        10.COLCST       14.STORE
  5.ABSEDM       21.HEX          15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:

 SYSTEM - DEFINE COMPONENTS IN SYSTEM

 MODELS FOR VAPOR ENTHALPY HV:
   1. IDEAL SOLUTION OF PERFECT GASES.
   2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
   3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR LIQUID ENTHALPY HL:
   1. IDEAL SOLUTION OF SATURATED LIQUIDS.
   2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
   3. EXCESS ENTHALPY FROM WILSON EQUATION.
   4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR VLE CALCULATIONS:
   1. LIQUID: WILSON ACTIVITY;VAPOR: VIRIAL EQN OF STATE.
   2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
   3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

 SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
 SELECT COMPONENTS (0 FOR HELP):

 SELECTED COMPONENTS:
   1. CHLOROBENZENE
   2. WATER

 VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
 LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
 K-VALUES: RAOULT'S LAW.

 PROCEDURES:
  1.KVALUE        7.SHTCUT       11.RETREV       17.HELP
  2.ENTHALPY      8.COLUMN       12.SYSTEM       18.STOP
  3.PHASE         9.CERDA        13.DEFINE       19.TIME AND DATE
  4.FLASH        10.COLCST       14.STORE
  5.ABSEDM       21.HEX          15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:

HEAT EXCHANGER CALCULATION

ENTER INPUT PARAMETERS
+(TH1,TH2,TC1,TC2,N,HO,HDO,HDI,HI,DI,DO
  SL,NTP,PT,B,Y,DE,MCOMP,KH,KC,VISH,VISC
  TETA,FLAG,EPS,SWCH,SWCH1,SWCH2,CPL)

+:
+:
+:
+:
+:
```

```
HEAT EXCHANGER RESULTS



     UD=       503.6849 J/(S*M**2*K)

     A=        30.1230M**2

     L=       504.6560 M

     NT=          104.0

     DIS=      299.8245MM

     HI=    6205.6770 J/(S*M**2*K)

     HO=      889.5244 J/(S*M**2*K)

     TW=       310.3139KELVIN

     F=           .9660

     CMTD=        56.2678 KELVIN

REPEAT? ( Y OR N ):
? SYSTEM IS UNDEFINED

 PROCEDURES:
  1.KVALUE        7.SHTCUT       11.RETREV       17.HELP
  2.ENTHALPY      8.COLUMN       12.SYSTEM       18.STOP
  3.PHASE         9.CERDA        13.DEFINE       19.TIME AND DATE
  4.FLASH        10.COLCST       14.STORE
  5.ABSEDM       21.HEX          15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:
   PROGRAM IS STOPPED
```

```
11
PUBDAT
N
HYDROGEN CHLORIDE
BENZENE
CHLOROBENZENE
WATER

12
113
0010020003
4
7
T=405.2,P=2.38,Z=10,40,50;
N
6
T=405.2,P=2.38,Z=10,40,50,HF=42918;
N
8
5
TT=326.37,TB=401.33,P=2.17,LT=100.68,VB=49.634,N=3,
XT=0.,0.0006683,0.99,YB=0.1995,0.5009,0.2996;
N
6
RATIO=1.3,ALPHA=3.878,Q=1,ETA=1,XF=.2103,XD=.9975,
F=190.289,D=40.056;
N
12
113
003004
21
TH1=425.9,TH2=321.88,TC1=299.6,TC2=305.2,N=1,HO=1570,HDO=5000,
HDI=1666,HI=6550,DI=16.5,DC=19,SL=4.88,NTP=2,PT=23.8,
B=305,Y=4.76,DE=14,MCOMP=4.697,15.145,KH=.1308,KC=.616,
VISH=.32,VISC=.85,TETA=0.,0.,
FLAG=1,EPS=.01,SWCH=0,SWCH1=0,SWCH2=0,CPL=178.8,75.5;
N
18
20.38.24.UCLP, BU, PC4     ,       0.374KLNS.
```

INPUT Data File of CASE 3.

```
DESPAC 5.8 (6-APR-81)

PROCEDURES:
 1.KVALUE       7.SHTCUT       11.RETREV      17.HELP
 2.ENTHALPY     8.COLUMN       12.SYSTEM      18.STOP
 3.PHASE        9.CERDA        13.DEFINE      19.TIME AND DATE
 4.FLASH       10.COLCST       14.STORE
 5.ABSEDM      21.HEX          15.ACTFIT
 6.MCCABE      22.EXT

SELECT PROCEDURE:

RETREV - RETRIEVE PHYSICAL CONSTANTS FROM DISK FILES

ENTER NAME OF FILE (RETURN FOR PUBLIC DATA):
+DATA WILL BE RETRIEVED FROM FILE PUBDAT
RETRIEVE ALL COMPONENTS FROM FILE? (Y OR N):

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  1 IS HYDROGEN CHLORIDE

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  2 IS BENZENE

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  3 IS CHLOROBENZENE

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  4 IS WATER

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
LIBRARY IS REDEFINED.  SYSTEM IS UNDEFINED.

PROCEDURES:
 1.KVALUE       7.SHTCUT       11.RETREV      17.HELP
 2.ENTHALPY     8.COLUMN       12.SYSTEM      18.STOP
 3.PHASE        9.CERDA        13.DEFINE      19.TIME AND DATE
 4.FLASH       10.COLCST       14.STORE
 5.ABSEDM      21.HEX          15.ACTFIT
 6.MCCABE      22.EXT

SELECT PROCEDURE:

SYSTEM - DEFINE COMPONENTS IN SYSTEM

MODELS FOR VAPOR ENTHALPY HV:
  1. IDEAL SOLUTION OF PERFECT GASES.
  2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
  3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR LIQUID ENTHALPY HL:
  1. IDEAL SOLUTION OF SATURATED LIQUIDS.
  2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
  3. EXCESS ENTHALPY FROM WILSON EQUATION.
  4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR VLE CALCULATIONS:
  1. LIQUID: WILSON ACTIVITY/VAPOR: VIRIAL EQN OF STATE.
  2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
  3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

SELECT MODELS FOR HV/HL/VLE (   BLANK THEN RETURN FOR 1 1 1):
SELECT COMPONENTS (0 FOR HELP):
```

CASE 4 - Computer Output of the Flowsheet (d) of Figure 4.2
(Flash Temperature = 280°F = 410.77°K).

```
SELECTED COMPONENTS:
  1. HYDROGEN CHLORIDE
  2. BENZENE
  3. CHLOROBENZENE

VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
K-VALUES: RAOULT'S LAW.

PROCEDURES:
 1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH        10.COLCST       14.STORE
 5.ABSEDM       21.HEX          15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

FLASH CALCULATIONS

SELECT TYPE OF FLASH:

+1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :
 ENTER INPUT PARAMETERS
+(T,P,Z,(GUESS,X,Y,V) ;   )

+:


 FLASH RESULTS
  HF =   4.9066E+04       T = 410.770
  HL =   3.6938E+04       P =   2.380
  HV =   5.5433E+04       V =    .6558

  I  COMPONENT            X(I)     Y(I)     Z(I)     XI(I)        K(I)
  1. HYDROGEN CHLORI     .0014    .1518    .1000    .9953        111.0
  2. BENZENE             .2532    .4770    .4000    .7821        1.884
  3. CHLOROBENZENE       .7454    .3712    .5000    .4868        .4980

 REPEAT? (Y OR N):
+1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :
 ENTER INPUT PARAMETERS
+(T,P,Z,HF,(GUESS,X,Y,V) ;   )

+:


 FLASH RESULTS
  HF =   4.9066E+04       T = 410.770
  HL =   3.6938E+04       P =   2.380
  HV =   5.5433E+04       V =    .6558
   Q = -2.7177E-01

  I  COMPONENT            X(I)     Y(I)     Z(I)     XI(I)        K(I)
  1. HYDROGEN CHLORI     .0014    .1518    .1000    .9953        111.0
  2. BENZENE             .2532    .4770    .4000    .7821        1.884
  3. CHLOROBENZENE       .7454    .3712    .5000    .4868        .4980

 REPEAT? (Y OR N):
+1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :
```

```
PROCEDURES:
 1.KVALUE          7.SHTCUT         11.RETREV         17.HELP
 2.ENTHALPY        8.COLUMN         12.SYSTEM         18.STOP
 3.PHASE           9.CERDA          13.DEFINE         19.TIME AND DATE
 4.FLASH          10.COLCST         14.STORE
 5.ABSEDM         21.HEX            15.ACTFIT
 6.MCCABE         22.EXT

SELECT PROCEDURE:

ABSEDM - GAS ABSORPTION (EDMISTER METHOD)

ENTER INPUT PARAMETERS (TT,TB,P,LT,VB,N,XT,YB ;  )

+:
+:


ABSEDM RESULTS
 TT = 326.370      LT =  100.68     VT =  10.096
 TB = 401.330      VB =  65.577     LB =  156.16
  P =   2.170
  N =   3

  I. COMPONENT            XT(I)   XB(I)    YT(I)   YB(I)    XIT(I)   XIB(I)
  1. HYDROGEN CHLORI      .0000   .0017    .9594   .1518    .99955   .02691
  2. BENZENE              .0007   .2004    .0050   .4770    .03115   .99845
  3. CHLOROBENZENE        .9993   .7979    .0356   .3712    .00357   .99999


REPEAT? (Y OR N):

PROCEDURES:
 1.KVALUE          7.SHTCUT         11.RETREV         17.HELP
 2.ENTHALPY        8.COLUMN         12.SYSTEM         18.STOP
 3.PHASE           9.CERDA          13.DEFINE         19.TIME AND DATE
 4.FLASH          10.COLCST         14.STORE
 5.ABSEDM         21.HEX            15.ACTFIT
 6.MCCABE         22.EXT

SELECT PROCEDURE:

MCCABE - MCCABE-THIELE BINARY DISTILLATION

ENTER INPUT PARAMETERS (RATIO,ALPHA,Q, ETA ,XF,XD,F,D ;  )

+:
+:


MCCABE INPUT PARAMETERS
 RATIO = 1.30           XF =  .2103
 ALPHA = 3.878          XD =  .9975
     Q = 1.000           F =  190.27
   ETA = 1.000           D =  40.056


MCCABE RESULTS
    XW =   .0004        LB =  275.87
     W =   150.21       VB =  125.65
     L =   85.599       NT =   9
     V =   125.65       NB =  12
```

```
 REPEAT? (Y OR N):

 PROCEDURES:
  1.KVALUE         7.SHTCUT       11.RETREV        17.HELP
  2.ENTHALPY       8.COLUMN       12.SYSTEM        18.STOP
  3.PHASE          9.CERDA        13.DEFINE        19.TIME AND DATE
  4.FLASH         10.COLCST       14.STORE
  5.ABSEDM        21.HEX          15.ACTFIT
  6.MCCABE        22.EXT

 SELECT PROCEDURE:

 SYSTEM - DEFINE COMPONENTS IN SYSTEM

 MODELS FOR VAPOR ENTHALPY HV:
   1. IDEAL SOLUTION OF PERFECT GASES.
   2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
   3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR LIQUID ENTHALPY HL:
   1. IDEAL SOLUTION OF SATURATED LIQUIDS.
   2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
   3. EXCESS ENTHALPY FROM WILSON EQUATION.
   4. RESICUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR VLE CALCULATIONS:
   1. LIQUID: WILSON ACTIVITY/VAPOR: VIRIAL EQN OF STATE.
   2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
   3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

 SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
 SELECT COMPONENTS (0 FOR HELP):

 SELECTED COMPONENTS:
   1. CHLOROBENZENE
   2. WATER

 VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
 LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
 K-VALUES: RAOULT'S LAW.

 PROCEDURES:
  1.KVALUE         7.SHTCUT       11.RETREV        17.HELP
  2.ENTHALPY       8.COLUMN       12.SYSTEM        18.STOP
  3.PHASE          9.CERDA        13.DEFINE        19.TIME AND DATE
  4.FLASH         10.COLCST       14.STORE
  5.ABSEDM        21.HEX          15.ACTFIT
  6.MCCABE        22.EXT

 SELECT PROCEDURE:

HEAT EXCHANGER CALCULATION

ENTER INPUT PARAMETERS
+(TH1,TH2,TC1,TC2,N,HO,HDO,HDI,HI,DI,DO
  SL,NTP,PT,B,Y,DE,MCOMP,KH,KC,VISH,VISC
  TETA,FLAG,EPS,SWCH,SWCH1,SWCH2,CPL)

+:
+:
+:
+:
+:
```

```
HEAT EXCHANGER RESULTS



       UD=      503.6515 J/(S*M**2*K)

       A=       30.1186M**2

       L=      504.5820 M

       NT=         104.0

       DIS=     299.8245 MM

       HI=    6205.6770 J/(S*M**2*K)

       HO=     889.4202 J/(S*M**2*K)

       TW=      310.3131KELVIN

       F=          .9660

       CMTD=       56.2678 KELVIN

REPEAT? ( Y OR N ):
? SYSTEM IS UNDEFINED

 PROCEDURES:
  1.KVALUE        7.SHTCUT       11.RETREV       17.HELP
  2.ENTHALPY      8.COLUMN       12.SYSTEM       18.STOP
  3.PHASE         9.CERDA        13.DEFINE       19.TIME AND DATE
  4.FLASH        10.COLCST       14.STORE
  5.ABSEDM       21.HEX          15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:
   PROGRAM IS STOPPED
```

```
11
PUBDAT
N
HYDROGEN CHLORIDE
BENZENE
CHLOROBENZENE
WATER

12
113
001002003
4
7
T=410.77,P=2.38,Z=10,40,50;
N
6
T=410.77,P=2.38,Z=10,40,50,HF=49066;
N
8
5
TT=326.37,TB=401.33,P=2.17,LT=100.68,VB=65.577,N=3,
XT=0.,0.0006683,0.99,YB=0.1518,0.4770,0.3712;
N
6
RATIO=1.3,ALPHA=3.878,Q=1,ETA=1,XF=0.2103,XD=0.9975,
F=190.269,D=40.056;
N
12
113
003004
21
TH1=425.9,TH2=321.88,TC1=299.6,TC2=305.2,N=1,HO=1570,HDO=5000,
HDI=1666,HI=6550,DI=16.5,DO=19,SL=4.88,NTP=2,PT=23.8,
B=305,Y=4.76,DE=14,NCOMP=4.696,15.145,KH=.1303,KC=.616,
VISH=.32,VISC=.85,TETA=0.,0.,
FLAG=1,EPS=.01,SWCH=0,SWCH1=0,SWCH2=0,CPL=178.8,75.5;
N
18
20.42.08.UCLP, BU, P04    ,        0.374KLNS.
```

INPUT Data File of CASE 4.

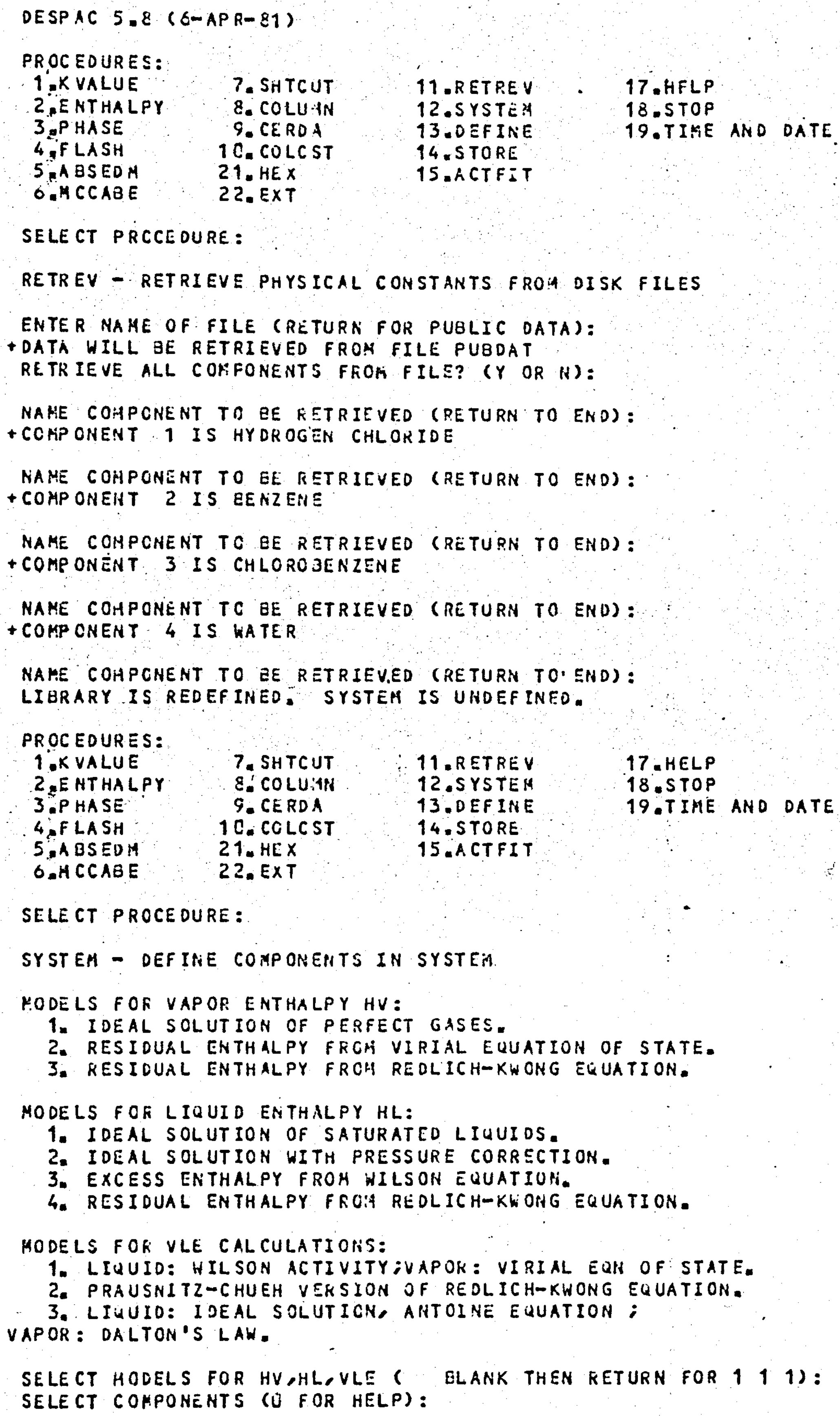
```
DESPAC 5.8 (6-APR-81)

PROCEDURES:
 1.KVALUE       7.SHTCUT      11.RETREV       17.HELP
 2.ENTHALPY     8.COLUMN      12.SYSTEM       18.STOP
 3.PHASE        9.CERDA       13.DEFINE       19.TIME AND DATE
 4.FLASH       10.COLCST      14.STORE
 5.ABSEDM      21.HEX         15.ACTFIT
 6.MCCABE      22.EXT

SELECT PROCEDURE:

RETREV - RETRIEVE PHYSICAL CONSTANTS FROM DISK FILES

ENTER NAME OF FILE (RETURN FOR PUBLIC DATA):
+DATA WILL BE RETRIEVED FROM FILE PUBDAT
RETRIEVE ALL COMPONENTS FROM FILE? (Y OR N):

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  1 IS HYDROGEN CHLORIDE

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  2 IS BENZENE

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  3 IS CHLOROBENZENE

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  4 IS WATER

NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
LIBRARY IS REDEFINED.  SYSTEM IS UNDEFINED.

PROCEDURES:
 1.KVALUE       7.SHTCUT      11.RETREV       17.HELP
 2.ENTHALPY     8.COLUMN      12.SYSTEM       18.STOP
 3.PHASE        9.CERDA       13.DEFINE       19.TIME AND DATE
 4.FLASH       10.COLCST      14.STORE
 5.ABSEDM      21.HEX         15.ACTFIT
 6.MCCABE      22.EXT

SELECT PROCEDURE:

SYSTEM - DEFINE COMPONENTS IN SYSTEM

MODELS FOR VAPOR ENTHALPY HV:
  1. IDEAL SOLUTION OF PERFECT GASES.
  2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
  3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR LIQUID ENTHALPY HL:
  1. IDEAL SOLUTION OF SATURATED LIQUIDS.
  2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
  3. EXCESS ENTHALPY FROM WILSON EQUATION.
  4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR VLE CALCULATIONS:
  1. LIQUID: WILSON ACTIVITY;VAPOR: VIRIAL EQN OF STATE.
  2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
  3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
SELECT COMPONENTS (0 FOR HELP):
```

CASE 5 - Computer Output of the Flowsheet (d) of Figure 4.2
(Flash Temperature = 300°F = 421.88°K).

```
        SELECTED COMPONENTS:
          1. HYDROGEN CHLORIDE
          2. BENZENE
          3. CHLOROBENZENE

        VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
        LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
        K-VALUES: RAOULT'S LAW.

        PROCEDURES:
         1.KVALUE          7.SHTCUT          11.RETREV          17.HELP
         2.ENTHALPY        8.COLUMN          12.SYSTEM          18.STOP
         3.PHASE           9.CERDA           13.DEFINE          19.TIME AND DATE
         4.FLASH          10.COLCST          14.STORE
         5.ABSEDM         21.HEX             15.ACTFIT
         6.MCCABE         22.EXT

        SELECT PROCEDURE:

        FLASH CALCULATIONS

        SELECT TYPE OF FLASH:

       +1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :
        ENTER INPUT PARAMETERS
       +(T,P,Z,(GUESS,X,Y,V) ;   )

       +:


        FLASH RESULTS
         HF =  6.2421E+04       T = 421.880
         HL =  3.6181E+04       P =   2.380
         HV =  6.2421E+04       V =  1.0000

         I  COMPONENT           X(I)     Y(I)     Z(I)     XI(I)        K(I)
         1. HYDROGEN CHLORI    .0009    .1000    .1000    1.000        125.3
         2. BENZENE            .1813    .4000    .4000    1.000        2.380
         3. CHLOROBENZENE      .8178    .5000    .5000    1.000        .6598


        REPEAT? (Y OR N):
       +1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :

        PROCEDURES:
         1.KVALUE          7.SHTCUT          11.RETREV          17.HELP
         2.ENTHALPY        8.COLUMN          12.SYSTEM          18.STOP
         3.PHASE           9.CERDA           13.DEFINE          19.TIME AND DATE
         4.FLASH          10.COLCST          14.STORE
         5.ABSEDM         21.HEX             15.ACTFIT
         6.MCCABE         22.EXT

        SELECT PROCEDURE:
          PROGRAM IS STOPPED
```

```
11
PUBDAT
N
HYDROGEN CHLORIDE
BENZENE
CHLOROBENZENE
WATER

12
113
001002003
4
7
T=421.88,P=2.38,Z=10,40,50;
 %FLSHTP: SYSTEM IS SUPERHEATED VAPOR.
21.42.36.UCLP, BU, P04    ,      C.176KLNS.
```

INPUT Data File of CASE 5.



```
 DESPAC 5.8 (6-APR-81)

 PROCEDURES:
  1.KVALUE        7.SHTCUT        11.RETREV   .    17.HFLP
  2.ENTHALPY      8.COLUMN        12.SYSTEM        18.STOP
  3.PHASE         9.CERDA         13.DEFINE        19.TIME AND DATE
  4.FLASH        10.COLCST        14.STORE
  5.ABSEDM       21.HEX           15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:

 RETREV - RETRIEVE PHYSICAL CONSTANTS FROM DISK FILES

 ENTER NAME OF FILE (RETURN FOR PUBLIC DATA):
+DATA WILL BE RETRIEVED FROM FILE PUBDAT
 RETRIEVE ALL COMPONENTS FROM FILE? (Y OR N):

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  1 IS HYDROGEN CHLORIDE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  2 IS BENZENE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  3 IS CHLOROBENZENE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  4 IS WATER

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
 LIBRARY IS REDEFINED.  SYSTEM IS UNDEFINED.

 PROCEDURES:
  1.KVALUE        7.SHTCUT        11.RETREV        17.HELP
  2.ENTHALPY      8.COLUMN        12.SYSTEM        18.STOP
  3.PHASE         9.CERDA         13.DEFINE        19.TIME AND DATE
  4.FLASH        10.COLCST        14.STORE
  5.ABSEDM       21.HEX           15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:

 SYSTEM - DEFINE COMPONENTS IN SYSTEM

 MODELS FOR VAPOR ENTHALPY HV:
   1. IDEAL SOLUTION OF PERFECT GASES.
   2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
   3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR LIQUID ENTHALPY HL:
   1. IDEAL SOLUTION OF SATURATED LIQUIDS.
   2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
   3. EXCESS ENTHALPY FROM WILSON EQUATION.
   4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR VLE CALCULATIONS:
   1. LIQUID: WILSON ACTIVITY;VAPOR: VIRIAL EQN OF STATE.
   2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
   3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

 SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
 SELECT COMPONENTS (0 FOR HELP):
```

CASE 6 - Computer Output of Flowsheet (e) of Figure 4.2
(Flash unit is removed).

```
SELECTED COMPONENTS:
  1. HYDROGEN CHLORIDE
  2. BENZENE
  3. CHLOROBENZENE

VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
K-VALUES: RAOULT'S LAW.

PROCEDURES:
 1.K VALUE        7.SHTCUT        11.RETREV        17.HELP
 2.ENTHALPY       8.COLUMN        12.SYSTEM        18.STOP
 3.PHASE          9.CERDA         13.DEFINE        19.TIME AND DATE
 4.FLASH         10.COLCST        14.STORE
 5.ABSEDM        21.HEX           15.ACTFIT
 6.MCCABE        22.EXT

SELECT PROCEDURE:

ABSEDM - GAS ABSORPTION (EDMISTER METHOD)

ENTER INPUT PARAMETERS (TT/TB/P/LT/VB/N/XT/YB ;  )

+:
+:


ABSEDM RESULTS
 TT = 326.370      LT =  100.68     VT =  10.255
 TB = 401.330      VB =  100.00     LB =  190.43
  P =   2.170
  N =   3

  I  COMPONENT              XT(I)    XB(I)     XT(I)    YB(I)     XIT(I)    XIB(I)
  1. HYDROGEN CHLORI        .0000    .0011     .9541    .1000     .99969    .02156
  2. BENZENE                .0007    .2099     .0089    .4000     .03479    .99778
  3. CHLOROBENZENE          .9993    .7889     .0370    .5000     .00376    .99998


REPEAT? (Y OR N):

PROCEDURES:
 1.K VALUE        7.SHTCUT        11.RETREV        17.HELP
 2.ENTHALPY       8.COLUMN        12.SYSTEM        18.STOP
 3.PHASE          9.CERDA         13.DEFINE        19.TIME AND DATE
 4.FLASH         10.COLCST        14.STORE
 5.ABSEDM        21.HEX           15.ACTFIT
 6.MCCABE        22.EXT

SELECT PROCEDURE:

MCCABE - MCCABE-THIELE BINARY DISTILLATION

ENTER INPUT PARAMETERS (RATIO/ALPHA/Q/ ETA /XF/XD/F/D ;  )

+:
+:


MCCABE INPUT PARAMETERS
 RATIO = 1.30              XF =  .2101
 ALPHA = 3.873             XD =  .9975
     Q = 1.000              F =   190.20
   ETA = 1.000              D =   40.056
```

```
MCCABE RESULTS
     XW =   .0000          LB =    275.88
      W =    150.14        VB =    125.74
      L =    85.681        NT =     9
      V =    125.74        NB =    17


REPEAT? (Y OR N):

PROCEDURES:
 1.KVALUE        7.SHTCUT        11.RETREV        17.HELP
 2.ENTHALPY      8.COLUMN        12.SYSTEM        18.STOP
 3.PHASE         9.CERDA         13.DEFINE        19.TIME AND DATE
 4.FLASH        10.COLCST        14.STORE
 5.ABSEDM       21.HEX           15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

SYSTEM - DEFINE COMPONENTS IN SYSTEM

MODELS FOR VAPOR ENTHALPY HV:
  1. IDEAL SOLUTION OF PERFECT GASES.
  2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
  3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR LIQUID ENTHALPY HL:
  1. IDEAL SOLUTION OF SATURATED LIQUIDS.
  2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
  3. EXCESS ENTHALPY FROM WILSON EQUATION.
  4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR VLE CALCULATIONS:
  1. LIQUID: WILSON ACTIVITY/VAPOR: VIRIAL EQN OF STATE.
  2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
  3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

SELECT MODELS FOR HV/HL/VLE (   BLANK THEN RETURN FOR 1 1 1):
SELECT COMPONENTS (0 FOR HELP):

SELECTED COMPONENTS:
  1. CHLOROBENZENE
  2. WATER

VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
K-VALUES: RAOULT'S LAW.

PROCEDURES:
 1.KVALUE        7.SHTCUT        11.RETREV        17.HELP
 2.ENTHALPY      8.COLUMN        12.SYSTEM        18.STOP
 3.PHASE         9.CERDA         13.DEFINE        19.TIME AND DATE
 4.FLASH        10.COLCST        14.STORE
 5.ABSEDM       21.HEX           15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

HEAT EXCHANGER CALCULATION

ENTER INPUT PARAMETERS
+(TH1,TH2,TC1,TC2,N,HO,HDO,HDI,HI,DI,DO
  SL,NTP,PT,B,Y,DE,MCOMP,KH,KC,VISH,VISC
  TETA,FLAG,EPS,SWCH,SWCH1,SWCH2,CPL)

+:
+:
+:
+:
+:
```

```
HEAT EXCHANGER RESULTS



     UD=      503.5828 J/(S*M**2*K)

     A=       30.1099M**2

     L=      504.4358 M

     NT=         104.0

     DIS=     299.8245MM

     HI=    6205.6770 J/(S*M**2*K)

     HO=     889.2119 J/(S*M**2*K)

     TW=      310.3115KELVIN

     F=          .9660

     CHTD=       56.2673 KELVIN


REPEAT? ( Y OR N ):
? SYSTEM IS UNDEFINED

 PROCEDURES:
  1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
  2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
  3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
  4.FLASH        10.COLCST       14.STORE
  5.ABSEDM       21.HEX          15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:
   PROGRAM IS STOPPED
```

```
11
PUBDAT
N
HYDROGEN CHLORIDE
BENZENE
CHLOROBENZENE
WATER

12
113
001002003
5
TT=326.37,TB=401.33,P=2.17,LT=100.68,VB=100.0,N=3,
XT=0.,0.0006683,0.99,YB=0.10,0.40,0.50;
N
6
RATIO=1.3,ALPHA=3.878,Q=1,ETA=1,XF=0.2101,XD=0.9975,
F=190.2,D=40.056;
N
12
113
003004
21
TH1=425.9,TH2=321.88,TC1=299.6,TC2=305.2,N=1,HO=1570,HDO=5000,
HDI=1666,HI=6550,DI=16.5,DO=19,SL=4.38,NTP=2,PT=23.8,
B=305,Y=4.76,DE=14,MCOMP=4.694,15.145,KH=.1303,KC=.616,
VISH=.32,VISC=.85,TETA=0.,0.,
FLAG=1,EPS=.01,SWCH=0,SWCH1=0,SWCH2=0,CPL=178.8,75.5;
N
18
20.20.09.UCLP, BU, P04     ,        0.311KLNS.
```

INPUT Data File of <u>CASE 6</u>.

```
 DESRAC 5.8 (6-APR-81)

 PROCEDURES:
  1.KVALUE         7.SHTCUT       11.RETREV        17.HELP
  2.ENTHALPY       8.COLUMN       12.SYSTEM        18.STOP
  3.PHASE          9.CERDA        13.DEFINE        19.TIME AND DATE
  4.FLASH         10.COLCST       14.STORE
  5.ABSEDM        21.HEX          15.ACTFIT
  6.MCCABE        22.EXT

 SELECT PROCEDURE:

 RETREV - RETRIEVE PHYSICAL CONSTANTS FROM DISK FILES

 ENTER NAME OF FILE (RETURN FOR PUBLIC DATA):
+DATA WILL BE RETRIEVED FROM FILE PUBDAT
 RETRIEVE ALL COMPONENTS FROM FILE? (Y OR N):

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  1 IS HYDROGEN CHLORIDE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  2 IS BENZENE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  3 IS CHLOROBENZENE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  4 IS WATER

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
 LIBRARY IS REDEFINED.  SYSTEM IS UNDEFINED.

 PROCEDURES:
  1.KVALUE         7.SHTCUT       11.RETREV        17.HELP
  2.ENTHALPY       8.COLUMN       12.SYSTEM        18.STOP
  3.PHASE          9.CERDA        13.DEFINE        19.TIME AND DATE
  4.FLASH         10.COLCST       14.STORE
  5.ABSEDM        21.HEX          15.ACTFIT
  6.MCCABE        22.EXT

 SELECT PROCEDURE:

 SYSTEM - DEFINE COMPONENTS IN SYSTEM

 MODELS FOR VAPOR ENTHALPY HV:
   1. IDEAL SOLUTION OF PERFECT GASES.
   2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
   3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR LIQUID ENTHALPY HL:
   1. IDEAL SOLUTION OF SATURATED LIQUIDS.
   2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
   3. EXCESS ENTHALPY FROM WILSON EQUATION.
   4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR VLE CALCULATIONS:
   1. LIQUID: WILSON ACTIVITY;VAPOR: VIRIAL EQN OF STATE.
   2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
   3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

 SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
 SELECT COMPONENTS (0 FOR HELP):
```

CASE 7 - Computer Output of the Flowsheet (e) of Figure 4.2
(Number of stages in the absorber is increased).

```
SELECTED COMPONENTS:
  1. HYDROGEN CHLORIDE
  2. BENZENE
  3. CHLOROBENZENE

VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
K-VALUES: RAOULT'S LAW.

PROCEDURES:
 1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH        10.COLCST       14.STORE
 5.ABSEDM       21.HEX          15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

ABSEDM - GAS ABSORPTION (EDMISTER METHOD)

ENTER INPUT PARAMETERS (TT/TB/P/LT/VB/N/XT/YB ;  )

+:
+:


ABSEDM RESULTS
 TT = 326.370      LT =  100.68      VT =  10.161
 TB = 401.330      VB =  100.00      LB =  190.52
  P =   2.170
  N =   6

  I  COMPONENT            XT(I)   XB(I)     YT(I)   YB(I)     XIT(I)   XIB(I)
  1. HYDROGEN CHLORI      .0000   .0011     .9629   .1000    1.00000   .02162
  2. BENZENE              .0007   .2103     .0003   .4000     .03448   .99999
  3. CHLOROBENZENE        .9993   .7886     .0369   .5000     .00372  1.00000

REPEAT? (Y OR N):

PROCEDURES:
 1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH        10.COLCST       14.STORE
 5.ABSEDM       21.HEX          15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

MCCABE - MCCABE-THIELE BINARY DISTILLATION

ENTER INPUT PARAMETERS (RATIO/ALPHA/Q/ ETA /XF/XD/F/D ;  )

+:
+:


MCCABE INPUT PARAMETERS
 RATIO = 1.30             XF =  .2105
 ALPHA = 3.878            XD =  .9975
     Q = 1.000             F =   190.31
   ETA = 1.000             D =   40.056
```

```
MCCABE RESULTS
    XW =    .0007       LB =    275.82
     W =    150.25      VB =    125.56
     L =    85.505      NT =      9
     V =    125.56      NB =    11


REPEAT? (Y OR N):

PROCEDURES:
 1.KVALUE         7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY       8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE          9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH         10.COLCST       14.STORE
 5.ABSEDM        21.HEX          15.ACTFIT
 6.MCCABE        22.EXT

SELECT PROCEDURE:

SYSTEM - DEFINE COMPONENTS IN SYSTEM

MODELS FOR VAPOR ENTHALPY HV:
  1. IDEAL SOLUTION OF PERFECT GASES.
  2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
  3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR LIQUID ENTHALPY HL:
  1. IDEAL SOLUTION OF SATURATED LIQUIDS.
  2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
  3. EXCESS ENTHALPY FROM WILSON EQUATION.
  4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR VLE CALCULATIONS:
  1. LIQUID: WILSON ACTIVITY;VAPOR: VIRIAL EQN OF STATE.
  2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
  3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
SELECT COMPONENTS (L FOR HELP):

SELECTED COMPONENTS:
  1. CHLOROBENZENE
  2. WATER

VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
K-VALUES: RAOULT'S LAW.

PROCEDURES:
 1.KVALUE         7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY       8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE          9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH         10.COLCST       14.STORE
 5.ABSEDM        21.HEX          15.ACTFIT
 6.MCCABE        22.EXT

SELECT PROCEDURE:

HEAT EXCHANGER CALCULATION

ENTER INPUT PARAMETERS
+(TH1,TH2,TC1,TC2,N,HO,HDO,HDI,HI,DI,DO
 SL,NTP,PT,B,Y,DE,MCOMP,KH,KC,VISH,VISC
 TETA,FLAG,EPS,SWCH,SWCH1,SWCH2,CPL)

+:
+:
+:
+:
+:
```

```
HEAT EXCHANGER RESULTS


        UD=       503.7109 J/(S*M**2*K)

        A=        30.1266M**2

        L=       504.7158 M

        NT=          104.0

        DIS=      299.8245MM

        HI=    6205.6770 J/(S*M**2*K)

        HO=      889.6077 J/(S*M**2*K)

        TW=       310.3146KELVIN

        F=           .9660

        CMTD=        56.2678 KELVIN

REPEAT? ( Y OR N ):
? SYSTEM IS UNDEFINED

 PROCEDURES:
  1.KVALUE        7.SHTCUT       11.RETREV       17.HELP
  2.ENTHALPY      8.COLUMN       12.SYSTEM       18.STOP
  3.PHASE         9.CERDA        13.DEFINE       19.TIME AND DATE
  4.FLASH        10.COLCST       14.STORE
  5.ABSEDM       21.HEX          15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:
   PROGRAM IS STOPPED
```

```
11
PUBDAT
N
HYDROGEN CHLORIDE
BENZENE
CHLOROBENZENE
WATER

12
113
001002003
5
TT=326.37,TB=401.33,P=2.17,LT=100.68,VB=100.0,N=6,
XT=0.,0.0006683,0.99,YB=0.10,0.40,0.50;
N
6
RATIO=1.3,ALPHA=3.878,Q=1,ETA=1,XF=0.21053,XD=0.9975,
F=190.31,D=40.056;
N
12
113
003004
21
TH1=425.9,TH2=321.88,TC1=299.6,TC2=305.2,N=1,HQ=1570,HDO=5000,
HDI=1666,HI=6550,DI=16.5,DO=19,SL=4.88,NTP=2,PT=23.8,
B=305,Y=4.76,DE=14,MCOMP=4.6978,15.145,KH=.1308,KC=.616,
VISH=.32,VISC=.85,TETA=0.,0.,
FLAG=1,EPS=.01,SWCH=0,SWCH1=0,SWCH2=0,CPL=178.8,75.5;
N
18
20.23.12.UCLP, BU, PC4     ,       0.311KLNS.
```

INPUT Data File of CASE 7.

```
 DESPAC 5.8 (6-APR-81)

 PROCEDURES:
  1.KVALUE          7.SHTCUT        11.RETREV         17.HELP
  2.ENTHALPY        8.COLUMN        12.SYSTEM         18.STOP
  3.PHASE           9.CERDA         13.DEFINE         19.TIME AND DATE
  4.FLASH          10.COLCST        14.STORE
  5.ABSEDM         21.HEX           15.ACTFIT
  6.MCCABE         22.EXT

 SELECT PROCEDURE:

 RETREV - RETRIEVE PHYSICAL CONSTANTS FROM DISK FILES

 ENTER NAME OF FILE (RETURN FOR PUBLIC DATA):
+DATA WILL BE RETRIEVED FROM FILE PUBDAT
 RETRIEVE ALL COMPONENTS FROM FILE? (Y OR N):

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  1 IS HYDROGEN CHLORIDE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  2 IS BENZENE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  3 IS CHLOROBENZENE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  4 IS WATER

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
 LIBRARY IS REDEFINED.  SYSTEM IS UNDEFINED.

 PROCEDURES:
  1.KVALUE          7.SHTCUT        11.RETREV         17.HELP
  2.ENTHALPY        8.COLUMN        12.SYSTEM         18.STOP
  3.PHASE           9.CERDA         13.DEFINE         19.TIME AND DATE
  4.FLASH          10.COLCST        14.STORE
  5.ABSEDM         21.HEX           15.ACTFIT
  6.MCCABE         22.EXT

 SELECT PROCEDURE:

 SYSTEM - DEFINE COMPONENTS IN SYSTEM

 MODELS FOR VAPOR ENTHALPY HV:
   1. IDEAL SOLUTION OF PERFECT GASES.
   2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
   3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR LIQUID ENTHALPY HL:
   1. IDEAL SOLUTION OF SATURATED LIQUIDS.
   2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
   3. EXCESS ENTHALPY FROM WILSON EQUATION.
   4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR VLE CALCULATIONS:
   1. LIQUID: WILSON ACTIVITY/VAPOR: VIRIAL EQN OF STATE.
   2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
   3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

 SELECT MODELS FOR HV/HL/VLE (   BLANK THEN RETURN FOR 1 1 1):
 SELECT COMPONENTS (0 FOR HELP):
```

CASE 8 - Computer Output of the Flowsheet (e) of Figure 4.2
(Solvent flow rate is increased).

```
SELECTED COMPONENTS:
  1. HYDROGEN CHLORIDE
  2. BENZENE
  3. CHLOROBENZENE

VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
K-VALUES: RAOULT'S LAW.

PROCEDURES:
 1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH        10.COLCST       14.STORE
 5.ABSEDM       21.HEX          15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

ABSEDM - GAS ABSORPTION (EDMISTER METHOD)

ENTER INPUT PARAMETERS (TT/TB/P/LT/VB/N/XT/YB ;  )

+:
+:


ABSEDM RESULTS
 TT = 326.370      LT =  110.68     VT =  10.216
 TB = 401.330      VB =  100.00     LB =  200.46
  P =   2.170
  N =   3

  I  COMPONENT           XT(I)    XB(I)     YT(I)    YB(I)     XIT(I)    XIB(I)
  1. HYDROGEN CHLORI     .0000    .0012     .9562    .1000     .99961    .02316
  2. BENZENE             .0007    .1995     .0072    .4000     .03091    .99822
  3. CHLOROBENZENE       .9993    .7993     .0366    .5000     .00338    .99999


REPEAT? (Y OR N):

PROCEDURES:
 1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH        10.COLCST       14.STORE
 5.ABSEDM       21.HEX          15.ACTFIT
 6.MCCABE       22.EXT

SELECT PROCEDURE:

MCCABE - MCCABE-THIELE BINARY DISTILLATION

ENTER INPUT PARAMETERS (RATIO/ALPHA/Q/ ETA /XF/XD/F/D ;  )

+:
+:


MCCABE INPUT PARAMETERS
 RATIO = 1.30            XF =  .1998
 ALPHA = 3.878           XD =  .9975
     Q = 1.000            F =   200.22
   ETA = 1.000            D =   40.056
```

```
MCCABE RESULTS
    XW =   .0003        LB =    290.33
     W =    160.16      VB =    130.17
     L =    90.112      NT =     9
     V =    130.17      NB =    13


REPEAT? (Y OR N):

PROCEDURES:
 1.KVALUE         7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY       8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE          9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH         10.COLCST       14.STORE
 5.ABSEDM        21.HEX          15.ACTFIT
 6.MCCABE        22.EXT

SELECT PROCEDURE:

SYSTEM - DEFINE COMPONENTS IN SYSTEM

MODELS FOR VAPOR ENTHALPY HV:
  1. IDEAL SOLUTION OF PERFECT GASES.
  2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
  3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR LIQUID ENTHALPY HL:
  1. IDEAL SOLUTION OF SATURATED LIQUIDS.
  2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
  3. EXCESS ENTHALPY FROM WILSON EQUATION.
  4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

MODELS FOR VLE CALCULATIONS:
  1. LIQUID: WILSON ACTIVITY;VAPOR: VIRIAL EQN OF STATE.
  2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
  3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

SELECT MODELS FOR HV,HL,VLE (   BLANK THEN RETURN FOR 1 1 1):
SELECT COMPONENTS (0 FOR HELP):

SELECTED COMPONENTS:
  1. CHLOROBENZENE
  2. WATER

VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
K-VALUES: RAOULT'S LAW.

PROCEDURES:
 1.KVALUE         7.SHTCUT       11.RETREV        17.HELP
 2.ENTHALPY       8.COLUMN       12.SYSTEM        18.STOP
 3.PHASE          9.CERDA        13.DEFINE        19.TIME AND DATE
 4.FLASH         10.COLCST       14.STORE
 5.ABSEDM        21.HEX          15.ACTFIT
 6.MCCABE        22.EXT

SELECT PROCEDURE:

HEAT EXCHANGER CALCULATION

ENTER INPUT PARAMETERS
+(TH1,TH2,TC1,TC2,N,HO,HDO,HDI,HI,DI,DO
  SL,NTP,PT,B,Y,DE,MCOMP,KH,KC,VISH,VISC
  TETA,FLAG,EPS,SWCH,SWCH1,SWCH2,CPL)

+:
+:
+:
+:
+:
```

```
HEAT EXCHANGER RESULTS



          UD=       508.1460 J/(S*M**2*K)

          A=        31.8165M**2

          L=      533.0271 M

          NT=          110.0

          DIS=      307.2684MM

          HI=    5933.3736 J/(S*M**2*K)

          HO=     908.8053 J/(S*M**2*K)

          TW=       310.7928KELVIN

          F=           .9660

          CMTD=        56.2678 KELVIN


REPEAT? ( Y OR N ):
? SYSTEM IS UNDEFINED

 PROCEDURES:
  1.KVALUE        7.SHTCUT       11.RETREV       17.HELP
  2.ENTHALPY      8.COLUMN       12.SYSTEM       18.STOP
  3.PHASE         9.CERDA        13.DEFINE       19.TIME AND DATE
  4.FLASH        10.COLCST       14.STORE
  5.ABSEDM       21.HEX          15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:
   PROGRAM IS STOPPED
```

```
11
PUBDAT
N
HYDROGEN CHLORIDE
BENZENE
CHLOROBENZENE
WATER

12
113
001002003
5
TT=326.37,TB=401.33,P=2.17,LT=110.68,VB=100.0,N=3,
XT=0.,0.0006683,0.99,YB=0.10,0.40,0.50;
N
6
RATIO=1.3,ALPHA=3.878,Q=1,ETA=1,XF=0.1998,XD=0.9975,
F=200.218,D=40.056;
N
12
113
003004
21
TH1=425.9,TH2=321.88,TC1=299.6,TC2=305.2,N=1,HO=1570,HDO=5000,
HDI=1666,HI=6550,DI=16.5,DO=19,SL=4.88,NTP=2,PT=23.8,
B=305,Y=4.76,DE=14,KCOMP=5.005,15.145,KH=.1308,KC=.616,
VISH=.32,VISC=.85,TETA=0.,0.,
FLAG=1,EPS=.01,SWCH=0,SWCH1=0,SWCH2=0,CPL=178.8,75.5;
N
18
20.27.34.UCLP, BU, PC4     ,       0.311KLNS.
```

INPUT Data File of CASE 8.

```
 DESPAC 5.8 (6-APR-81)

 PROCEDURES:
  1.KVALUE        7.SHTCUT        11.RETREV        17.HELP
  2.ENTHALPY      8.COLUMN        12.SYSTEM        18.STOP
  3.PHASE         9.CERDA         13.DEFINE        19.TIME AND DATE
  4.FLASH        10.COLCST        14.STORE
  5.ABSEDM       21.HEX           15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:

 RETREV - RETRIEVE PHYSICAL CONSTANTS FROM DISK FILES

 ENTER NAME OF FILE (RETURN FOR PUBLIC DATA):
+DATA WILL BE RETRIEVED FROM FILE PUBDAT
 RETRIEVE ALL COMPONENTS FROM FILE? (Y OR N):

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  1 IS HYDROGEN CHLORIDE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  2 IS BENZENE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  3 IS CHLOROBENZENE

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
+COMPONENT  4 IS WATER

 NAME COMPONENT TO BE RETRIEVED (RETURN TO END):
 LIBRARY IS REDEFINED.  SYSTEM IS UNDEFINED.

 PROCEDURES:
  1.KVALUE        7.SHTCUT        11.RETREV        17.HELP
  2.ENTHALPY      8.COLUMN        12.SYSTEM        18.STOP
  3.PHASE         9.CERDA         13.DEFINE        19.TIME AND DATE
  4.FLASH        10.COLCST        14.STORE
  5.ABSEDM       21.HEX           15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:

 SYSTEM - DEFINE COMPONENTS IN SYSTEM

 MODELS FOR VAPOR ENTHALPY HV:
   1. IDEAL SOLUTION OF PERFECT GASES.
   2. RESIDUAL ENTHALPY FROM VIRIAL EQUATION OF STATE.
   3. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR LIQUID ENTHALPY HL:
   1. IDEAL SOLUTION OF SATURATED LIQUIDS.
   2. IDEAL SOLUTION WITH PRESSURE CORRECTION.
   3. EXCESS ENTHALPY FROM WILSON EQUATION.
   4. RESIDUAL ENTHALPY FROM REDLICH-KWONG EQUATION.

 MODELS FOR VLE CALCULATIONS:
   1. LIQUID: WILSON ACTIVITY/VAPOR: VIRIAL EQN OF STATE.
   2. PRAUSNITZ-CHUEH VERSION OF REDLICH-KWONG EQUATION.
   3. LIQUID: IDEAL SOLUTION, ANTOINE EQUATION ;
VAPOR: DALTON'S LAW.

 SELECT MODELS FOR HV/HL/VLE (   BLANK THEN RETURN FOR 1 1 1):
 SELECT COMPONENTS (U FOR HELP):
```

Computer Output of the Flowsheet (a) of Figure 4.2.

```
 SELECTED COMPONENTS:
   1. HYDROGEN CHLORIDE
   2. BENZENE
   3. CHLOROBENZENE

 VAPOR ENTHALPY: IDEAL SOLUTION OF PERFECT GASES.
 LIQUID ENTHALPY: IDEAL SOLUTION OF SATURATED LIQUIDS.
 K-VALUES: RAOULT'S LAW.

 PROCEDURES:
  1.KVALUE        7.SHTCUT       11.RETREV        17.HELP
  2.ENTHALPY      8.COLUMN       12.SYSTEM        18.STOP
  3.PHASE         9.CERDA        13.DEFINE        19.TIME AND DATE
  4.FLASH        10.COLCST       14.STORE
  5.AESEDM       21.HEX          15.ACTFIT
  6.MCCABE       22.EXT

 SELECT PROCEDURE:

 FLASH CALCULATIONS

 SELECT TYPE OF FLASH:

+1.PQ 2.TQ 3.GV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :
 ENTER INPUT PARAMETERS
+(T,P,Z,(GUESS,X,Y,V) ;  )

+:


 FLASH RESULTS
  HF =  4.2918E+04       T = 405.200
  HL =  3.7698E+04       P =   2.380
  HV =  4.8216E+04       V =   .4963

  I  COMPONENT            X(I)     Y(I)    Z(I)     XI(I)        K(I)
  1. HYDROGEN CHLORI     .0019    .1995   .1000    .9904       104.2
  2. BENZENE             .3006    .5009   .4000    .6215       1.666
  3. CHLOROBENZENE       .6975    .2996   .5000    .2974       .4295

 REPEAT? (Y OR N):
+1.PQ 2.TQ 3.GV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :
 ENTER INPUT PARAMETERS
+(T,P,Z,HF,(GUESS,X,Y,V) ;  )

+:


 FLASH RESULTS
  HF =  4.2918E+04       T = 405.200
  HL =  3.7698E+04       P =   2.380
  HV =  4.8216E+04       V =   .4963
   Q =  9.6915E-02

  I  COMPONENT            X(I)     Y(I)    Z(I)     XI(I)        K(I)
  1. HYDROGEN CHLORI     .0019    .1995   .1000    .9904       104.2
  2. BENZENE             .3006    .5009   .4000    .6215       1.666
  3. CHLOROBENZENE       .6975    .2996   .5000    .2974       .4295

 REPEAT? (Y OR N):
+1.PQ 2.TQ 3.GV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :
 ENTER INPUT PARAMETERS
+(T,P,Z,(GUESS,X,Y,V) ;  )
```

```
+:


 FLASH RESULTS
  HF =   3.7025E+04       T  = 394.100
  HL =   4.0003E+04       P  =   2.380
  HV =   3.5794E+04       V  =    .7075

  I   COMPONENT              X(I)     Y(I)     Z(I)     XI(I)        K(I)
  1.  HYDROGEN CHLORI       .0031    .2807    .1995    .9955       91.42
  2.  BENZENE               .4159    .5361    .5009    .7571       1.289
  3.  CHLOROBENZENE         .5810    .1832    .2996    .4326       .3153


 REPEAT? (Y OR N):
+1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :
 ENTER INPUT PARAMETERS
+(T,P,Z,HF,(GUESS,X,Y,V) ;   )

+:


 FLASH RESULTS
  HF =   3.7025E+04       T  = 394.100
  HL =   4.0017E+04       P  =   2.380
  HV =   3.5867E+04       V  =    .7094
   Q =   4.7688E+01

  I   COMPONENT              X(I)     Y(I)     Z(I)     XI(I)        K(I)
  1.  HYDROGEN CHLORI       .0031    .2803    .1998    .9955       91.42
  2.  BENZENE               .4163    .5366    .5016    .7589       1.289
  3.  CHLOROBENZENE         .5806    .1831    .2986    .4350       .3153


 REPEAT? (Y OR N):
+1.PQ 2.TQ 3.QV 4.TV 5.PV 6.TP 7.ENTHALPY 8.DONE :

 PROCEDURES:
  1.KVALUE         7.SHTCUT        11.RETREV        17.HELP
  2.ENTHALPY       8.COLUMN        12.SYSTEM        18.STOP
  3.PHASE          9.CERDA         13.DEFINE        19.TIME AND DATE
  4.FLASH         10.COLCST        14.STORE
  5.ABSEDM        21.HEX           15.ACTFIT
  6.MCCABE        22.EXT

 SELECT PROCEDURE:
   PROGRAM IS STOPPED
```

```
11
PUBDAT
N
HYDROGEN CHLORIDE
BENZENE
CHLOROBENZENE
WATER

12
113
00100 2003
4
7
T=405.2,P=2.38,Z=10,40,50;
N
6
T=405.2,P=2.38,Z=10,40,50,HF=42918;
N
7
T=394.1,P=2.38,Z=9.902,24.862,14.87;
N
6
T=394.1,P=2.38,Z=9.902,24.862,14.8,HF=37025;
N
8
18
18.43.19.UCLP, EU, FU4    ,       0.241KLNS.
```

INPUT Data File for Flowsheet (a) of Figure 4.2.

APPENDIX I

THE INPUT DATA REQUIRED FOR THE PROCESS FLOWSHEET DEVELOPMENT EXAMPLE

APPENDIX I

The Input Data Required for the Process Flowsheet Development Example

The input data required for the process flowsheet development example is obtained from FLOWTRAN [15].

ABSORBER UNIT:

The temperature at the top of the absorber = 128°F (326.37°K)

The temperature at the bottom of the absorber = 263°F (401.33°K)

Pressure = 32 psia (2.17 bar)

Solvent used in the absorber = Mainly MCB

Flowrate of solvent = 100.68 kmol/h

Composition of the solvent = 0.067281 kmol/h of benzene
100.61 kmol/h MCB

Number of theoretical stages = 3

DISTILLATION UNIT:

Distillate rate = 40.056 kmol/h

Bottom product rate = 150.26 kmol/h

Column pressure = 25 psia (1.7 bar)

Number of theoretical stages = 20

Quality of feed = 1 (saturated liquid)

HEAT EXCHANGER:

Hot stream inlet temperature = 307.36°F (425.9°K)

Hot stream outlet temperature = 120°F (321.88°K)

Cooling fluid = water

Cold stream inlet temperature = 80°F (299.6°K)

Cold stream outlet temperature =90°F (305.2°K)