

AN INTERACTIVE FACILITY FOR THERMODYNAMIC  
PROPERTY PREDICTIONS

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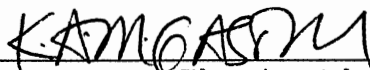
1989

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Oklahoma State University  
in partial fulfillment of  
the requirements for  
the Degree of  
MASTER OF SCIENCE  
JULY, 1992

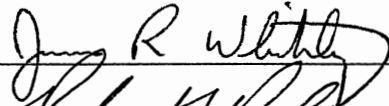
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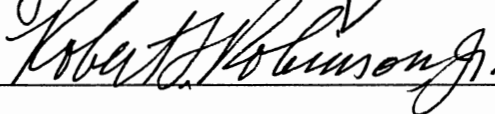
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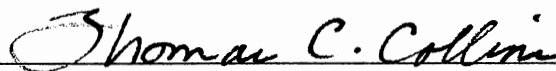
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## PREFACE

This study involves the development of an interactive facility for thermodynamic property prediction software GEOS (Generalized Equation of State). The interface was developed along with necessary on-line help documentation and graphics to enable the users to conveniently explore the various aspects of phase behavior problem formulation and thermodynamic property prediction.

I extend my sincere thanks to my advisor Dr. K. A. M. Gasem, for introducing me to this area of work and his continued guidance during the different stages of the development of the software. I deem it my privilege to work under his supervision.

I would like to thank Dr. R. L. Robinson, Jr., for his recommendations and critical assessment of this work. Dr. Rob Whitely, as the third member of my committee, has reviewed this work and his comments are greatly appreciated.

My appreciation goes to my wife for her patience during my entire tenure in this institution. I am also grateful to my mother and my in-laws for their moral encouragement at times when I needed it most.

Finally, I would like to gratefully acknowledge the financial support received from the School of Chemical Engineering.



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## NOMENCLATURE

A,B	cubic equation of state parameters; Helmholtz energy, kJ/Mole
AAD	arithmetic average of the absolute values of the deviation of n observations about the mean
a	activity; equation of state cohesive energy parameter
BIAS	arithmetic average of deviations of n observations
b	equation of state covolume parameter
C	number of components
$C_{ij}$	equation of state binary interaction parameter
$D_{ij}$	equation of state binary interaction parameter
D	phase density, gm/cc
DEV	deviation of the calculated value from experimental value, $X_{calc} - X_{exp}$
E1..E4	activity coefficient parameters
F	number of degrees of freedom
f	fugacity, bar
G	specific Gibbs free energy, kJ/mole
H	enthalpy, kJ/mole
$K_i$	equilibrium constant for component i
L	total moles of liquid
N	total number of moles
NPTS	number of points
P,p	pressure, bar
Q	group area parameter

$Q_k$  surface parameter in the UNIFAC equation  
 $q_i$  pure component parameter in the UNIFAC equation  
 $R$  gas constant  
 $R_k$  group volume parameter in the UNIFAC equation  
 RMSE root mean square error  
 $S$  entropy, kJ/mole/K  
 $T$  temperature, K  
 $U$  internal energy, kJ/mole  
 $v, V$  molar volume; total moles of vapor  
 $\mu$  chemical potential  
 $U, W$  constants in generalized form of cubic EOS  
 $x_i$  liquid mole fraction of component  $i$   
 $y_i$  vapor mole fraction of component  $i$   
 $z_i$  feed mole fraction of component  $i$   
 $Z$  compressibility factor  
 $z$  lattice coordination number in UNIFAC equation

### Greek Letters

$\gamma_i$  activity coefficient of component  $i$   
 $\theta$  area fraction  
 $\psi$  group interaction parameter  
 $\Lambda_{ij}$  Wilson Parameter, Table II  
 $\Lambda_{ji}$  Wilson Parameter, Table II  
 $\lambda_{ij}$  exponential parameters in Wilson equation, cal/gmol, Table II  
 $\lambda_{ji}$  exponential parameters in Wilson equation, cal/gmol, Table II  
 $\Phi_i$  segment fraction

## CHAPTER I

### INTRODUCTION

Phase equilibrium and volumetric properties are essential in many chemical engineering operations. Numerous separation processes such as distillation, absorption and extraction involve the transfer of chemical species between coexisting liquid and vapor phases. Rational design, operation, simulation, and optimization of such a process require the knowledge of equilibrium compositions of the existing phases over wide ranges of operating conditions of temperature and pressure. In the absence of reliable theoretical predictions, one has to resort to either experimental data or to thermodynamic correlations derived from such data.

This study is concerned with the development of an interactive facility for the thermodynamic property prediction software entitled GEOS (Gasem, 1988).

GEOS is a thermodynamic software for calculating volumetric and phase equilibrium properties. A generalized cubic equation of state and a number of activity coefficient models have been incorporated into the software to allow for flexible formulation and solution of realistic phase equilibrium problems of nonelectrolyte fluid mixtures.

The motivation for the development of an interactive



facility for GEOS is to develop a user-friendly educational tool supported by good graphics and help screens. Such a facility is specifically designed to enable users to conveniently explore the various aspects of phase behavior problem formulation and property prediction.

A computer interface can be developed by using a commercial interface development software or the computer language in which the application software has been developed. A market survey conducted for a suitable interfacing software resulted in the selection of "HI-SCREEN" by Softway, Inc. (1990), which is described in Chapter IV. The interface routines for GEOS.FOR were written mostly in Fortran. Functions requiring system calls, however, were written in 'C' computer language.

## CHAPTER II

### THERMODYNAMIC PRINCIPLES

#### Phase Equilibria

In this chapter, a brief review of the vapor-liquid phase equilibrium problem is presented. The main emphasis is on the use of both the single equation of state and the activity coefficient models for predicting equilibrium properties of nonelectrolyte fluids.

#### Equilibrium Criteria

The first and second laws of thermodynamics assert that, at equilibrium, the Gibbs free energy is minimum at a fixed temperature and pressure, or

$$(dG)_{T,p} \leq 0 \quad (2.1)$$

Based on the above statement, a criterion for equilibrium between two heterogeneous phases (liquid and vapor) may be given as:

$$T^V = T^L \quad (2.2)$$

$$P^V = P^L \quad (2.3)$$

$$\hat{\mu}_i^V = \hat{\mu}_i^L \quad (i = 1, N) \quad (2.4)$$

The component fugacity,  $\hat{f}_i$ , can be used in equilibrium calculations as a substitute for  $\mu_i$ , thus Equation 2.4 is replaced by

$$\hat{f}_i^V = \hat{f}_i^L \quad (i = 1, N) \quad (2.5)$$

The component fugacity in general is defined in terms of residual or excess functions, where:

$$\hat{f}_i = x_i \Phi_i P \quad (2.6)$$

or

$$\hat{f}_i = x_i \gamma_i \hat{f}_i^r \quad (2.7)$$

The fugacity coefficient,  $\Phi_i$ , and the activity coefficients,  $\gamma_i$ , are related to volumetric properties as

$$\ln \Phi_i = \frac{1}{RT} \int_0^P \left( \bar{v}_i - \frac{RT}{P} \right) dP \quad (2.8)$$

$$\ln \gamma_i = \frac{1}{RT} \int_0^P (\bar{v}_i - \bar{v}_i^L) dP \quad (2.9)$$

Where  $\bar{v}_i$  is the component partial molar volume and  $\bar{v}_i^L$  is the liquid molar volume of that component.

Using residual properties, i.e., the equation of state approach, Equation 2.6 is rewritten as:

$$\Phi_i^V P y_i = \Phi_i^L P x_i \quad (i = 1, N) \quad (2.10)$$

where  $\Phi_i$  is obtained from the equation of state models. While this approach works well for normal fluids at high pressure, when dealing with highly polar or associative

fluids, the split approach is preferred. In such a case, the component liquid phase fugacity is defined through the excess property  $\gamma_i$  and the vapor phase component fugacity using  $\hat{\phi}_i$ . Using Equation 2.7 to define the liquid phase fugacity, Equation 2.5 may be recast as

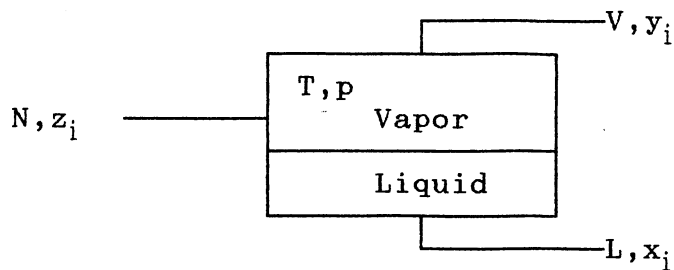
$$\hat{\phi}_i^V p y_i = \gamma_i f_i^R x_i \quad (i = 1, N) \quad (2.11)$$

where  $\gamma_i$  is obtained from activity coefficient models and the reference fugacity,  $f_i^R$ , is the ideal solution fugacity for the component.

The different thermodynamic models used in GEOS will be discussed in Chapter III.

### VLE Iteration Functions

The calculation of vapor-liquid equilibrium using an iteration function approach is discussed in this section. The general computational problem as shown below is that of vapor-liquid phase equilibrium. Given  $N$  moles of a fluid with composition  $z_i$ , at fixed  $T$  and  $p$ , the phase equilibrium problem is to determine whether or not the fluid is in the two-phase state, and, if so, to calculate the amount of liquid (L) and vapor (V) and their compositions ( $x_i$ 's and  $y_i$ 's), respectively (Gasem and Robinson, 1990).



Where

$z_i$  = feed composition at (T, p)

$x_i$  = Liquid phase composition

$y_i$  = Vapor phase composition

The overall and component molar material balance for the system shown above is

$$N = L + V \quad (2.12)$$

$$Nz_i = Lx_i + Vy_i \quad (2.13)$$

Where  $N$  = total moles

$L$  = amount in liquid phase, moles

$V$  = amount in vapor phase, moles

The "vapor-liquid equilibrium constant" or "K-value" for component "i" is defined as

$$K_i = \frac{y_i}{x_i} \quad (2.14)$$

Eliminating  $y_i$  from the molar material balance equation, we get

$$Nz_i = Lx_i + V(Kx_i) \quad (2.15)$$

Further, solving for  $x_i$  and  $y_i$  using Equation 2.13, we get

$$x_i = \frac{z_i}{\left(\frac{L}{N}\right) + \left[1 - \left(\frac{L}{N}\right)\right] K_i} \quad (2.16)$$

$$y_i = \frac{K_i z_i}{\left(\frac{L}{N}\right) + \left[1 - \left(\frac{L}{N}\right)\right] K_i} \quad (2.17)$$

At equilibrium

$$\sum_i x_i = \sum_i y_i = 1.0 \quad (2.18)$$

and

$$\sum_i (x_i - y_i) = 0 \quad (2.19)$$

or

$$F = \sum_i \frac{z_i (1 - K_i)}{\left(\frac{L}{N}\right) + \left[1 - \left(\frac{L}{N}\right)\right] K_i} = 0 \quad (2.20)$$

The above equation is called the Rice-Rachford iteration function for the flash calculation. The functional dependence of  $F$  on  $(L/N)$  is given for various states of the fluid (Gasem and Robinson, 1990) as

1.  $F > 0$  for  $0 \leq (L/N) \leq 1$       the fluid is a subcooled liquid at  $T, p$
2.  $F = 0$  at  $(L/N) = 1.0$       the fluid is at its bubble point at  $T, p$
3.  $F = 0$  for  $(L/N) 0 < (L/N) < 1$       the fluid is two phase at  $T, p$  with the molar fraction of liquid given by  $(L/N)$
4.  $F = 0$  at  $(L/N) = 0$ , or  $V = N$       the fluid is at its dew point at  $T, p$
5.  $F < 0$  for  $0 \leq (L/N) \leq 1$       the fluid is a superheated vapor at  $T, p$

The dew point iteration function is given as

$$\sum_I \frac{z_i}{K_i} = 1.0 \quad (2.21)$$

Which expresses the fact that  $[(L/N) = 0.0]$

Similarly, the bubble point iteration function is derived as

$$\sum_I z_i K_i = 1.0 \quad (2.22)$$

for the limiting condition  $(L/N) = 1.0$

### Calculation Procedure

The flash calculation procedure used to characterize a two-phase system at a given T and p is as follows:

1. Estimate initial K-values for first iteration,

where 
$$K_i = \frac{y_i}{x_i}$$

2. Calculate  $\sum_I K_i z_i$  ; if
  - < 1.0, all liquid
  - = 1.0, bubble-point fluid
  - > 1.0, proceed to step 3

3. Calculate  $\sum_I \frac{z_i}{K_i}$  ; if
  - < 1.0, all vapor
  - = 1.0, dew-point
  - > 1.0, proceed to 4

4. Both  $\sum_I K_i z_i$  and  $\sum_I \frac{z_i}{K_i}$  are > 1.0, thus the mixture is in the two-phase region.

5. Solve Equation 2.20 for  $L/N$
6. Calculate  $x_i$ 's and  $y_i$ 's from Equation 2.16 and 2.17.
7. Calculate  $v^v, v^L$ .
8. Calculate  $\hat{\phi}_i^v$  and  $\hat{\phi}_i^L$  for all  $i$ .
9. Calculate  $K_i^+$ , where

$$K_i^+ = \frac{\hat{\phi}_i^L}{\hat{\phi}_i^v}$$

or

$$K_i^+ = \frac{\gamma_i f_i^r}{\hat{\phi}_i^v P}$$

10. Check if  $K_i^+$  (step 9) =  $K_i$  (step 1). If so, stop,  
otherwise set  $K_i = K_i^+$  and repeat steps 2-10.

The flow diagrams for the flash calculation procedure, the bubble and dew point procedures are outlined in Appendix A.



## CHAPTER III

### THERMODYNAMIC MODELS

In this chapter the equation of state models and the activity coefficient models used in the GEOS program are briefly described.

#### Equation of State Models

The generic expression for the currently popular cubic equations of state is given in this general form (Abbot, 1979):

$$P = \frac{RT}{v-b} - \frac{a}{v^2 + Ubv + Wb^2} \quad (3.1)$$

The definitions of  $a$ ,  $b$ ,  $U$ , and  $W$  are specified for the various equations of state in Table I (Gasem, 1986). For mixtures, the following mixing rules are applied:

$$a = \sum_i \sum_j z_i z_j (a_{ii} a_{jj})^{\frac{1}{2}} (1 - C_{ij}) \quad (3.2)$$

$$b = \sum_i \sum_j z_i z_j \left( \frac{b_{ii} + b_{jj}}{2} \right) \quad (3.3)$$

where  $a_{ii}$ ,  $a_{jj}$ ,  $b_{ii}$ ,  $b_{jj}$  = pure component parameters,  
 $C_{ij}$  = binary interaction parameter,  
 $C_{ii}$ ,  $C_{jj}$  = 0.0, and  
 $z_i$  = mole fraction of component  $i$ .

TABLE I

## FEATURES OF GENERALIZED CUBIC EQUATION OF STATE

<i>EOS</i>	<i>U</i>	<i>W</i>	<i>a</i>	<i>b</i>	$\alpha$
<i>VDW</i>	0	0	$(\frac{27}{64}) (\frac{RT_c^2}{P_c})$	$\frac{RT_c}{8P_c}$	-
<i>RK</i>	1	0	$0.42748\alpha \frac{(RT_c)^2}{P_c}$	$0.08664 \frac{RT_c}{P_c}$	$T_r^{-0.5}$
<i>SRK</i>	1	0	$0.42728\alpha \frac{(RT_c)^2}{P_c}$	$0.08664 \frac{RT_c}{P_c}$	$\alpha_{SRK}$
<i>PR</i>	2	-1	$0.457235\alpha \frac{(RT_c)^2}{P_c}$	$0.077796 \frac{RT_c}{P_c}$	$\alpha_{PR}$

Where *VDW* = van der Waals  
*RK* = Redlich Kwong  
*SRK* = Soave-Redlich-Kwong  
*PR* = Peng-Robinson

$$\alpha_{SRK} = (1 + (0.485 + 1.574\omega - 0.176\omega^2) (1 - T_r^{0.5}))^2$$

$$\alpha_{PR} = (1 + (0.37646 + 1.54226\omega - 0.266772\omega^2) (1 - T_r^{0.5}))^2$$

## Activity Coefficient Models

Models for the activity coefficient,  $\gamma_i$ , must be specified in order to solve phase equilibrium problems using the VLE split approach. The activity coefficient models selected for inclusion in GEOS, as described in Table II, can be classified into three groups:

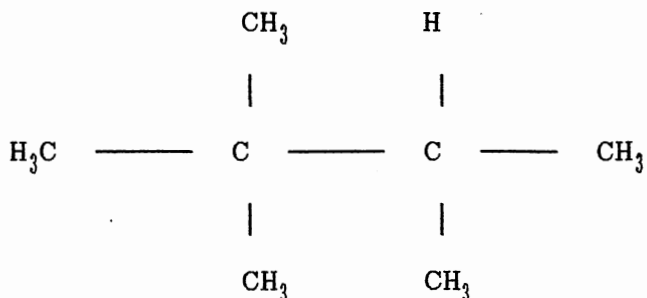
1. simple models,
2. multicomponents models, and
3. predictive models.

From among the historically important models, van Laar and the Margules equations have been chosen for this study because of their simplicity. The Wilson equation, which uses the local composition concept, is selected to perform predictions for both binary and multicomponent mixtures.

As shown in Table II, the van Laar, the Margules, and the Wilson models all require two regressed parameters per binary system. However, the Wilson model (1964) has several advantages; specifically, the equation's representation of highly nonideal systems is better than the other two models, it extends directly to multicomponent systems using only the binary parameters and is more capable of predicting activity coefficients at high dilution (less than 0.1 mole%).

A good predictive model utilizes existing phase equilibrium data to predict phase equilibria of systems for which no experimental data are available. Group contribution methods offer an attractive vehicle for the development of predictive models. Group contribution

methods typically express the phase behavior model parameters in terms of the sum of contributions from groups rather than molecules (Rasmussen, 1979). For example,



consists of

5 - CH<sub>3</sub> groups

1 - CH group

1 - C group

and similarly, benzene yields six aromatic CH (ACH) groups. This method can represent many mixtures in terms of only a few interactions. For example, "CH<sub>3</sub>", "CH<sub>2</sub>", and "OH" could describe all mixtures of n-paraffins and n-alcohols.

Some of the group contribution models which are in use include the ASOG (Analytic Solution Of Groups) method based on the Wilson equation (Wilson, 1962) and the UNIFAC (UNIQUAC Functional Group Activity Coefficients) method based on the UNIQUAC (Universal Quasi-Chemical) model (Abrams, 1975). The UNIFAC method is probably the more widely used method. In this method, there are two contributions to the activity coefficient: combinatorial (C) and residual (R) (Rasmussen, 1979). Thus, the UNIFAC equation is given as:

$$\ln \gamma_i = \ln \gamma_i^C + \ln \gamma_i^R \quad (3.1)$$

where

$$\ln \gamma_i^C = \ln \frac{\Phi_i}{x_i} + \frac{z}{2} q_i \ln \frac{\theta_i}{\Phi_i} + l_i - \frac{\Phi_i}{x_i} \sum_j x_j l_j \quad (3.2)$$

$$\ln \gamma_i^R = -q_i \left[ 1 - \ln \left( \sum_j \theta_j \tau_{ji} \right) - \frac{\sum_j (\theta_j \tau_{i,j} / \sum_k \theta_k \tau_{kj})}{\sum_k \theta_k \tau_{kj}} \right] \quad (3.3)$$

$$l_i = \frac{z}{2} (r_i - q_i) - (r_i - 1) ; z = 10 \quad (3.4)$$

$$\theta_i = \frac{q_i x_i}{\sum_j q_j x_j} ; \quad \Phi_i = \frac{r_i x_i}{\sum_j r_j x_j} \quad (3.5)$$

$$\tau_{ji} = \exp - \left( \frac{u_{ji} - u_{ii}}{R T} \right) \quad (3.6)$$

In the above equations,  $z$  is the lattice coordination number, a constant set equal to ten;  $x_i$  is the mole fraction of component  $i$ , and the summations in Equations 3.2, 3.3 and 3.5 are over all components, including component  $i$ ;  $\theta_i$  is the area fraction, and  $\Phi_i$  is the segment fraction, which is similar to the volume fraction. The two adjustable parameters,  $\tau_{ij}$  and  $\tau_{ji}$  appearing in Equation 3.3 must be evaluated from experimental phase equilibrium data. Pure component parameters,  $r_i$  and  $q_i$ , in Equation 3.4 are measures of molecular van der Waals volumes and molecular surface areas, they are determined as,

$$r_i = \sum_k v_k^{(i)} R_k \quad \text{and} \quad q_i = \sum_k v_k^{(i)} Q_k \quad (3.7)$$

where  $v_k^{(i)}$ , always an integer, is the number of groups of type  $k$  in molecule  $i$ .  $R_k$  and  $Q_k$  are group parameters which are given by Bondi (1968).

The version which has been currently implemented with GEOS is that of Freduslund (1982). The interaction parameters for prediction of vapor liquid equilibria are stored in the program GEOS.

A summary of the activity coefficient models used in this study is shown in Table II (Walas, 1985).

TABLE II  
ACTIVITY COEFFICIENTS MODELS EMPLOYED IN GEOS

---

BINARY MODELS	
<i>Margules</i>	$\ln \gamma_1 = [A_{12} + 2(A_{21} - A_{12})x_1]x_2^2$ $\ln \gamma_2 = [A_{21} + 2(A_{12} - A_{21})x_2]x_1^2$
<i>van Laar</i>	$\ln \gamma_1 = A_{12} \left( \frac{A_{21}x_2}{A_{12}x_1 + A_{21}x_2} \right)^2$ $\ln \gamma_2 = A_{21} \left( \frac{A_{12}x_1}{A_{12}x_1 + A_{21}x_2} \right)^2$
<i>Wilson</i>	$\ln \gamma_1 = -\ln(x_1 + \Lambda_{12}x_2) + x_2 \left( \frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{\Lambda_{21}x_1 + x_2} \right)$
<i>Wilson</i>	$\ln \gamma_2 = -\ln(x_1 + \Lambda_{21}x_2) + x_1 \left( \frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{\Lambda_{21}x_1 + x_2} \right)$
MULTICOMPONENT MIXTURE MODELS	
<i>Wilson</i>	$\ln \gamma_i = -\ln \left( \sum_{j=1}^m x_j \Lambda_{ij} \right) + 1 - \frac{\sum_{k=1}^m x_k \Lambda_{ki}}{\sum_{j=1}^m x_j \Lambda_{kj}}$
	$\Lambda_{ii} = \Lambda_{jj} = 1$
PREDICTIVE GROUP CONTRIBUTION MODEL	
<i>UNIFAC</i>	$\ln \gamma_i = \ln \gamma_i^C + \ln \gamma_i^R$
	$\ln \gamma_i^C$ given in Equation 3.2
	$\ln \gamma_i^R$ given in Equation 3.3

---

## CHAPTER IV

### LITERATURE REVIEW FOR INTERFACE DEVELOPMENT

A literature survey concerning the development of a user-friendly interface for GEOS was conducted. The search was focused on two areas of direct use in this study: (1) guidelines for interface design and (2) types of interface development software available.

#### Interface Design

One cannot mathematically derive an interface design from a set of equations. Moreover, it is difficult to define the characteristics of an interface in rigorous terms. In the absence of an accepted theory, seven design guidelines for the development of an effective interface are explained in the following section. The desired characteristics of interface design include (Newell, 1986),

1. putting the user in control,
2. addressing the users's level of skill and experience,
3. being consistent,
4. protecting the user from the inner workings of the hardware and software,
5. providing online documentation,



6. minimizing the burden on the user's memory, and
7. following the principles of good graphics design.

These guidelines have been roughly ordered based on their importance to the design of an effective interface. Since they have not been derived from a theory of human-computer interaction (Newell, 1986), there is no way to measure their relative importance. The guidelines at the top of the list, however, have a broader impact on the quality of the user interface than those at the bottom.

### User Control

The guideline of putting the user in control is most important. Making users feel that they are in control has two components: cognitive and behavioral. The cognitive component addresses the user's understanding of the structure of the software interface and his ability to predict its response to given directions. The word "direction" here refers to any means available to users that tells the software what has to be done (Newell, 1986), including menus, function keys, commands, etc. The behavioral component deals with the user's knowledge of what actions they need to perform to accomplish tasks.

An effective interface allows users to form an accurate and detailed cognitive representation of the structure of the software and to learn quickly how to operate it. A poor interface does just the opposite. It frustrates and confuses the user's attempts to understand it, which leaves the user in constant doubt about where they are in the

structure of the application; it makes users unsure that they can predict how the software will respond to their direction; it creates difficulties in operating the software; and makes it easy to make errors and difficult to recover from them.

Putting the user in control is the broadest and most important guideline. Many of the practices that are described below contribute to its importance. This includes providing,

1. online help that informs the users about the structure and operation of the application,
2. effective prompts and status messages that guide the user through procedures and keep them informed about program status,
3. error messages that allow the users to understand both what went wrong and how to recover from the error,
4. the means to move freely within and between screens and the ability to move easily to major selection menus and to quickly exit from the application or sub-section of the program, and
5. consistency in the use of words, formats and procedures.

### User's Skill and Experience

Most software is created by the people who are heavily involved in computer technology. From their point of view,

most applications do not come close to pushing the limits of the available technology.

On the other hand, most users are at the opposite end of the spectrum. While one may be familiar with an application area, their experience with computers can vary from having used a few basic applications to none at all. The percentage of people who have hands-on experience with computers is still relatively small as the availability of computers is still a factor. One of the most difficult problems for software developers is accommodating the limited computer skills of most users. If the software application developed will be used by people with virtually no computer experience, then its design must favor these users over the more experienced ones regardless of their computer skills. All users must, however, be aware of the technical aspects of the subject covered in the software.

This does not mean, however, that one must ignore the needs of the more experienced users. Such users need a design that takes advantage of their experience. They should be able to take shortcuts and should be provided with online documentation that jogs their memory when they need it rather than a lengthy explanation of basics.

The practices that contribute most to the above guidelines are

1. The interface must contain words, phrases, and examples that reflect the users point of view and not that of the developer. All computer terms and other technical jargon that are not familiar to

users must either be eliminated from the interface or explained to the user. In addition, the design must be subjected to a usability test to ensure that potential users understand the words contained in menus, messages, help text, and tutorials.

2. Use of appropriate transaction control procedures. The means by which users tell the software what they want to do must be compatible with their level of skill and experience with computers. New users will be most comfortable with menus or simple question and answer dialogue. Experienced users can use these methods, but they may want to be able to string together sequences of commands and use function keys to speed up the operation of an application.
3. Use of several levels of details for error and help messages. Experienced users need error and help messages to remind them of what they already know. New users, however, need step-by-step procedures and examples that instruct them in the operation of the application. The needs of both of these groups can be met by providing more than one level of help and error messages. The first level should be short and provide the essential information. At this level the user then has the option of accessing and displaying subsequent levels that are more detailed.

## Consistency

Consistency is an important feature that should be built into every interface and, whenever possible, it should be maintained across applications. Consistency helps the user to learn an application more easily, use it more easily, and recover more easily when there is a problem. In short, consistency is one of the factors that helps the user to feel in control of the software.

## Protecting User from Workings of the Software

The computer hardware which is used to help in ones work and play in the 1990s is both powerful and flexible. The general purpose computer allows users to create an unlimited number of applications to meet their needs. To take advantage of this flexibility, however, applications software are required to harness the power of the computer. An application software itself is created using a more basic set of software tools.

When an application is created, use is made of such software tools as a high level language, system utilities, various libraries, and a database manager to compliment it. These tools provide a buffer between the user and the registers, memories, and other components of the hardware. Consequently, the user does not have to deal with the details of machine operation directly.

The practices that contribute most to this principle are avoiding:

1. jargon, by using plain English rather than words and phrases that refer directly to the software tools one is using,
2. status messages such as "LINK MAIN" or "FORTRAN END" or " C END." These messages describe the inner workings of the software in terms that the user cannot interpret, and
3. passing error messages generated by the software tools directly to the user. Translating such messages to plain English first and then displaying them will enhance the usability.

### Online Help

An extensive, well-designed, and well-written online help system has now become an accepted goal of major software applications. Further, there is evidence that a well-designed help system improves the productivity of users and increases their satisfaction with a software product (Magers, 1983). Users should not have to search continually through a shelf of manuals to make their way through an application. Printed documentation is necessary to allow users to begin using an application. Once they have started, however, users should be able to complete most of their routine work with online documentation and, perhaps, a Quick Reference Guide included in the Help.

The online documentation that users need consists of more than just online help messages. All messages that are displayed are part of the online documentation. As we will

see in the later sections of this chapter, status messages, prompts, and error messages are also components of online documentation. These messages inform users about the status of the operation of the application completed or in progress, and they help them to know how to proceed and how to recover from errors. In short, these messages are critical contributors to giving the user a sense of being in control.

#### User's Memory.

Human beings are poor at recalling detailed information but are remarkably good at recognizing it (McNulty, 1965). In addition, the nature of the computer terminal screen puts an extra burden on a user's memory. Unlike working with printed documents or even working on the top of a desk, a computer application typically consists of a sequence of screens that users can display in various orders. When one screen is displayed, the others cannot be seen. Even when the technology allows the screen to display multiple windows, there is a limit to how much information can be displayed and used at one time. Consequently, the user of a computer application is often forced to memorize information and recall it later.

A good interface design should minimize the need for the user to memorize and later recall information. Whenever possible, users should be able to choose from lists so they can use their recognition memory rather than their primary recall memory. The widespread acceptance of menus as a

primary means to control the users interaction with the software is an example of an application of this principle.

There is more to minimizing memory load, however, than using menus. There are several other practices that also contribute to this principle:

1. Consistency in one's use of words, formats, and procedures for the layout of the screens.  
Consistency reduces the user's need to learn and remember new information. For example, when the same exit keys are used on all menus, a user has to learn it only once, and it is therefore easier to remember.
2. Display of status messages that remind users where they are in an application and what options are in effect. For example, the current option of the process selected can be displayed at the time of the execution of the problem.
3. Providing online help that is designed as an aid to memory. This helps users to remember information on infrequently used procedures or the details of a data entry format without having to search through their memory or a manual.
4. Use of memory aids in prompts and data entry captions. For example, telling users how to enter the data. Many of the details of the entry of the data in the respective screens are simply not important to the users of the information, so one quickly forgets them. But these details are



important to the software that stores and manages the data files information. One of the first things that new users learn about computers is that they must be careful about these details. A good interface design helps users with these details by including memory aids in messages that request information.

### Screen Layout

It is essential that one put a meaningful title at the top of every data display, menu, help, and data entry screen. Titles have an important function. Numerous research studies have shown that organizing features, such as titles, increase the comprehension and retention of information (Ausubel, 1978).

When creating a screen, one should start designing the general layout of the screen. The screen is designed using screen layout features such as semi-graphic characters, colors, frames, large fonts, shading, highlighting, etc.

In producing a magazine or a book, strict information layout practices are followed. For example, tables and figures are centered and informative headings, consistent in format, are used. These practices are not important only because of their aesthetic nature. A large amount of research had been done on the relationship between how information is displayed and how the users of the software, both good and poor, process it (Engel, 1975). An analysis

of this research indicates that there are principles of information display that help users to find what they want easily and to understand it. An effective interface must also follow these good information layout practices.

Displays should be formatted such that the users can find what they want with ease.

In general, displaying information on a terminal screen imposes additional constraints on the design of layouts. A screen is substantially smaller than the pages of most documents that accompany it. Also, the contrast on video screens is, in general, much poorer than the contrast available with printed documents. One cannot put as much information on a screen as there is in the document, but judicious organization of the screen will keep it as legible as possible. Finally, most users will not read large blocks of text on a screen, hence information can be spread out relevant to the screen, and kept to the point. Moreover, users do not like to read long instructions or other information given on screens. These characteristics of the computer screen medium pose a challenge to the interface designer. The design of every screen should maximize the likelihood that the user's eye will be able to find the important information easily and quickly.

The practices that contribute to this guideline are:

1. using the whole screen rather than putting everything on one side,
2. using highlighting techniques to emphasize important information without distracting the user

- with unnecessary blinking and flashing lights,
3. breaking up blocks of text and results by using bulleted lists, different screens and numbered steps,
  4. putting titles on each screen and headings on lists, and
  5. aligning lists of textual and numeric data to facilitate visually pleasing screens.

Menus have become, perhaps, the most frequently used method of option selection in inputting data to a program. Menus are usually the preferred method for software that is intended for new or casual users. Despite their widespread use, however, menus are a relatively new feature of applications software. A comprehensive summary of user-interface guidelines published about ten years ago (Engel, 1975) does not include guidelines for menus, which were not then in common use.

For new users, menus have two major advantages over other control methods. First, they provide an obvious structure to the software. In a well designed interface that is controlled by menus, the user can quickly develop an understanding of how the software is structured from the organization of the options on menus and from the organization of the menus themselves. The ability of new users to form an accurate mental model of the structure of the software is a major contributor to their feeling about being in control (Norman, 1983). Second, menus take advantage of people's superior ability to recognize

information rather than recall it from memory (McNulty, 1965).

### Interface Development Software

There are many software companies that offer customized interface development software, the basic features of which are common to all. Some of the features are:

1. Screens,
2. Icons,
3. Mouse cursor,
4. Graphs,
5. Menus,
6. Function keys,
7. Image screens,
8. Help documentation, etc.

The above features of an interface-development software are called objects in a user interface terminology. Graphic images are usually used to enhance the appearance of an application. Icon objects are graphical representations of various items. For example, in a data validation screen, different choices or methods can be represented by different icons. A mouse interface usually accelerates data entry and selection process. It allows users to move freely among fields. An interface to a technical program is developed using the language in which the application program is written or that supported by the interface development software.

Typically, two steps are involved in the creation of an

interface, object creation and linking objects.

The user interfaces are made of objects which interact with the end-user and the technical program (GEOS.FOR in our case). Different interface objects are created using the editor which is part of the interface development software. These objects are linked to the technical program using a set of object management functions usually provided by the editor. These functions are the same for all programming languages. The objects can replace several lines of "conventional" source code, since they contain various information about the position, color, format of the character, type of character (integer, real or alphanumeric), etc., of the screen that need to be displayed. For example, one can manage data entry to a screen with a couple of commands. Tasks such as data validation, context-sensitive help, formats, etc., are also taken care of by these functions.

#### Interface Commands

After extensive survey, HI-Screen (Softway Inc., 1991) was selected for the purpose of design of an interface for GEOS. For more details on the different interface functions, the reader is advised to refer to the users guides or the technical reference manuals of the interface development software. A number of the basic features are explained below:

1. displaying of screens and windows,
2. merging of screens and windows,

3. opening screens and windows,
4. using help screens,
5. managing standard menus,
6. displaying values to a field,
7. full screen input,
8. recovering field values, and
9. managing arrays.

Displaying Screens and Windows: The "USE" function of the interface-development software allows one to display a screen (or window), and to activate its fields. One can then provide input to these fields or display default values. For example, in Fortran language, the interface call statement will read as follows,

```
WRITE (*,*) BEGH, 'USE,FILENAME.AID',ENDH
```

This line brings up the screen or displays the screen FILENAME.AID with all its screen parameters (i.e., text, fields (arrays), etc.,).

Merging Screens and Windows: The fields of the merged window become active while the fields of the previous screen remain active. The fields of both screens are therefore active at the same time. For example, use of this interface code,

```
WRITE(*,*) BEGH, 'MERGE,FILENAME.AID',ENDH
```

will merge FILENAME.AID with an already active screen.

Opening Screens and Windows: The OPEN function allows

one to display a window without erasing the contents of the previous screen. Only the fields of the opened window are active. The fields of the previous screen are temporarily inactive.

The CLOSE function erases the opened window and restores the contents of the previous screen. The fields of the previous screen become active again and still display whatever values were current at the time the window was open.

Opening and closing of windows is similar to the use of parentheses in algebra. One can open multiple windows on top of each other, and close them one by one. This software can handle up to 26 levels of open windows. Before each OPEN function, the contents of the previous screen are saved. The previous screen will be restored when the second window is closed using the CLOSE function. For example,

```
WRITE (*,*) , 'OPEN,FILENAME.AID',ENDH  
WRITE (*,*) , 'CLOSE,FILENAME.AID',ENDH
```

Using Help Screens: Help screens are automatically managed by this software package based on user request. Function key F1 is used as a default for help. However, one can associate a different key to the help screens. The EXIT function is used to specify the help key.

To leave a help screen, users can press any key or click with the mouse button. The previous screen will automatically be restored, and its fields will become active again. For example, in the following statement,

```
WRITE (*,*) , 'EXIT, FK1=H, RET=V',ENDH
```

the function key f1 is defined as the help key.

Managing Standard Menus: When a menu screen is displayed, one must use a "MENU,INPUT" function to activate the menu management procedure. This function returns to the application program a numeric value representing the index of the menu option selected. The command used in this case is

```
WRITE (*,*) , 'MENU,INPUT',ENDH
```

Displaying Values to a Field: To display a value to a field one must use the DISPLAY function, with the name of the field and its value as parameters. For example, this call statement,

```
WRITE (*,*) , 'BEGH,DISPLAY,FIELDNAME',VALUE,ENDH
```

may be used where FIELDNAME is the name declared in the screen and VALUE is the value assigned to be displayed.

Full-Screen Input: Full-screen input is performed using the SCREEN,INPUT function. Unless otherwise specified, a full screen input involves all the fields defined as active for full screen input under the screen editor. In full screen mode, a single command is needed to perform input on multiple fields. For example,

```
WRITE(*,*) , 'BEGH,SCREEN,INPUT',ENDH
```

activates all the fields of the screen.

Exiting Full Screen Input: Full screen input is usually terminated when the user presses a key to accept or abandon



input. Some temporary interruptions requested by the technical program are also possible.

There are different situations of temporary or permanent exit from full screen input. Each exit is associated with a code belonging to one of the following categories:

1. Predefined key codes. Each of these codes corresponds to a specific key pressed by the user. For example, the function key "FK0" code corresponds to the F10 function key, and is usually used to validate input; the ESC code corresponds to the [ESC] key, and usually means abandonment of the input. The programmer can change the description of these keys.
2. Specific codes attached to a mouse/dialogue box.

Recovering Field Values: To recover the value of a field in the technical program one must use the SCREEN,RECOVER function with the field name as parameter. For example, one may use

```
WRITE(*,*) , 'BEGH,SCREEN,RECOVER',FIELDNAME,ENDH
READ(*,*) VARIABLE
```

to recover the value. Usually the FIELDNAME and the variable used in the program will be the same.

These were a few examples of the Fortran interface code used in GEOS.

## CHAPTER V

### STRUCTURE OF GEOS INTERFACE

This chapter deals with the software structure for the application software GEOS.FOR and its relationship with the different interface routines. This interface has been developed to implement GEOS in an interactive format, which is supported by an adequate graphics capability.

Four types of software routines constitute the entire structure of the GEOS program:

1. Fortran application routines,
2. interface routines,
3. graphic routines, and
4. utility routines.

Figure 19 in Appendix A illustrates the interaction between these routines.

#### Fortran Application Routines

The GEOS.FOR (Gasem, 1988) is an application program consisting of routines for calculating volumetric, calorimetric and equilibrium properties of nonelectrolyte mixtures. The flow sheets describing a few of the application subroutines used in design GEOS are given in Appendix B.

## Interface Routines

The GEOS interface is an editor developed (or tailored) for GEOS.FOR which, unlike other commercial editors, cannot be used as a text editor. The interface routines were developed in Fortran language and the functions requiring disk operating system (DOS) calls were coded in "C" language. In general, an interface can be developed in two ways using:

1. Independent coding, where the interface routines are coded independently without altering the application code (GEOS.FOR in our case). This may be accomplished by passing the parameters as global variables using common blocks or by passing parameters through the call statement in fortran. This method preserves the integrity of the application program as the interface becomes modular and portable to other programs.

2. Dependent coding, where the interface code is merged with the application routines thereby modifying the original program structure. This approach has the advantage that the number of variables declared and the size of the program are relatively small in comparison to that of the independent coding technique.

In the GEOS interface the independent coding technique was adopted to a large degree, since some source code modifications were undertaken. These modifications, however, were limited to the INPUT and OUTPUT subroutines.

## Graphic routines

Graphic routines have been incorporated in the GEOS program to enhance the presentation of the predicted volumetric, calorimetric and phase equilibrium properties. GRAPHER is the commercial software which has been linked to the GEOS interactively to produce various descriptive and deviation plots. Specifically, there are fifteen graphs which accompany the various calculation options. Figures 33 - 36 in Appendix C illustrate some of them. The user also has an option to interactively produce the graphs to their requirements using GRAPHER directly. The graphs currently generated include the following descriptive and deviation plots:

1. liquid/vapor composition plot,
2. pressure, composition plot,
3. temperature, composition plot,
4. liquid/vapor density plot,
5. liquid/vapor enthalpy plot,
6. liquid/vapor entropy plot,
7. activity coefficient, liquid composition plot,
8. pressure deviation plot,
9. temperature deviation plot,
10. liquid composition deviation plot,
11. vapor composition deviation plot,
12. liquid density deviation plot,
13. vapor density deviation plot,
14. enthalpy deviation plot, and

15. entropy deviation plot.

### Utility routines

Two popular editors XTREE GOLD and SPFPC have been included with this software to enable the user to switch over to another program, or to edit one. These editors can be accessed interactively without exiting from the GEOS program. This option can be selected directly from the opening main menu, as shown in Figure 1 of Appendix A.

### GEOS Interface Operation

There are basically five major tasks that govern the operation of the GEOS interface:

1. problem setup,
2. problem execution,
3. output,
4. option change,
5. intermediate output, and
6. the configure option.

#### Problem setup

The problem can be set up in two steps by selecting:

1. a data file from the database, and
2. the option needed to calculate volumetric, calorimetric or the phase equilibrium properties.

The different options are as given in Table III:

TABLE III  
INPUT FILE DESCRIPTION

LINE ENTRY NO	NAME	SELECTION
1	CALCULATION MODE	0 OPTIMIZE 1 PREDICT
	VOLUMETRIC OR PHASE EQUILIBRIUM CALCULATION	1 LIQUID DENSITY 2 VAPOR DENSITY 3 LIQUID AND VAPOR DENSITY 4 FLASH CALCULATIONS 5 BUBBLE POINT PRESSURE 6 BUBBLE POINT TEMP 7 DEW POINT PRESSURE 8 DEW POINT TEMPERATURE
	EQUATION OF STATE	0 IDEAL GAS 1 VIRIAL 2 VAN DER WAALS 3 REDLICH-KWONG 4 SOAVE-REDLICH-KWONG 5 PENG-ROBINSON
	LIQUID SOLUTION MODEL	0 IDEAL SOLUTION 1 WILSON 2 VAN LAAR 3 MARGULES 4 UNIFAC
	REFERENCE FUGACITY	1 FL(T,P) 2 FL(T,VP) 3 FL(T,P,X)
	VAPOR PRESSURE MODEL	1 SVRC (SCALED-VARIABLE- REDUCED-COORDINATE) (Shaver, 1990) 2 ANTOINE
	VAPOR PRESSURE GENERALIZED	1 YES 2 NO
	VOLUME TRANSLATION (Sudibandriyo, 1991)	1 YES 2 NO

TABLE III (continued)

LINE ENTRY NO	NAME	SELECTION
	NO OF COMPONENTS	NC MAXIMUM = 20
	NO OF POINTS	NPTS MAXIMUM = 20
	INPUT MODE	INPT 1 T,P,X1,ID,IRF,Y1,DL,DV 2 T,P,(ZE(I,J),J=1,NC)
	UNITS	IUNIT 1 T(K), P(BAR), DEN(GM/CC) 2 T(F), P(PSIA),DEN(GM/CC) 3 T(C), P(MMHG),DEN(GM/CC)
2	PURE- FLUID PHYSICAL PROPERTIES	NAME TC(J) PC(J) OMG(J) TB(J) ZRA(J) WT(J) NAME OF THE COMPONENT CRITICAL TEMPERATURE CRITICAL PRESSURE ACENTRIC FACTOR BOILING TEMPERATURE COMPRESSIBILITY FACTOR MOLECULAR WEIGHT
3	HEAT CAPACITY PARAMETERS CP(J)	
4	ESTIMATES FOR INTERACTION PARAMETER  C(I,J) D(I,J)	
5	MASKING PARAMETERS FOR OPTIMIZATION  MASK(J)	
6	ACTIVITY COEFFICIENTS PARAMETERS  Q(I,J)	
7	EXPERIMENTAL DATA	1 T(I),PE(I),XE(I),ID.. 2 T(I),PE(I),(ZE(I,J),J=1,NC)

### Problem Execution

Once the problem has been set up, the next step is to execute the program. This is done by selecting the RUN option from the main menu. The necessary steps that should be taken to implement this are shown in sequence in Figures 1-14 of Appendix A.

### Output screen description

The sequence of outputs that can be generated individually by this program are:

1. activity coefficients,
2. liquid composition,
3. vapor composition,
4. bubble/dew point temperature,
5. bubble/dew point pressure,
6. liquid density,
7. vapor density,
8. enthalpy and entropy, and
9. ZOOM data output for a selected data point.

Sample outputs generated are shown in the Figures 15-18 of Appendix A. If a particular output is selected and the problem which has been setup does not generate that output, then the message "The option chosen for this run does not produce this output" is displayed.

The ZOOM output option has the facility to calculate and display all the volumetric, calorimetric and phase equilibrium values for a single experimental data point all



in one screen, followed by its depiction in the graphic mode.

In addition, a multicomponent output screen can be viewed for calculations having more than two components. The output consists of the liquid and vapor compositions and the liquid and vapor densities at a given temperature and pressure.

#### Intermediate output

This option is an important tool as one can closely look into the workings of the different convergence routines of the GEOS program. It enables one to determine the quality of convergence of the various routines implemented for a particular data point. This option, however, slows down the execution time of the problem, since information has to be continuously displayed onto the screen; whenever any information has to be displayed on to the screen the central processing unit (CPU) of the computer is interrupted and the processing is transferred to the input/output (I/O) processor; therefore, no further calculation can take place until the I/O operation is completed.

#### Change Options

There are two ways of changing the options in the current problem setup. One is to change the settings in the data file by editing the input screens, which makes a permanent change in the data file. The second and the more

convenient way to change a particular option is to select the "CHANGE OPTIONS" in the main menu as shown in Figure 13, Appendix A. The changes made using this method, however, are temporary.

#### Configure Option

This option gives the user an opportunity to design their own convergence routines and to link them to the GEOS program, keeping every other subroutine the same.

## CHAPTER VI

### HELP AND TROUBLE SHOOTING

In this chapter an attempt is made to outline some of the problems that a user may face when executing the GEOS program and the different help options available to the user.

#### Help

On-line help is an important part of an application development. Two levels of help have been introduced:

1. a general help screen attached to the main screen, and
2. a help screen specific to each field.

The first level of help is useful in providing general guidelines and information. Whenever one needs to be more specific, one can use the field-specific help level. When the user requests help, the current task is interrupted, and the appropriate help screen is displayed. When the user exits the help screen, the original task resumes where it left off. Apart from the above mentioned help there is yet another help documentation which has been included in the GEOS software, i.e., general help, which explains the input data file setup and on the trouble shooting as explained above. This can be accessed from the main help as well as

the output screens.

Function key F1 is the default help key configured for the GEOS interface. One can return to the calling program by either pressing any key from the key board or clicking with the left button of the mouse after accessing the help screen.

Displaying of status messages on tasks in progress is another important aspect of help included in GEOS. These messages inform the user when the calculations for a given task are completed.

Sample HELP screens for data file setup, trouble shooting and interface use have been included in Appendix C.

### Trouble Shooting

Aside from the problems that may occur due to errors in the setup and in the input data, eight possible causes of calculation failure are outlined here. Detailed discussion for means to avoid these and other calculation failures are given elsewhere (Gasem, 1990).

1. Poor choice of solution model. The user must know how to select the appropriate models for the mixtures at hand. For example, in equilibrium calculations two decisions must be made; first whether to use a single equation of state for both the vapor and the liquid phase (EOS method) or to use the split method, where a liquid solution model is used for the liquid phase along with an equation of state for the

vapor phase. The second decision is that in either case which equation of state or which solution model to use. The use of a single equation of state is considered thermodynamically more efficient. The van der Waals-type equation such as (SRK) and (PR) are capable of representing all types of fluid behavior (Modell, 1979). Their inherent simplicity, however, precludes their use for accurate calculations except for normal fluids.

2. Improper specification of calculation option. For example, one may not specify (fix) the vapor composition for a bubble point calculation. Similarly, one may not fix both temperature and pressure for a pure component two phase calculation. Use of phase rule and familiarity with phase diagrams is required for meaningful computations.

3. Improper specification of equilibrium conditions. For example, one may not specify the flash option outside the two-phase region and expect property predictions for both the liquid and the vapor phase.

4. Improper specification of independent variables. Some phase conditions require strict choice of fixed (independent) variables (and thus the iteration variables). For examples, if a bubble point pressure calculation fails to converge for a given mixture, the bubble point temperature option should be used.

5. Poor initial guesses. Reasonable initial estimates are required for the property convergence routines such as that for the solution of the cubic equation of state, the bubble

point, and the dew point predictions. Typically equal molar phase distribution among the phases present is assumed in the flash calculation and ideal solution equilibrium constants are used as initial guesses. Although any of the above initial guess methods can be used, provisions are made for the use of experimental values.

6. Convergence to trivial solutions. During equilibrium calculations to obtain values of  $f_j$ , one needs to solve the cubic equation for the compressibility factor,  $Z$ . Below the pseudocritical point, there is a range of temperatures for a given pressure and composition over which there exists three real roots for the compressibility. Over this range one assigns the largest root for the vapor phase and the smallest one for the liquid phase. During early iterations, however, where only rough estimates of the dependent variable are available a single root may be obtained which does not correspond to the desired phase. This leads to the convergence of a trivial solution where both phases have identical properties and thus satisfying the equations given in Chapter II and Chapter III. To alleviate this problem, better estimates for the corresponding conditions should be provided and then the calculations may be attempted again.

7. Near critical predictions. While cubic equations of state are inherently inadequate for accurate predictions near the critical point, some property estimates can still be made by such equations. To avoid failures in such regions, a series of calculations are performed starting at

lower pressures and then proceeding to higher pressures in smaller steps using the results of a previous calculation as an initial guess for the next (stair-casing). While not recommended, this procedure can also be used to estimate the critical point.

8. Retrograde behavior, where the possibility of two solutions exists for a given bubble or dew point condition. Here the user must be aware of the possibility for such conditions and based on the required information one should decide which of the two solutions is the right one. Typically, tracing the p-T projection for the desired composition is helpful in exploring retrograde behavior.

## CHAPTER VII

### TEST CASES

This chapter describes the different stages in the set up of a problem, and compares the results generated by the interface version of GEOS with that of the original Fortran version without the interface.

To describe the different input and output that can be generated using this program, a test case was selected. The data file CDBZ.CAT involving the binary mixture CO<sub>2</sub> + benzene was selected from the selection menu of the FILE OPTION. Once the file has been selected the user is given the option to either return to the main menu or to view the different sections of the data file. As shown in Figure 5, of Appendix A, the data file has been divided for convenience of display into four sections:

- Input options,
- Physical properties,
- E O S interaction parameters,
- V L E data, and
- UNIFAC parameters.

By providing this menu one need not go through the entire data file to access the V L E data screen, instead the user can select the V L E DATA option in the selection menu to directly view the desired data. The dividing of the data



file into different sections simplifies the structure of the data file for the user.

On exiting from the file selection menu, one can either run the problem, as seen in the input option of the data file screen Figure 14 of Appendix A, or can change the input options before running the present setup. For example, the present setup to calculate the phase compositions using the Peng-Robinson Equation of state shown can be changed by selecting the CHANGE OPTIONS icon from the main menu (Figure 2, Appendix A) and the METHOD icon of the CHANGE OPTIONS screen (Figure 13, Appendix A).

When the changes are completed, the user can select the RUN option of the main screen to run the problem that has been setup. On selecting this option a status message appears as shown in Figure 14 of Appendix A indicating that the calculation is under progress and specifying the data file used, method and the option selected for execution of the problem. On completion of the execution the screen displays that the calculation has been completed and puts the user in the main menu.

The user now has an option to either view the output screens generated by this program or the associated graphs. On selecting the OUTPUT option the program switches to the OUTPUT menu showing the different outputs available as explained in Chapter VI. In addition, the ZOOM option may be requested to give the user the facility to view all the phase equilibrium and volumetric properties of a single data

point followed by its depiction in the graphic mode. The details of the results of this case are shown in the Figures XV-XVIII in Appendix A.

#### Comparison of results

Four test cases have been identified to compare the results generated by the GEOS interface program with that of the original GEOS without the interface. The results are tabulated in sequence as given below in Tables IV-X:

1. Pure CO<sub>2</sub>,
2. Pure Propane,
3. CO<sub>2</sub> + Benzene, and
4. n-Hexane + Toluene.

Corresponding graphs for the test case CO<sub>2</sub> + benzene have been included in Appendix C.

TABLE IV

TEST CASE 1: PURE CO<sub>2</sub>  
 DATA POINT 1 (INTERFACE VERSION)

---

PURE CO<sub>2</sub> :

---

## LIQUID/VAPOR PHASE PROPERTIES

DATA NO = 1            T(K)= 298.812            P(BAR)= 3.447

MOLE FRACTION FEED,	Z1...ZN:	1.0000
LIQUID,	X1...XN:	1.0000
VAPOR,	Y1...YN:	1.0000
EQUILIBRIUM CONSTANT,	K1...KN:	1.0000
COMPONENT FUGACITY (L/V),	FL1...FLN:	3.3828
	FV1...FVN:	3.3828

	LIQUID	VAPOR	OVERALL
PHASE MOLAR RATIO, (L/N)	0.0000	1.0000	1.0000
COMPRESSIBILITY FACTOR, Z	.9811E+00	.9811E+00	---
MOLAR VOLUME, V(CC/MOL)	.7071E+04	.7071E+04	.7071E+04
PHASE DENSITY, D(GM/CC)	.0062	.0062	---
ENTHALPY, H(KJ/MOL)	.9246E+01	.9246E+01	.9246E+01
ENTROPY, S(KJ/MOL/K)	.2033E+00	.2033E+00	.2033E+00
INTERNAL ENERGY, U(KJ/MOL)	.6808E+01	.6808E+01	.6808E+01
HELMHOLTZ ENERGY, A(KJ/MOL)	-.5395E+02	-.5395E+02	-.5395E+02
GIBBS FREE ENERGY, G(KJ/MOL)	-.5152E+02	-.5152E+02	-.5152E+02

TABLE IV CONTINUED  
 DATA POINT 1 (ORIGINAL GEOS VERSION)

---

PURE CO<sub>2</sub>:

---

LIQUID/VAPOR PHASE PROPERTIES

DATA NO = 1            T(K)= 298.812            P(BAR)= 3.447

MOLE FRACTION FEED,	Z1...ZN:	1.0000
LIQUID,	X1...XN:	1.0000
VAPOR,	Y1...YN:	1.0000
EQUILIBRIUM CONSTANT,	K1...KN:	1.0000
COMPONENT FUGACITY (L/V),	FL1...FLN:	3.3828
	FV1...FVN:	3.3828

	LIQUID	VAPOR	OVERALL
PHASE MOLAR RATIO, (L/N)	0.0000	1.0000	1.0000
COMPRESSIBILITY FACTOR, Z	.9811E+00	.9811E+00	---
MOLAR VOLUME, V(CC/MOL)	.7071E+04	.7071E+04	.7071E+04
PHASE DENSITY, D(GM/CC)	.0062	.0062	---
ENTHALPY, H(KJ/MOL)	.9246E+01	.9246E+01	.9246E+01
ENTROPY, S(KJ/MOL/K)	.2033E+00	.2033E+00	.2033E+00
INTERNAL ENERGY, U(KJ/MOL)	.6808E+01	.6808E+01	.6808E+01
HELMHOLTZ ENERGY, A(KJ/MOL)	-.5395E+02	-.5395E+02	-.5395E+02
GIBBS FREE ENERGY, G(KJ/MOL)	-.5152E+02	-.5152E+02	-.5152E+02

---

TABLE V

TEST CASE 1: PURE CO<sub>2</sub>  
 DATA POINT 2 (INTERFACE VERSION)

---

PURE CO<sub>2</sub>:

---

LIQUID/VAPOR PHASE PROPERTIES

DATA NO = 2            T(K)= 298.800            P(BAR)= 34.470

MOLE FRACTION FEED,	Z1...ZN:	1.0000
LIQUID,	X1...XN:	1.0000
VAPOR,	Y1...YN:	1.0000
EQUILIBRIUM CONSTANT,	K1...KN:	1.0000
COMPONENT FUGACITY (L/V),	FL1...FLN:	28.2902
	FV1...FVN:	28.2902

	LIQUID	VAPOR	OVERALL
PHASE MOLAR RATIO, (L/N)	0.0000	1.0000	1.0000
COMPRESSIBILITY FACTOR, Z	.7891	.7891	---
MOLAR VOLUME, V(CC/MOL)	.5687E+03	.5687E+03	.5687E+03
PHASE DENSITY, D(GM/CC)	.0774	.0774	---
ENTHALPY, H(KJ/MOL)	.7708E+01	.7708E+01	.7708E+01
ENTROPY, S(KJ/MOL/K)	.1805E+00	.1805E+00	.1805E+00
INTERNAL ENERGY, U(KJ/MOL)	.5747E+01	.5747E+01	.5747E+01
HELMHOLTZ ENERGY, A(KJ/MOL)	-.4820E+02	-.4820E+02	-.4820E+02
GIBBS FREE ENERGY, G(KJ/MOL)	-.4624E+02	-.4624E+02	-.4624E+02

TABLE V CONTINUED  
DATA POINT 2 (ORIGINAL GEOS VERSION)

---

PURE CO<sub>2</sub>:

---

LIQUID/VAPOR PHASE PROPERTIES

DATA NO = 2            T(K)= 298.800            P(BAR)= 34.470

MOLE FRACTION FEED,	Z1...ZN:	1.0000
LIQUID,	X1...XN:	1.0000
VAPOR,	Y1...YN:	1.0000
EQUILIBRIUM CONSTANT,	K1...KN:	1.0000
COMPONENT FUGACITY (L/V),	FL1...FLN:	28.2902
	FV1...FVN:	28.2902

	LIQUID	VAPOR	OVERALL
PHASE MOLAR RATIO, (L/N)	0.0000	1.0000	1.0000
COMPRESSIBILITY FACTOR, Z	.7891	.7891	---
MOLAR VOLUME, V(CC/MOL)	.5687E+03	.5687E+03	.5687E+03
PHASE DENSITY, D(GM/CC)	.0774	.0774	---
ENTHALPY, H(KJ/MOL)	.7708E+01	.7708E+01	.7708E+01
ENTROPY, S(KJ/MOL/K)	.1805E+00	.1805E+00	.1805E+00
INTERNAL ENERGY, U(KJ/MOL)	.5747E+01	.5747E+01	.5747E+01
HELMHOLTZ ENERGY, A(KJ/MOL)	-.4820E+02	-.4820E+02	-.4820E+02
GIBBS FREE ENERGY, G(KJ/MOL)	-.4624E+02	-.4620E+02	-.4620E+02

---

TABLE VI

TEST CASE: 2 PURE PROPANE  
 DATA POINT 1 (INTERFACE VERSION)

---

PURE PROPANE:

---

LIQUID/VAPOR PHASE PROPERTIES

DATA NO = 1            T(K)= 250.000            P(BAR)= 2.176

MOLE FRACTION FEED,	Z1...ZN:	1.0000
LIQUID,	X1...XN:	1.0000
VAPOR,	Y1...YN:	1.0000
EQUILIBRIUM CONSTANT,	K1...KN:	1.0000
COMPONENT FUGACITY (L/V),	FL1...FLN:	2.0527
	FV1...FVN:	2.0527

	LIQUID	VAPOR	OVERALL
PHASE MOLAR RATIO, (L/N)	1.0000	.0000	1.0000
COMPRESSIBILITY FACTOR, Z	.0077	.9404	---
MOLAR VOLUME, V(CC/MOL)	.7395E+02	.8983E+04	.7395E+02
PHASE DENSITY, D(GM/CC)	.5962	.0049	---
ENTHALPY, H(KJ/MOL)	-.6791E+00	.1108E+02	-.6791E+01
ENTROPY, S(KJ/MOL/K)	.1794E+00	.2509E+00	.1794E+00
INTERNAL ENERGY, U(KJ/MOL)	-.6807E+01	.9128E+01	.6807E+01
HELMHOLTZ ENERGY, A(KJ/MOL)	-.5166E+02	-.5360E+02	-.5166E+02
GIBBS FREE ENERGY, G(KJ/MOL)	-.5165E+02	-.5165E+02	-.5165E+02

## TABLE VI CONTINUED

## DATA POINT 1 (ORIGINAL GEOS VERSION)

---

 PURE PROPANE:
 

---

## LIQUID/VAPOR PHASE PROPERTIES

DATA NO = 1            T(K)= 250.000            P(BAR)= 2.178

MOLE FRACTION FEED,	Z1...ZN:	1.0000
LIQUID,	X1...XN:	1.0000
VAPOR,	Y1...YN:	1.0000
EQUILIBRIUM CONSTANT,	K1...KN:	1.0000
COMPONENT FUGACITY (L/V),	FL1...FLN:	2.0527
	FV1...FVN:	2.0527

	LIQUID	VAPOR	OVERALL
PHASE MOLAR RATIO, (L/N)	1.00000	.0000	1.0000
COMPRESSIBILITY FACTOR, Z	.7742E-02	.9404E+00	-----
MOLAR VOLUME, V(CC/MOL)	.7395E+02	.8983E+05	.7395E+02
PHASE DENSITY, D(GM/CC)	.5962	.0049	-----
ENTHALPY, H(KJ/MOL)	-.6791E+01	.1108E+02	-.6791E+01
ENTROPY, S(KJ/MOL/K)	.1794E+00	.2507E+00	.1794E+00
INTERNAL ENERGY, U(KJ/MOL)	-.6807E+01	.9117E+01	-.6807E+01
HELMHOLTZ ENERGY, A(KJ/MOL)	-.5166E+02	-.5360E+02	-.5166E+02
GIBBS FREE ENERGY, G(KJ/MOL)	-.5165E+02	-.5165E+02	-.5165E+02

---



TABLE VII

TEST CASE 2: PURE PROPANE  
DATA POINT 2 (INTERFACE VERSION)

---

PURE PROPANE:

---

LIQUID/VAPOR PHASE PROPERTIES

DATA NO = 2            T(K)= 350.000            P(BAR)= 29.713

MOLE FRACTION FEED,	Z1...ZN:	1.0000
LIQUID,	X1...XN:	1.0000
VAPOR,	Y1...YN:	1.0000
EQUILIBRIUM CONSTANT,	K1...KN:	1.0000
COMPONENT FUGACITY (L/V),	FL1...FLN:	20.8869
	FV1...FVN:	20.8869

	LIQUID	VAPOR	OVERALL
PHASE MOLAR RATIO, (L/N)	1.0000	.0000	1.0000
COMPRESSIBILITY FACTOR, Z	.1248	.5683	---
MOLAR VOLUME, V(CC/MOL)	.1222E+03	.5565E+03	.1222E+03
PHASE DENSITY, D(GM/CC)	.3607	.0792	---
ENTHALPY, H(KJ/MOL)	.6269E+01	.1483E+02	.6269E+01
ENTROPY, S(KJ/MOL/K)	.2218E+00	.2463E+00	.2218E+00
INTERNAL ENERGY, U(KJ/MOL)	.5906E+01	.1317E+02	.5906E+01
HELMHOLTZ ENERGY, A(KJ/MOL)	-.7173E+02	-.7302E+02	-.7173E+02
GIBBS FREE ENERGY, G(KJ/MOL)	-.7137E+02	-.7137E+02	-.7137E+02

## TABLE VII CONTINUED

## DATA POINT 2 (ORIGINAL GEOS VERSION)

---

 PURE PROPANE:
 

---

## LIQUID/VAPOR PHASE PROPERTIES

DATA NO = 2            T(K)= 350.000            P(BAR)= 29.713

MOLE FRACTION FEED,	Z1...ZN:	1.0000
LIQUID,	X1...XN:	1.0000
VAPOR,	Y1...YN:	1.0000
EQUILIBRIUM CONSTANT,	K1...KN:	1.0000
COMPONENT FUGACITY (L/V),	FL1...FLN:	20.8869
	FV1...FVN:	20.8869

	LIQUID	VAPOR	OVERALL
PHASE MOLAR RATIO, (L/N)	1.0000	.0000	1.0000
COMPRESSIBILITY FACTOR, Z	.1248E+00	.5783E+00	---
MOLAR VOLUME, V(CC/MOL)	.1222E+03	.5565E+03	.1222E+03
PHASE DENSITY, D(GM/CC)	.3606	.0777	---
ENTHALPY, H(KJ/MOL)	.6269E+01	.1483E+02	.6269E+01
ENTROPY, S(KJ/MOL/K)	.2218E+00	.2463E+00	.2218E+00
INTERNAL ENERGY, U(KJ/MOL)	.5906E+01	.1317E+02	.5906E+01
HELMHOLTZ ENERGY, A(KJ/MOL)	-.7173E+02	-.7302E+02	-.7173E+02
GIBBS FREE ENERGY, G(KJ/MOL)	-.7137E+02	-.7137E+02	-.7137E+02

---

TABLE VIII

TEST CASE 3: CO<sub>2</sub> + BENZENE  
 DATA POINT 1 (INTERFACE VERSION)

---

 CO<sub>2</sub> + BENZENE:
 

---

## LIQUID/VAPOR PHASE PROPERTIES

DATA NO = 1            T(K)= 344.300            P(BAR)= 73.068

MOLE FRACTION FEED,	Z1...ZN:	.9702	.0298
LIQUID,	X1...XN:	.5070	.4930
VAPOR,	Y1...YN:	.9702	.0298
EQUILIBRIUM CONSTANT,	K1...KN:	1.9137	0.0604
COMPONENT FUGACITY (L/V),	FL1...FLN:	54.6728	.5391
	FV1...FVN:	54.3728	.5391

	LIQUID	VAPOR	OVERALL
PHASE MOLAR RATIO, (L/N)	1.0000	.0000	1.0000
COMPRESSIBILITY FACTOR, Z	.1854	.6903	---
MOLAR VOLUME, V(CC/MOL)	.7261E+02	.2704E+03	.7261E+02
PHASE DENSITY, D(GM/CC)	.8374	.1665	---
ENTHALPY, H(KJ/MOL)	-.5161E+01	.8082E+01	-.5161E+01
ENTROPY, S(KJ/MOL/K)	.1784E+00	.1797E+00	.1784E+00
INTERNAL ENERGY, U(KJ/MOL)	-.5692E+01	.6106E+01	-.5692E+01
HELMHOLTZ ENERGY, A(KJ/MOL)	-.6712E+02	-.5575E+02	-.6712E+02
GIBBS FREE ENERGY, G(KJ/MOL)	-.6659E+02	-.5377E+02	-.6659E+02

TABLE VIII CONTINUED  
 DATA POINT 1 (ORIGINAL GEOS VERSION)

---

CO<sub>2</sub> + BENZENE:

---

LIQUID/VAPOR PHASE PROPERTIES

DATA NO = 1            T(K)= 344.300            P(BAR)= 73.068

MOLE FRACTION FEED,	Z1...ZN:	.9702	.0298
LIQUID,	X1...XN:	.5070	.4930
VAPOR,	Y1...YN:	.9702	.0298
EQUILIBRIUM CONSTANT,	K1...KN:	1.9137	0.0604
COMPONENT FUGACITY (L/V),	FL1...FLN:	54.6728	.5391
	FV1...FVN:	54.3728	.5391
	LIQUID	VAPOR	OVERALL
PHASE MOLAR RATIO, (L/N)	1.0000	.0000	1.0000
COMPRESSIBILITY FACTOR, Z	.1854E+00	.6903E+00	---
MOLAR VOLUME, V(CC/MOL)	.7261E+02	.2704E+03	.7261E+02
PHASE DENSITY, D(GM/CC)	.8374	.1665	---
ENTHALPY, H(KJ/MOL)	-.5161E+01	.8082E+01	-.5161E+01
ENTROPY, S(KJ/MOL/K)	.1784E+00	.1797E+00	.1784E+00
INTERNAL ENERGY, U(KJ/MOL)	-.5692E+01	.6106E+01	-.5692E+01
HELMHOLTZ ENERGY, A(KJ/MOL)	-.6712E+02	-.5575E+02	-.6712E+02
GIBBS FREE ENERGY, G(KJ/MOL)	-.6659E+02	-.5377E+02	-.6659E+02

---

TABLE IX

TEST CASE 3: CO<sub>2</sub> + BENZENE  
 DATA POINT 2 (INTERFACE VERSION)

---

 CO<sub>2</sub> + BENZENE:
 

---

## LIQUID/VAPOR PHASE PROPERTIES

DATA NO = 2	T(K)= 344.300	P(BAR)= 105.739	
MOLE FRACTION FEED,	Z1...ZN:	.9523	.0477
LIQUID,	X1...XN:	.6730	.2370
VAPOR,	Y1...YN:	.9523	.0477
EQUILIBRIUM CONSTANT,	K1...KN:	1.2481	0.2013
COMPONENT FUGACITY (L/V),	FL1...FLN:	69.3935	.4494
	FV1...FVN:	69.3935	.4494
	LIQUID	VAPOR	OVERALL
PHASE MOLAR RATIO, (L/N)	1.0000	.0000	1.0000
COMPRESSIBILITY FACTOR, Z	.2576	.4901	---
MOLAR VOLUME, V(CC/MOL)	.6974E+02	.1327E+03	.6974E+02
PHASE DENSITY, D(GM/CC)	.7467	.3439	---
ENTHALPY, H(KJ/MOL)	.9804E+00	.5348E+01	.9804E+00
ENTROPY, S(KJ/MOL/K)	.1688E+00	.1713E+00	.1688E+00
INTERNAL ENERGY, U(KJ/MOL)	.1718E+01	.3945E+01	.1718E+01
HELMHOLTZ ENERGY, A(KJ/MOL)	-.5985E+02	-.5505E+02	-.5985E+02
GIBBS FREE ENERGY, G(KJ/MOL)	-.5911E+02	-.5364E+02	-.5911E+02

TABLE IX CONTINUED  
 DATA POINT 2 (ORIGINAL GEOS VERSION)

---

CO<sub>2</sub> + BENZENE:

---

LIQUID/VAPOR PHASE PROPERTIES

DATA NO = 2

T(K)= 344.300

P(BAR)= 105.739

MOLE FRACTION FEED,	Z1...ZN:	.9523	.0477
LIQUID,	X1...XN:	.6730	.2370
VAPOR,	Y1...YN:	.9523	.0477
EQUILIBRIUM CONSTANT,	K1...KN:	1.2481	0.2013
COMPONENT FUGACITY (L/V),	FL1...FLN:	69.3935	.4494
	FV1...FVN:	69.3935	.4494
	LIQUID	VAPOR	OVERALL
PHASE MOLAR RATIO, (L/N)	1.0000	.0000	1.0000
COMPRESSIBILITY FACTOR, Z	.2576E+00	.4901E+00	---
MOLAR VOLUME, V(CC/MOL)	.6974E+02	.1327E+03	.6974E+02
PHASE DENSITY, D(GM/CC)	.7467	.3439	---
ENTHALPY, H(KJ/MOL)	.9804E+00	.5348E+01	.9804E+00
ENTROPY, S(KJ/MOL/K)	.1688E+00	.1713E+00	.1688E+00
INTERNAL ENERGY, U(KJ/MOL)	.1718E+01	.3945E+01	.1718E+01
HELMHOLTZ ENERGY, A(KJ/MOL)	-.5985E+02	-.5505E+02	-.5985E+02
GIBBS FREE ENERGY, G(KJ/MOL)	-.5911E+02	-.5364E+02	-.5911E+02

---

TABLE X

TEST CASE 4: n-HEXANE + TOLUENE (INTERFACE VERSION)

1VIRIAL-2G EQUATION OF STATE PREDICTIONS						
DATA	PRESS (BAR)	BT(EXP) (K)	XEXP(1)	BT(CAL)	DEV	%DEV
1	1.0130	383.7200	.0000	383.6723	-.0477	-.01
2	1.0130	377.8200	.0571	377.8282	.0082	.00
3	1.0130	373.4200	.1091	373.4222	.0022	.00
4	1.0130	369.1800	.1682	369.2139	.0339	.01
5	1.0130	366.4400	.2133	366.4489	.0089	.00
6	1.0130	363.7800	.2631	363.7521	-.0279	-.01
7	1.0130	358.6600	.3774	358.6237	-.0363	-.01
8	1.0130	360.2300	.3383	360.2382	.0082	.00
9	1.0130	356.9500	.4220	356.9262	-.0238	-.01
10	1.0130	354.1600	.5032	354.1573	-.0027	.00
11	1.0130	351.6400	.5867	351.6463	.0063	.00
12	1.0130	349.1600	.6781	349.1854	.0254	.01
13	1.0130	346.8500	.7717	346.8914	.0414	.01
14	1.0130	343.8100	.9064	343.8617	.0517	.02
15	1.0130	341.8000	1.0000	341.8795	.0795	.02
CIJ=	.0000	E1=	.3298000E+00	E2=	.3429000E+00	
DIJ=	.0000	E3=	.1000000E+01	E4=	.1000000E+01	
PCM=	1.00					
RMSE =	.0344	AAD =	.0269	%AAD =	.01	
BIAS =	.0085			NPTS =	15	
FUGACITY REFERENCE MODEL	=	REFERENCE-2	(PHIV*PV)			
ACTIVITY COEFFICIENT MODEL	=	VAN LAAR				

TABLE X CONTINUED  
(ORIGINAL GEOS VERSION)

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1VIRIAL-2G EQUATION OF STATE PREDICTIONS

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DATA	PRESS (BAR)	BT(EXP) (K)	XEXP(1)	BT(CAL)	DEV	%DEV
1	1.0130	383.7200	.0000	383.6723	-.0477	-.01
2	1.0130	377.8200	.0571	377.8282	.0082	.00
3	1.0130	373.4200	.1091	373.4222	.0022	.00
4	1.0130	369.1800	.1682	369.2139	.0339	.01
5	1.0130	366.4400	.2133	366.4489	.0089	.00
6	1.0130	363.7800	.2631	363.7521	-.0279	-.01
7	1.0130	358.6600	.3774	358.6237	-.0363	-.01
8	1.0130	360.2300	.3383	360.2382	.0082	.00
9	1.0130	356.9500	.4220	356.9262	-.0238	-.01
10	1.0130	354.1600	.5032	354.1573	-.0027	.00
11	1.0130	351.6400	.5867	351.6463	.0063	.00
12	1.0130	349.1600	.6781	349.1854	.0254	.01
13	1.0130	346.8500	.7717	346.8914	.0414	.01
14	1.0130	343.8100	.9064	343.8617	.0517	.02
15	1.0130	341.8000	1.0000	341.8795	.0795	.02

CIJ= .0000 E1= .3298000E+00 E2= .3429000E+00

DIJ= .0000 E3= .1000000E+01 E4= .1000000E+01

PCM= 1.00

RMSE = .0344 AAD = .0269 %AAD = .01

BIAS = .0085 NPTS = 15

FUGACITY REFERENCE MODEL = REFERENCE-2 (PHIV\*PV)

ACTIVITY COEFFICIENT MODEL= VAN LAAR

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## CHAPTER VIII

### DISCUSSION

A modular approach in the design of the interface was adopted. Using this approach, the modification to the original application program was limited to the INPUT and OUTPUT routines thereby preserving the original application program. The facility for separate viewing of the different sections of the INPUT and OUTPUT data file contents through the GEOS interface editor is one of the unique features of this interface. Help documentation at the INPUT and OUTPUT stage has been provided to aid in the interpretation of the INPUT and OUTPUT data files. Also a section on general help and trouble shooting has been included.

A provision was made for viewing the intermediate results of the different convergence subroutines as the actual calculations are taking place. As expected, viewing intermediate results causes a reduction in the speed of the program execution.

Interactive graphics routines have been provided to present the predicted volumetric, calorimetric and phase equilibrium properties. However the use of Fortran language for the online display of graphs as the calculation are in progress was not possible, due to the limitations in the Fortran language.

Detailed help with the thermodynamic subject matter was not provided. This can be attributed to the fact that the size of the interface and the total number of features that can be included in the interface were limited by the available memory of the personal computer which is 640KB.

The interface development software used for the GEOS interface had its own limitations. The time taken to develop a 3D screen with icons was considerable, the interface code required flexibility of character manipulation and access to memory management which unlike C language was not available in Fortran language.

The compilation and linking of the Fortran GEOS routines and the interface routines produced an executable code which exceeded the DOS limit of 640 KB. This problem relating to PC memory limitation was overcome by overlaying some of the routines, which resulted in the increase of the execution time. Currently, another possible solution to memory requirement is to compile the routines with a commercial software called as "DOS Extender" by PHARLAP Inc. This software does not involve overlays, will not slow the execution of the program, and also allows larger programs to be run.

Another option that has been made available in this program is the ZOOM option which can display all the volumetric, calorimetric and phase equilibrium values of a single data point in one single screen. The detailed information provided by this option will enable the user to

obtain additional thermodynamic properties typically not available in similar routines. In addition, some of the information provided are most useful in investigating calculation failures.

## CHAPTER IX

### CONCLUSIONS AND RECOMMENDATIONS

This work has dealt with the design and development of a user interface for the GEOS software (Gasem, 1988) used for predicting volumetric, calorimetric and phase equilibrium properties of nonelectrolyte fluids. The pertinent conclusions and recommendations arising from this work are given below.

#### Conclusions

1. A user interface for the GEOS program was developed using the interface development software HI-Screen. Unique interactive panels were developed to render GEOS a more accessible program for the prediction of volumetric, calorimetric, and equilibrium properties of nonelectrolyte fluids using both the equation of state and the split approach.
2. The results obtained using the interface version of the GEOS were found to be identical numerically to those of the original Fortran code without the interface.
3. The CPU time for execution of the GEOS program increased as the size of the program was increased to accommodate the interface routines.
4. The limitations on the base memory of the personal

computer, which is 640KB, restricted the use of GEOS without having to overlay the Fortran routines to accommodate the necessary interface features.

### Recommendations

Efforts should be undertaken to:

1. develop the HELP screens into a knowledge-based system to assist in problem formulation and error interpretation,
2. use the commercial software "DOS Extender" which will help overcome some of the present memory limitations and speed up the execution of the program,
3. develop the GEOS graphic routines in "C" to provide for the online graphs and interactive graphic input facility,
4. add a pure-fluid database to GEOS to facilitate the input of the required physical properties, and
5. develop a unit analysis capability based on the GEOS facility. This will enable users to analyze process units of a given flow sheet more efficiently, prior to implementing a full process simulator.

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APPENDIX A  
INTERFACE SCREENS

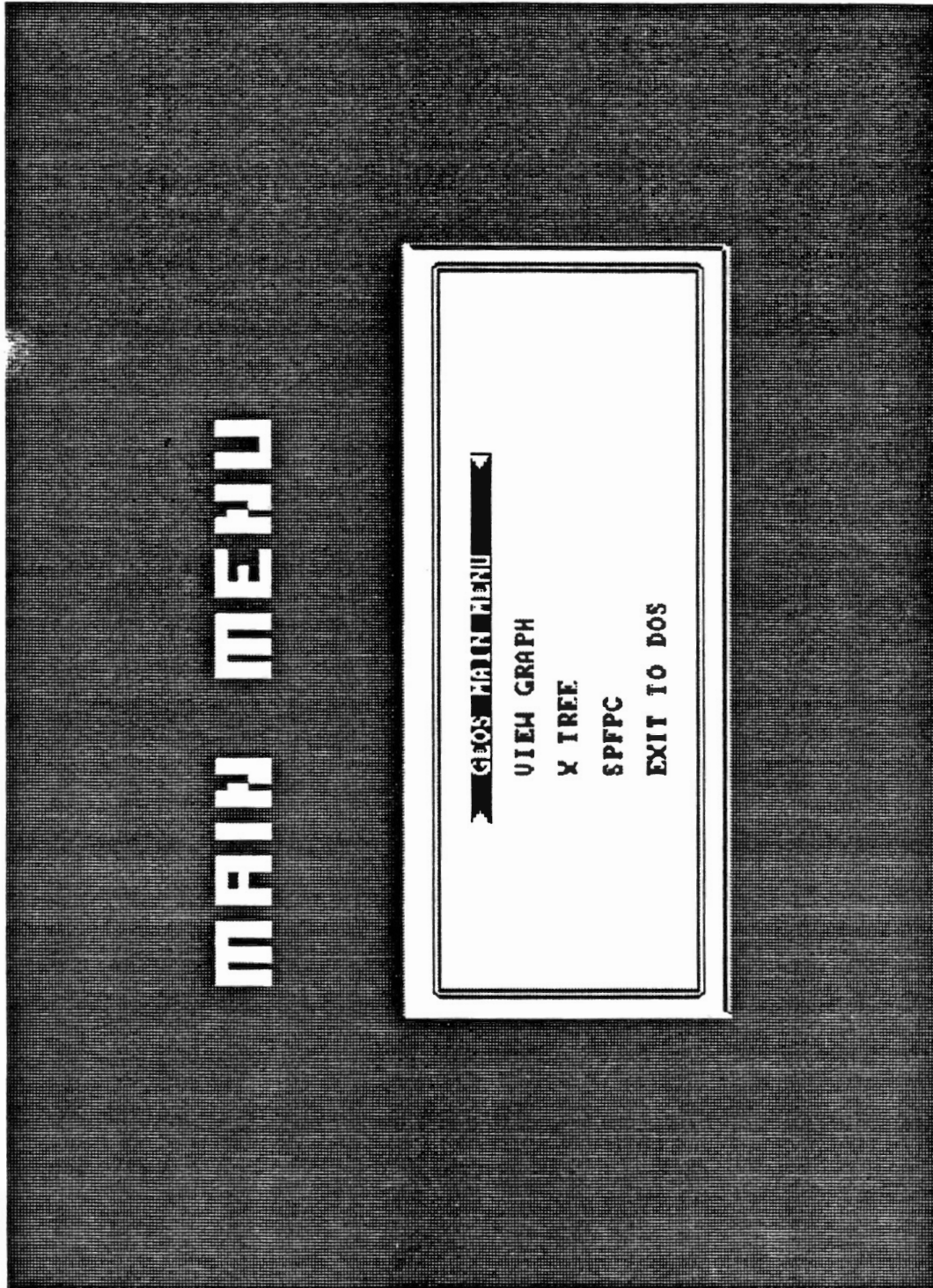


Figure 1. G E O S Opening Menu



Figure 2. G E O S Main Menu

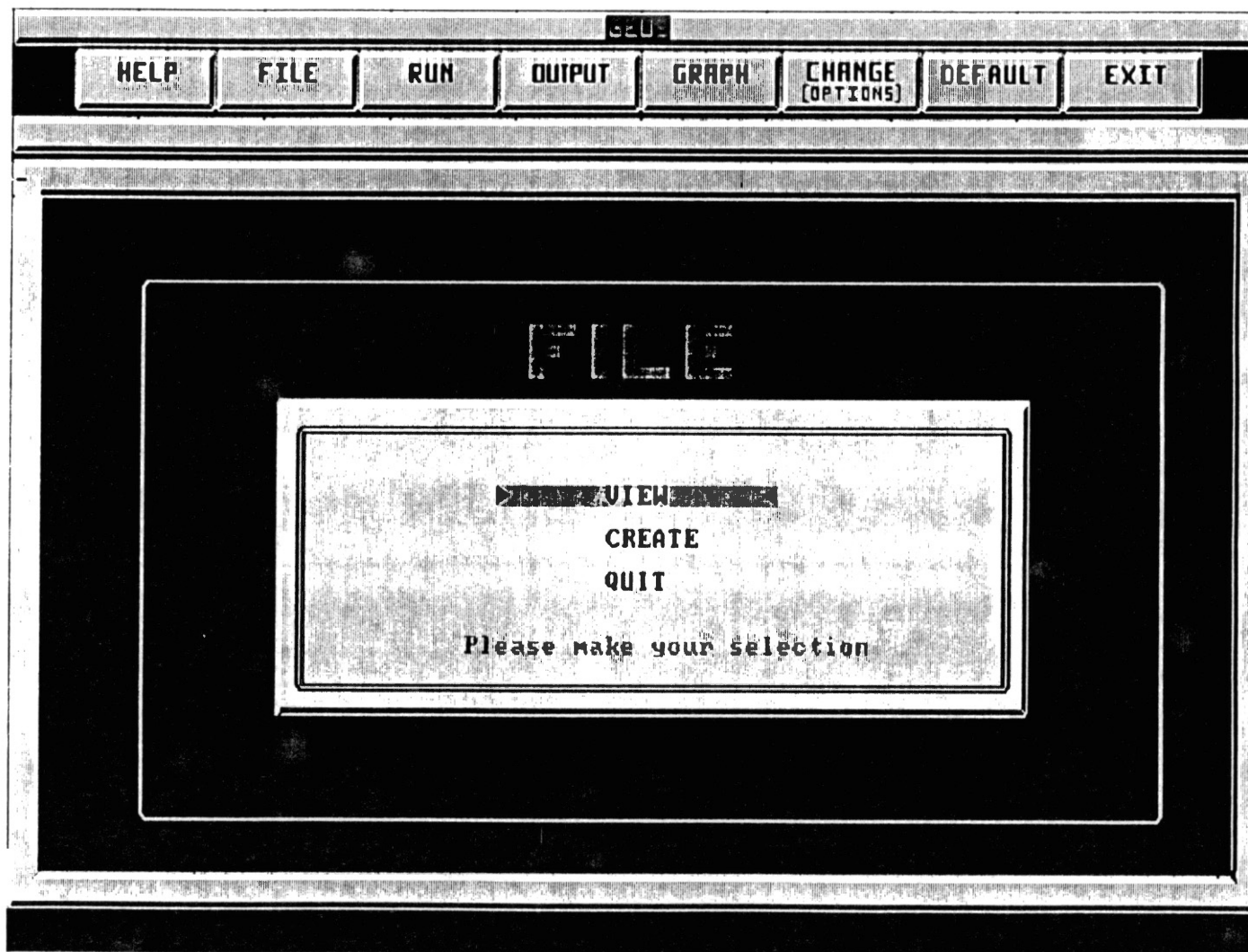


Figure 3. File View / Create Menu

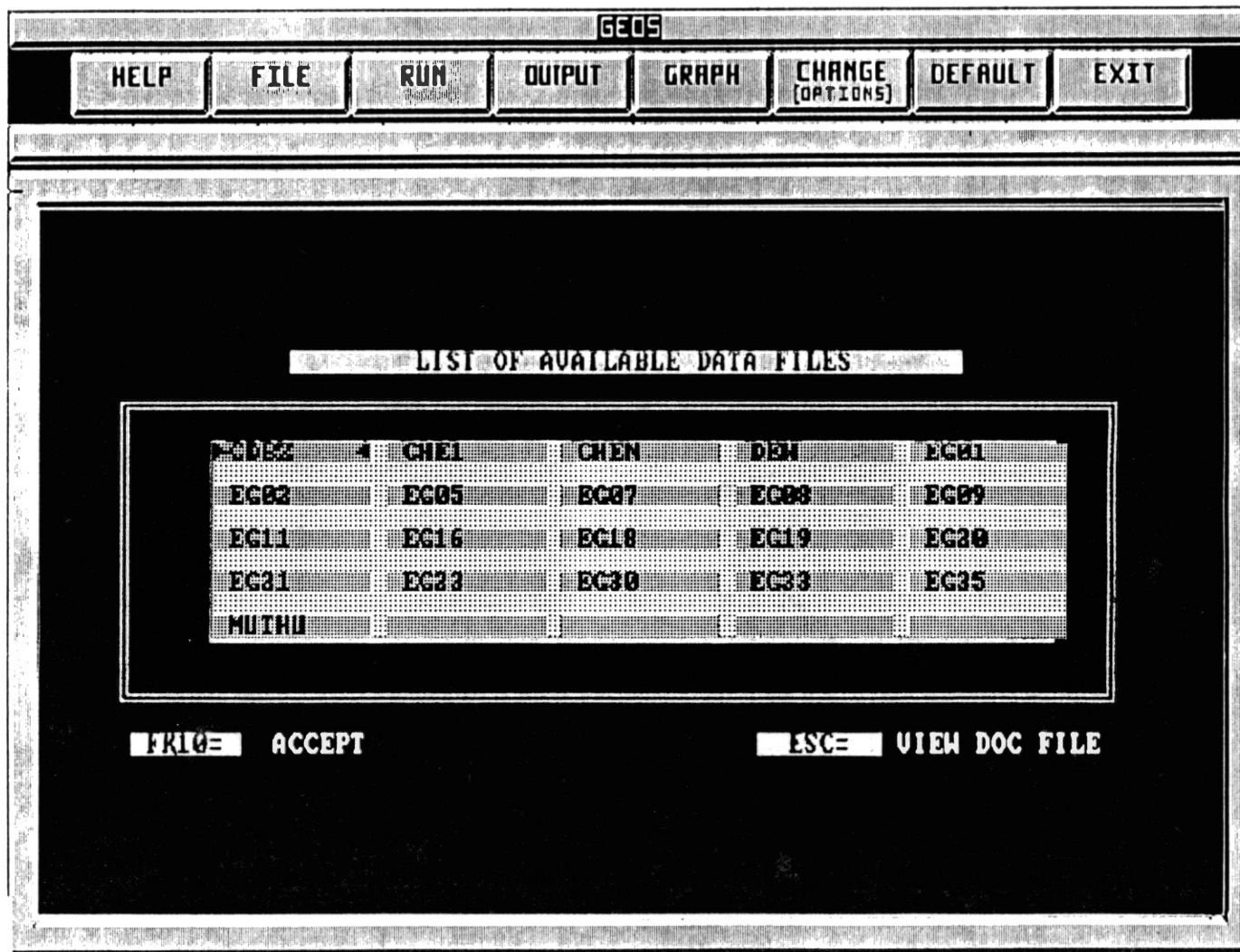


Figure 4. List of Data Files Menu

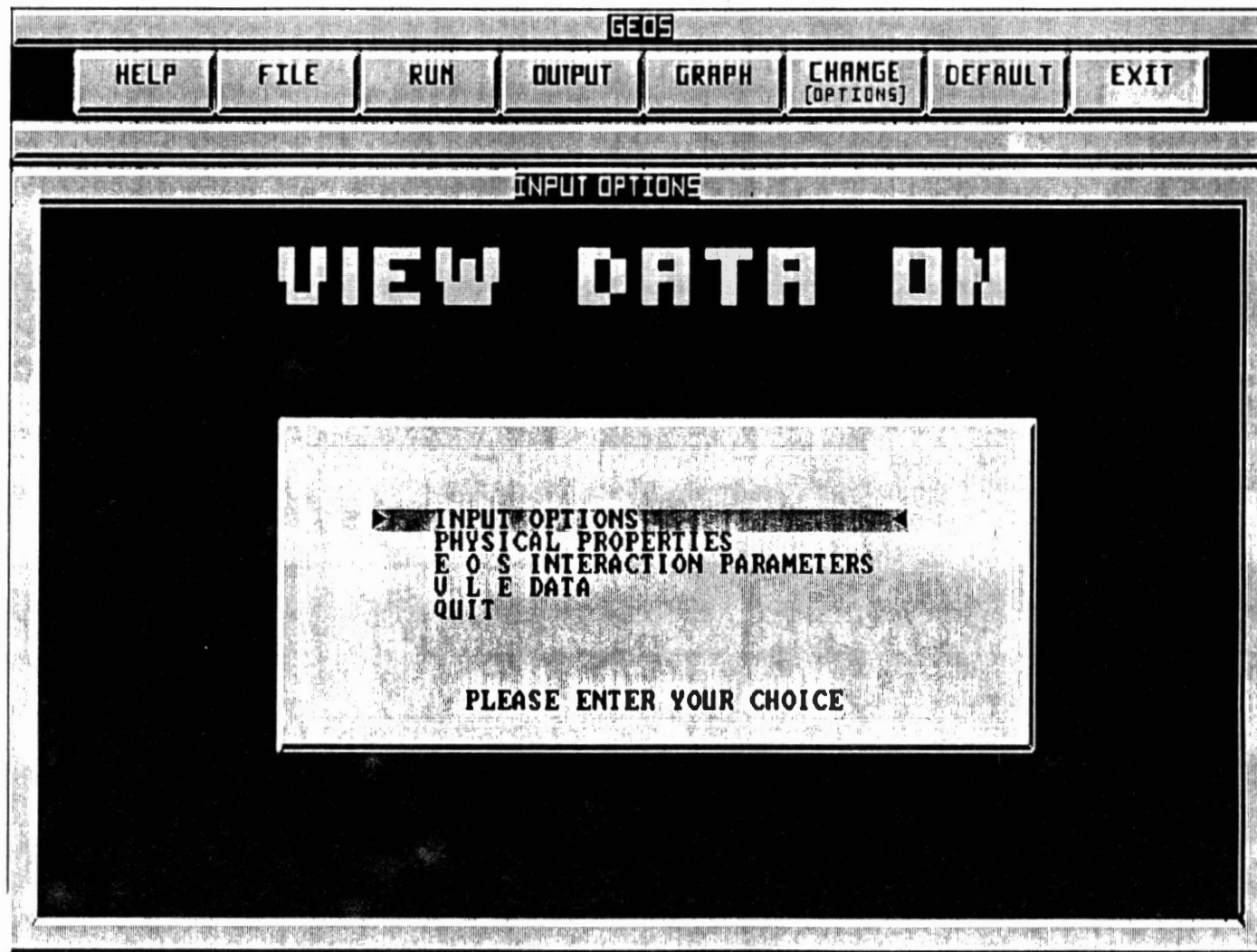


Figure 5. Input Options Selection Menu

GEOS

HELP    FILE    RUN    OUTPUT    GRAPH    CHANGE (OPTIONS)    DEFAULT    EXIT

---

HELP (PRESS F1)    CANCEL (ESC)    EDIT (FK2)    VALIDATE (F10)

FILE = EG01

MODE	OPTION	METHOD	EOS	MODEL	F-REF	UP-MOD	UP-GN	UOL-T
1	4	1	5	5	2	2	0	0
NC	NPTS	INPUT	UNITS	I-OUT	HEIGHT	TRIVIAL		
2	10	1	1	0	0	0		

<b>MODE</b>	0	OPTIMIZE	1	PREDICT	<b>EOS</b>	0	IDEAL GAS	<b>F-REF</b>	1	FL(T,P)
						1	UIRIAL		2	FL(T,UP)
<b>OPTION</b>	1	LIQUID VOLUME(S & H)				2	VAN DER WAALS		3	FL(T,P,X)
	2	VAPOR VOLUME				3	REDLICH-KWONG			
	3	LIQ & VAP VOLUME				4	SOAVE-REDLICH-KWONG	<b>UP-MOD</b>	1	SURC
	4	ISOTHERMAL FLASH				5	PENG-ROBINSON		2	ANTOINE
	5	BUBBLE-P PRESSURE						<b>UP-GN</b>	1	YES
	6	BUBBLE-P TEMPERATURE	<b>MODEL</b>	1	IDEAL SOLUTION				0	NO
	7	DEW-P PRESSURE		2	WILSON			<b>UOL-T</b>	1	YES
	8	DEW-P TEMPERATURE		3	VAN LAAR				0	NO
	9	Z MAPPING		4	MARGULES					
				5	UNIFAC					
<b>METHOD</b>	1	SINGLE MODEL								
	2	TWO MODEL								

Figure 6. Input Options Screen



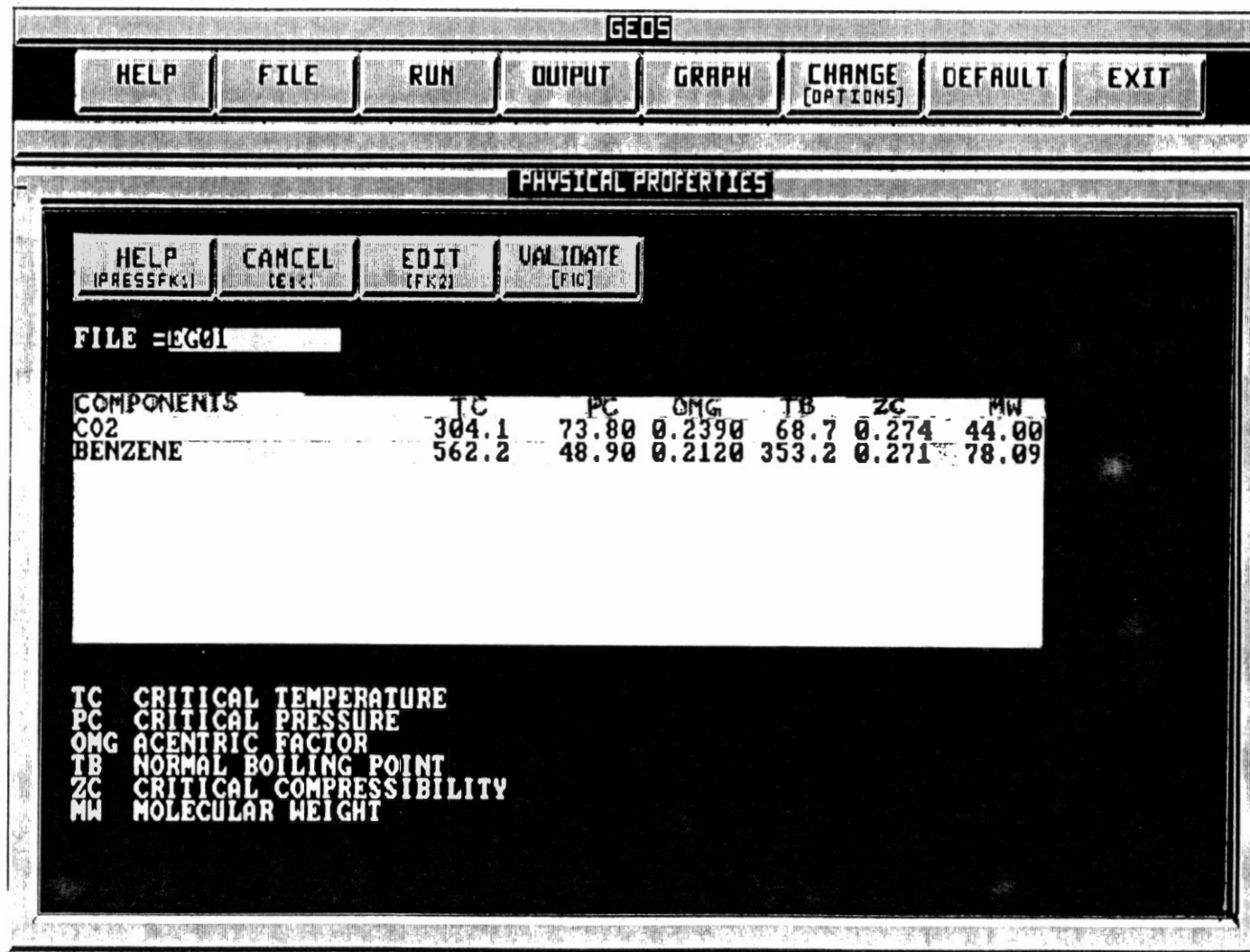


Figure 7. Physical Properties Screen



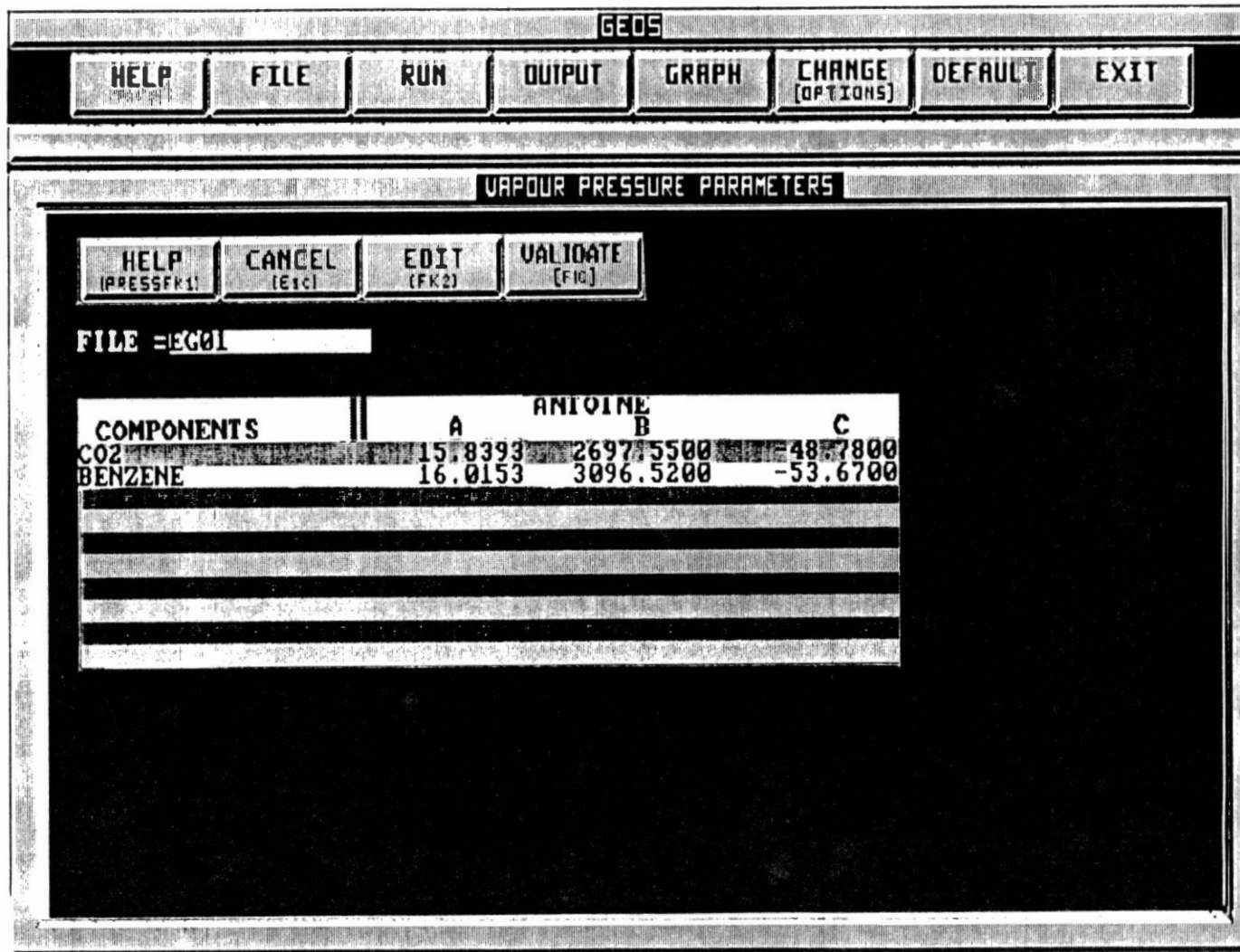


Figure 8. Vapor Pressure Parameters Screen

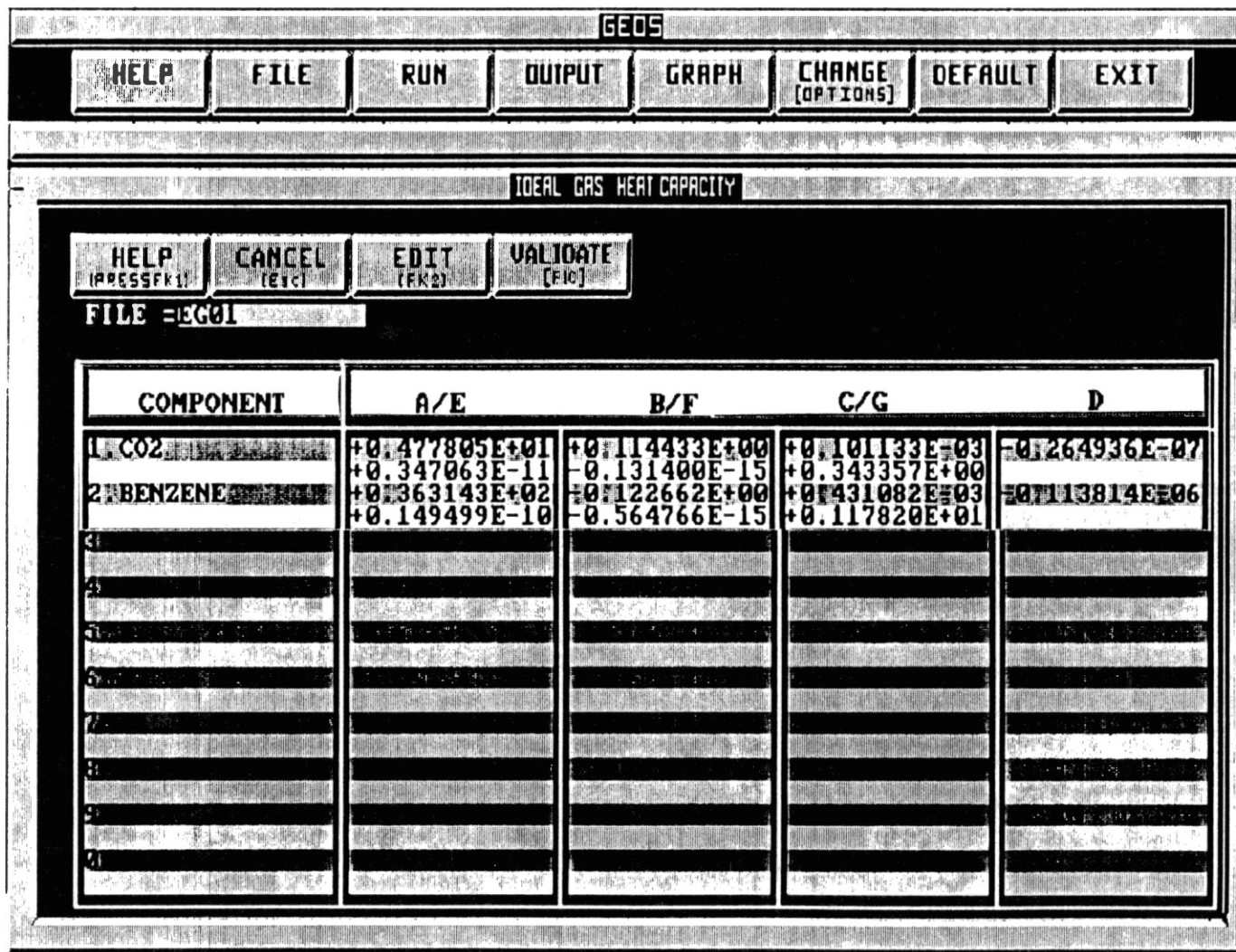


Figure 9. Ideal Gas Heat Capacity Screen

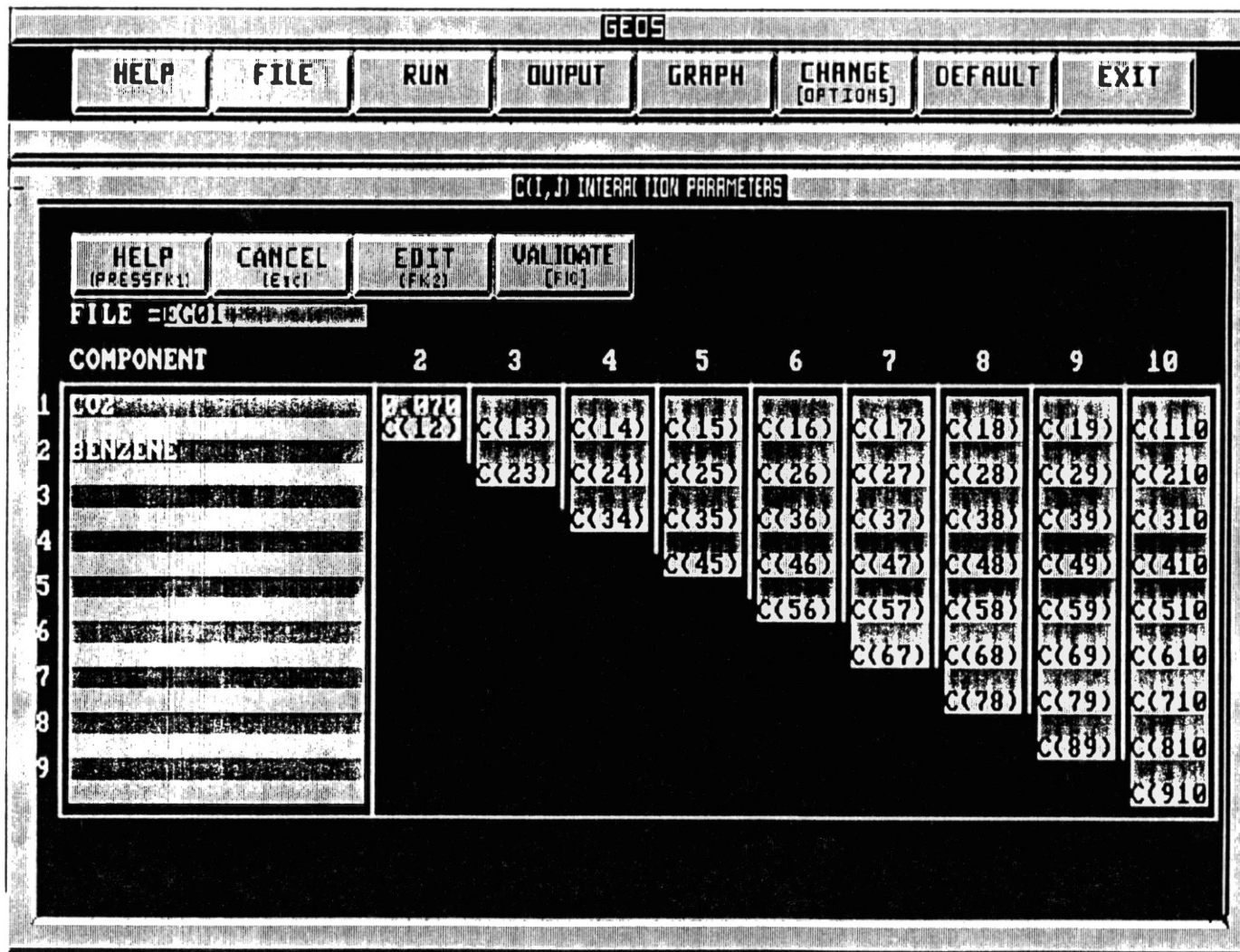


Figure 10. C(i,j) Interaction Parameters Screen

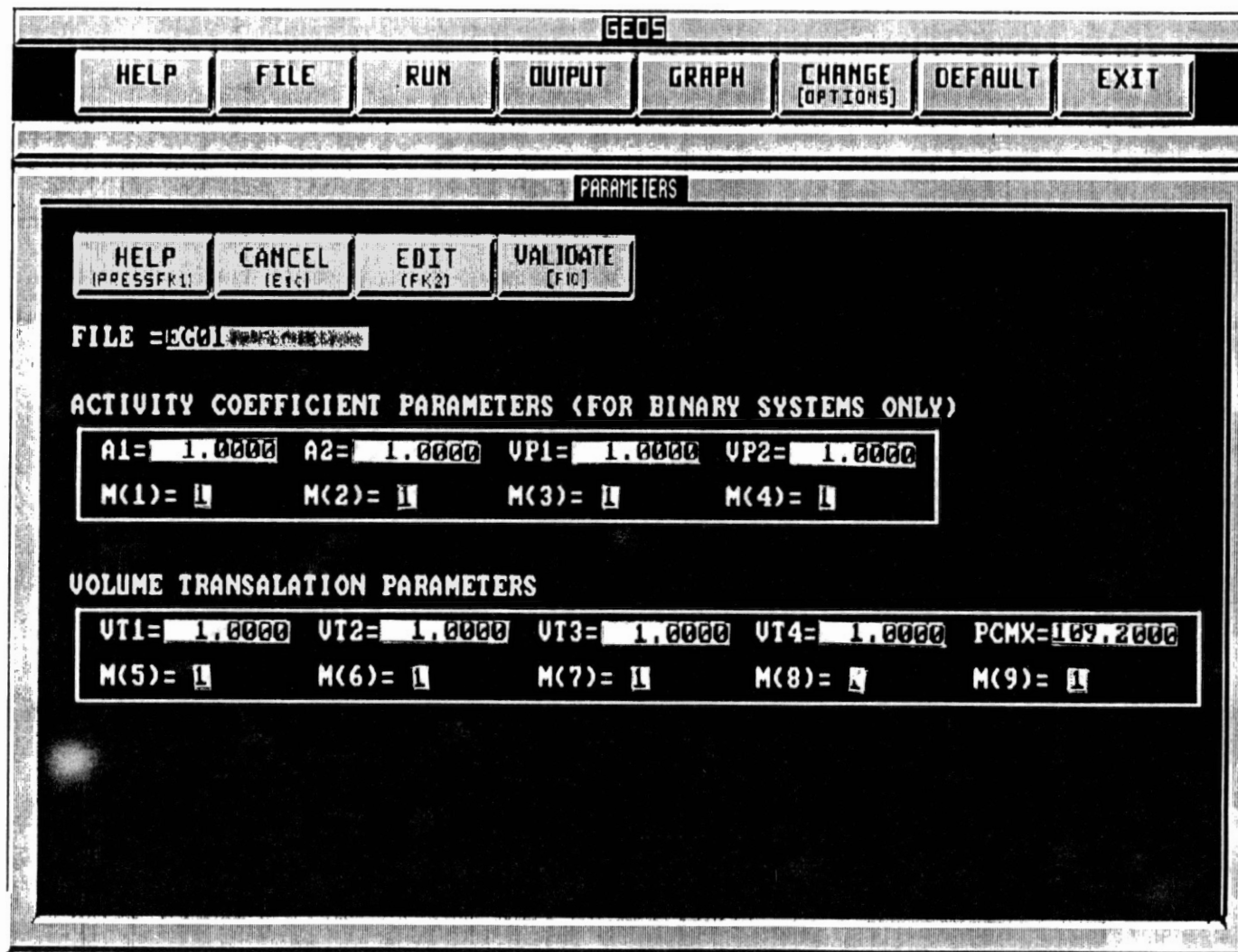


Figure 11. Activity Coefficient Parameters

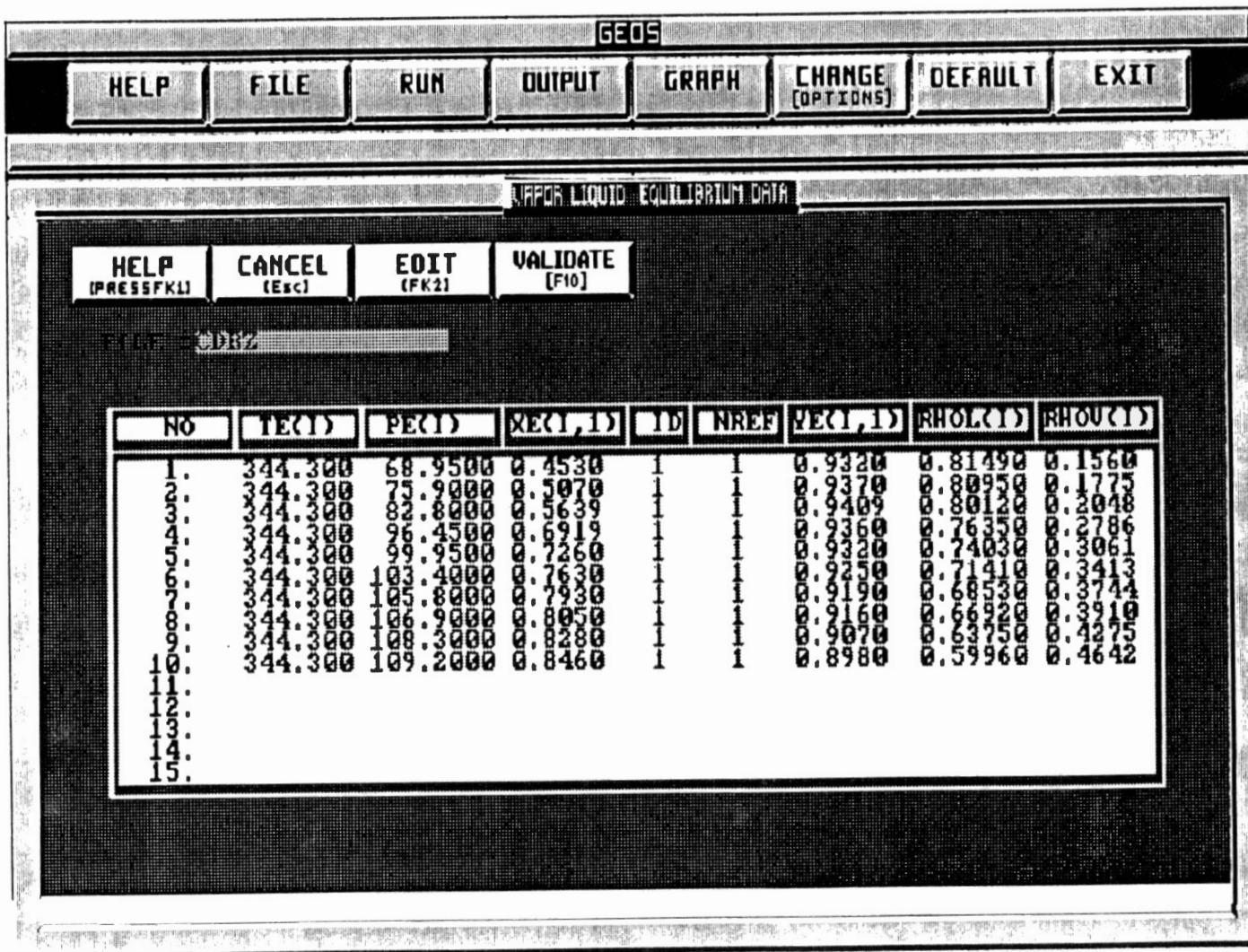


Figure 12. Vapor-Liquid Equilibrium Data Screen

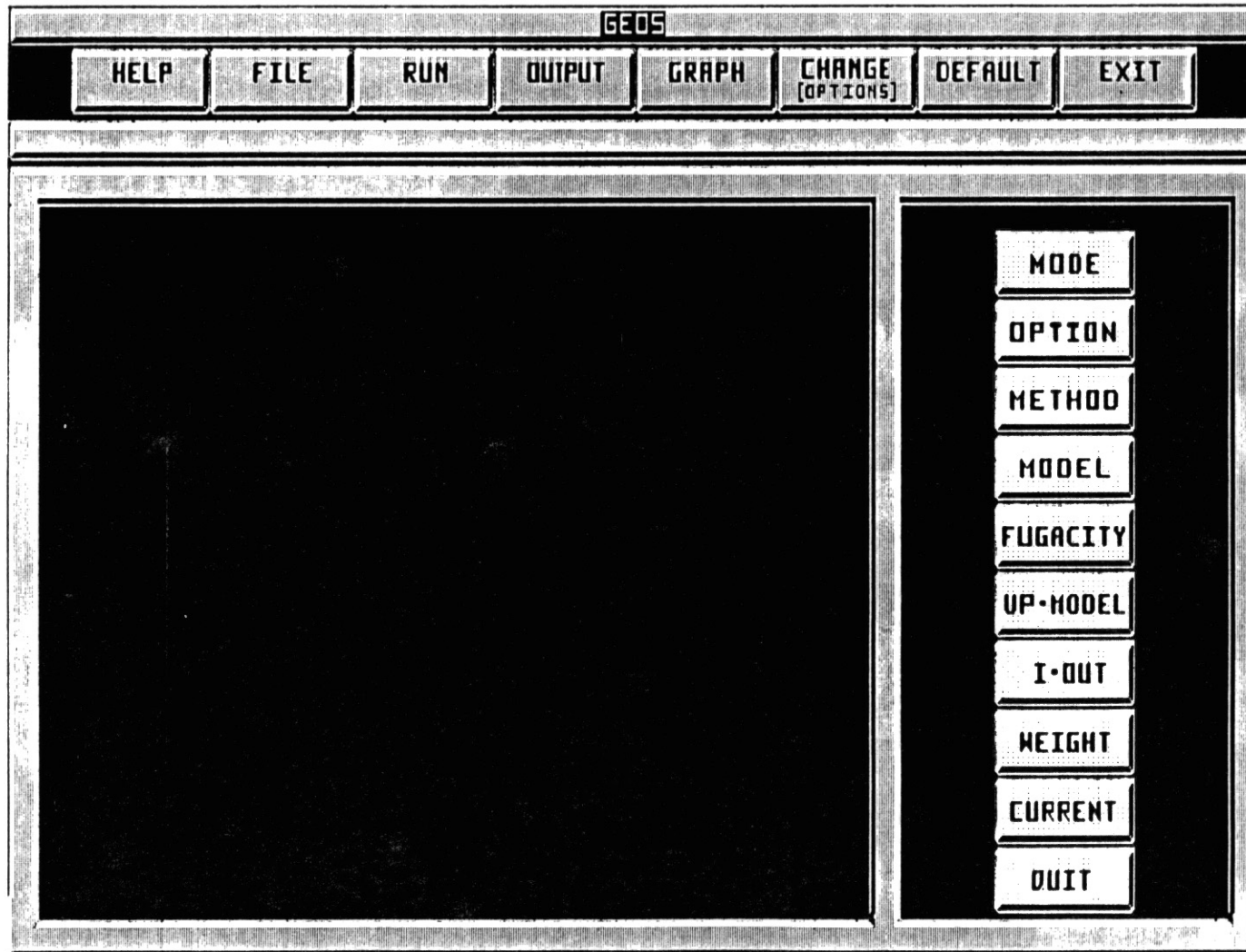


Figure 13. Change Options Menu



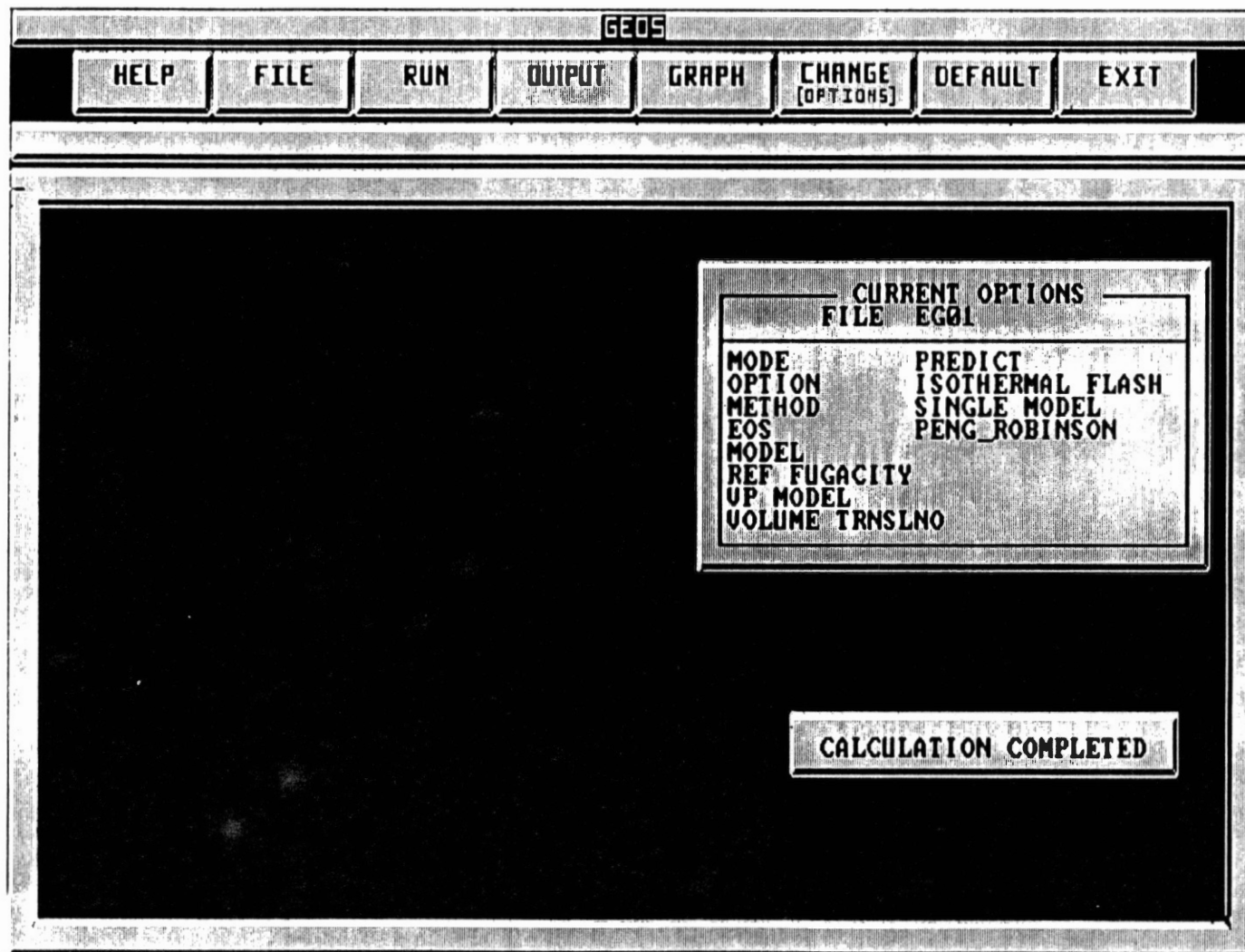


Figure 14. Display of Current Options for Run

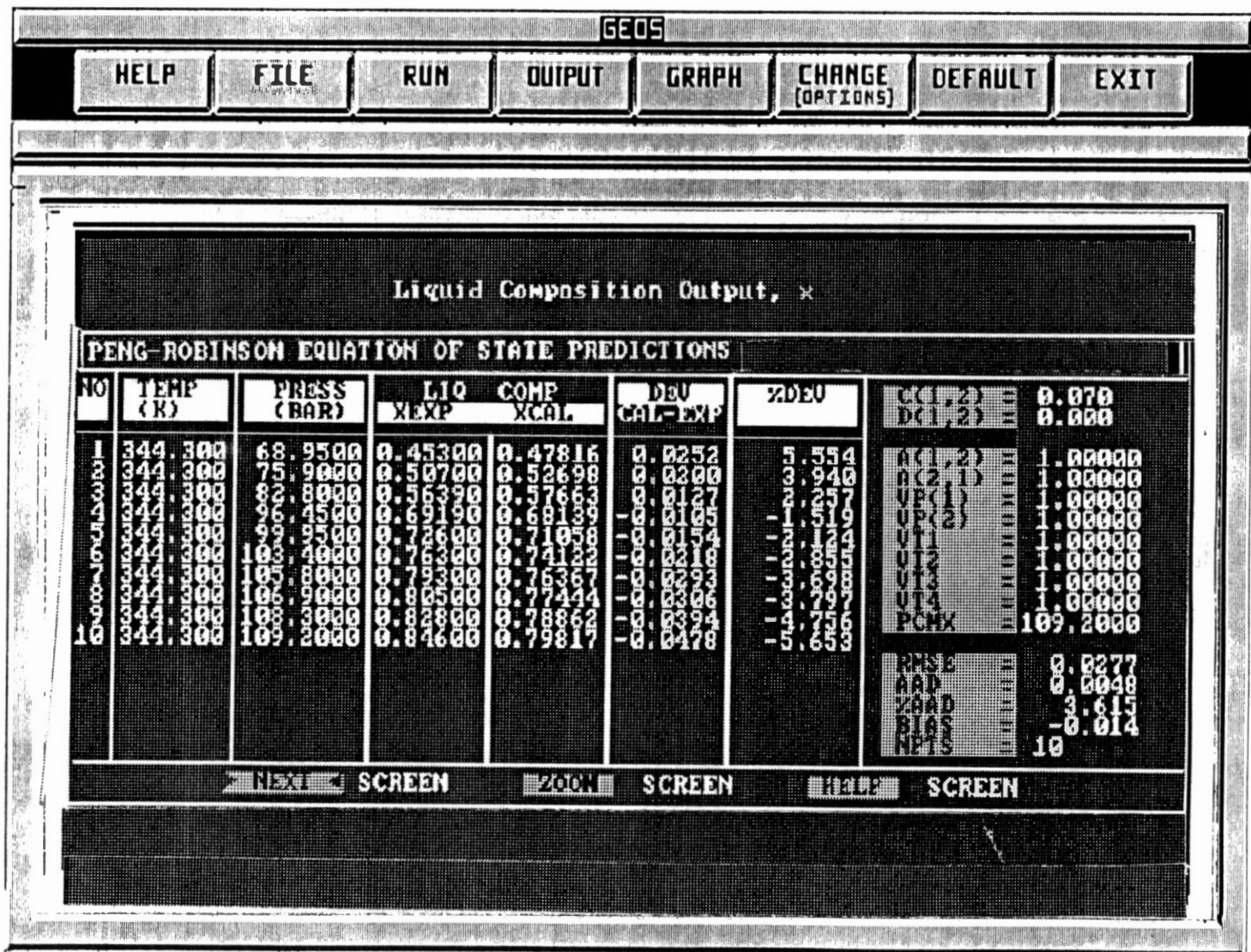


Figure 15. Liquid Composition Output Screen



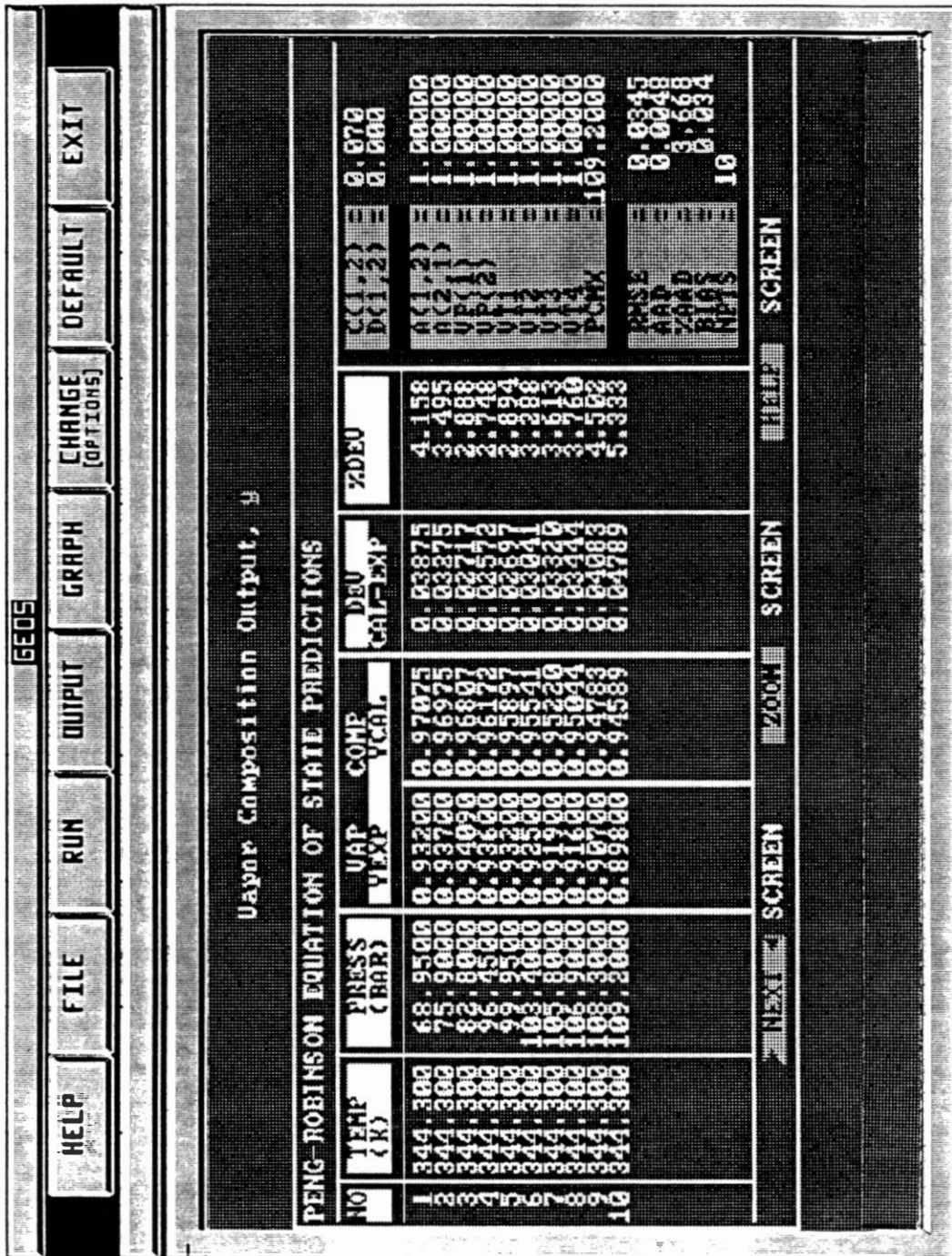


Figure 16. Vapor Composition Output Screen

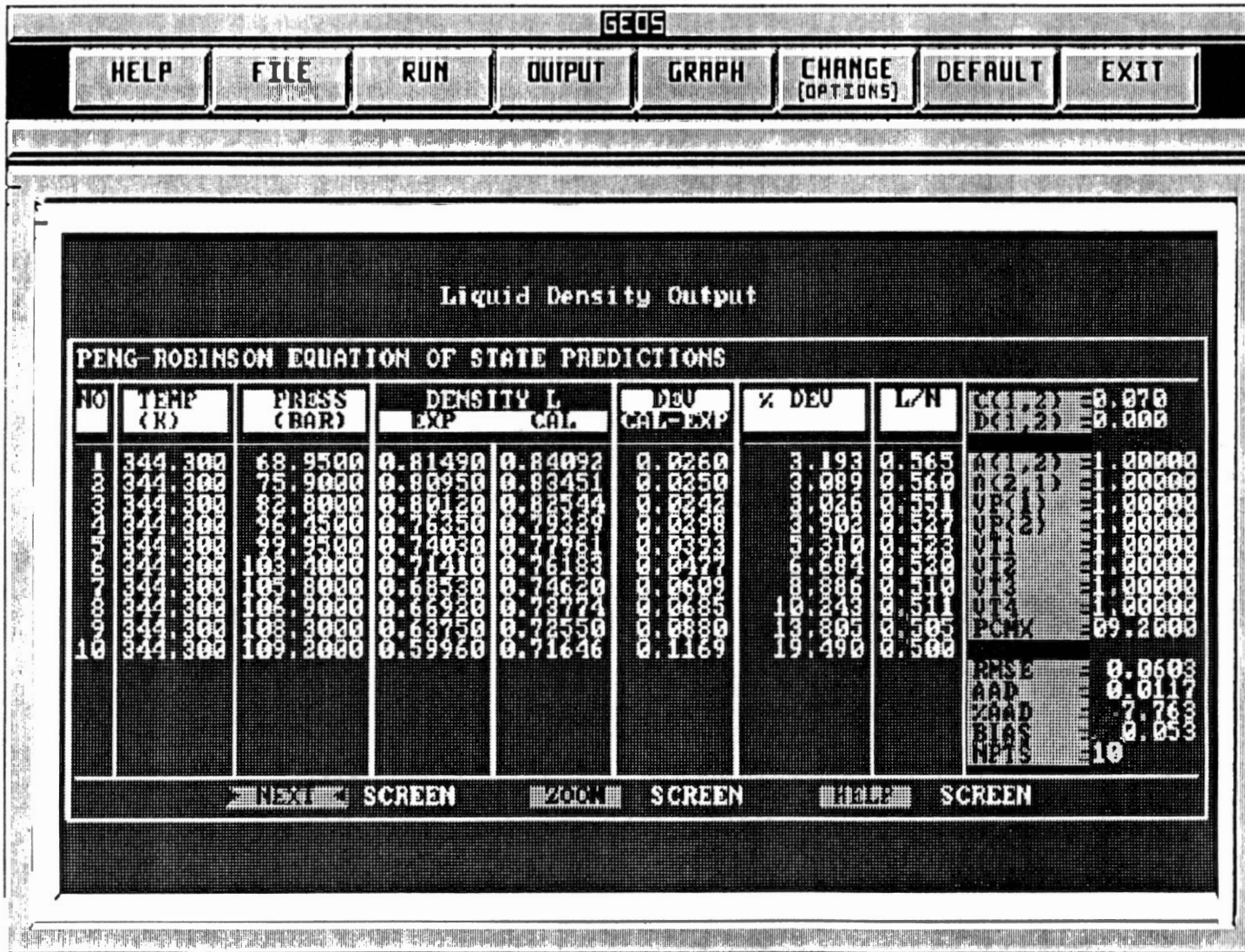


Figure 17. Liquid Density Output Screen

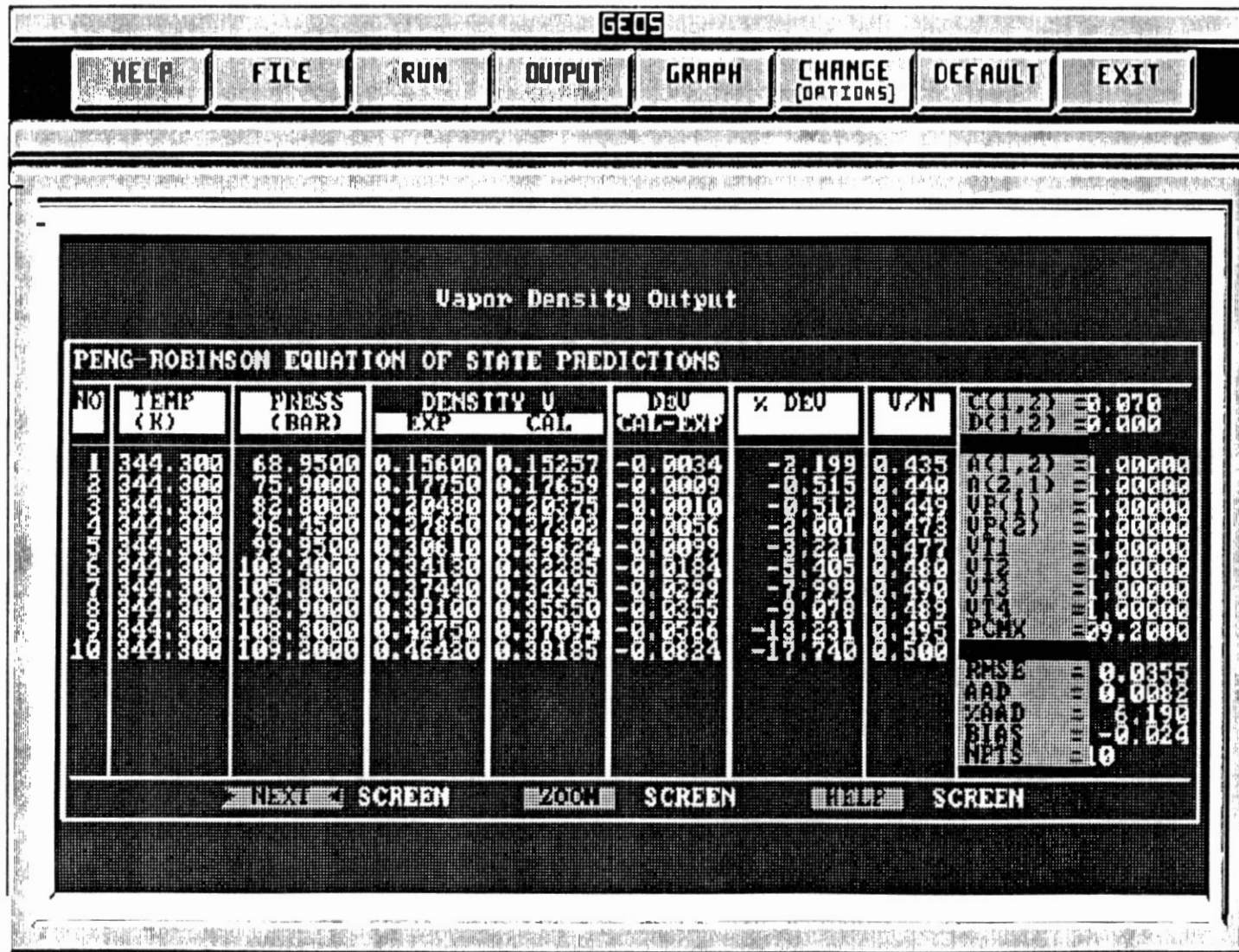


Figure 18. Vapor Density Output Screen

HELP

FILE

RUN

OUTPUT

GRAPH

CHANGE  
[OPTIONS]

DEFAULT

EXIT

```

UPDATE I, KM, J, DLC(I), DUC(I), KC(I, J)
2 8 2 .834518 .176586 .063955
UPDATE PHU(I, J), ACL(I, J), FLR(I, J)
2 2 8 .231438 .000000 .000000
UPDATE UP(J), PHIPURE
2 2 8 .000000 .000000
ALFA=..... .559539
FLASH KM, I, J, XC(I, J), YC(I, J), ALFA
2 8 2 .473024 .030252 .559539
    
```

```

CUBIC:  I KK      ZC      TEST
CUBIC:  3  1      .707682 .085818
    
```

— CURRENT OPTIONS —  
FILE CDBZ

```

MODE          PREDICT
OPTION         ISOTHERMAL FLASH
METHOD        SINGLE MODEL
EOS           PENG_ROBINSON
MODEL
REF FUGACITY
UP MODEL
VOLUME TRNSLNO
    
```

CALCULATION IN PROGRESS

Figure 19. Intermediate Option Screen



GEOS

HELP	FILE	RUN	OUTPUT	GRAPH	CHANGE [OPTIONS]	DEFAULT	EXIT
------	------	-----	--------	-------	---------------------	---------	------

ZOOM FOR DATA POINT NO

TEMPERATURE =  PRESSURE =

COMPONENTS	MOLE FRACTION			EQUIL. CONSTANT K	FUGACITY, f	
	FEED z	LIQUID x	VAPOR y		LIQUID	VAPOR
CO2	0.958969	0.710577	0.958969	1.3496	67.21638	67.21462
BENZENE	0.041031	0.289423	0.041031	0.1418	0.46583	0.46586

PROPERTIES	LIQUID	VAPOR	OVERALL
PHASE MOLAR RATIO	0.523241	0.476759	1.000000
COMPRESSIBILITY FACTOR Z	0.241256	0.535103	--
PHASE DENSITY D(GM/CC)	0.779607	0.296239	--
MOLAR VOLUME U(CC/MOL)	+0.691E+02	+0.153E+03	+0.109E+03
ENTHALPY H(KJ/MOL)	+0.799E+01	+0.745E+01	+0.773E+01
ENTROPY S(KJ/MOL/K)	+0.238E+00	+0.150E+00	+0.196E+00
INTERNAL ENERGY U(KJ/MOL)	+0.730E+01	+0.591E+01	+0.664E+01
HELMHOLTZ ENERGY A(KJ/MOL)	-0.746E+02	-0.456E+02	-0.608E+02
GIBBS FREE ENERGY G(KJ/MOL)	-0.739E+02	-0.440E+02	-0.597E+02

←NEXT SCREEN

ZOOM SCREEN

HELP SCREEN

Figure 20. Zoom Option Screen

APPENDIX B

FORTRAN FLOW SHEETS

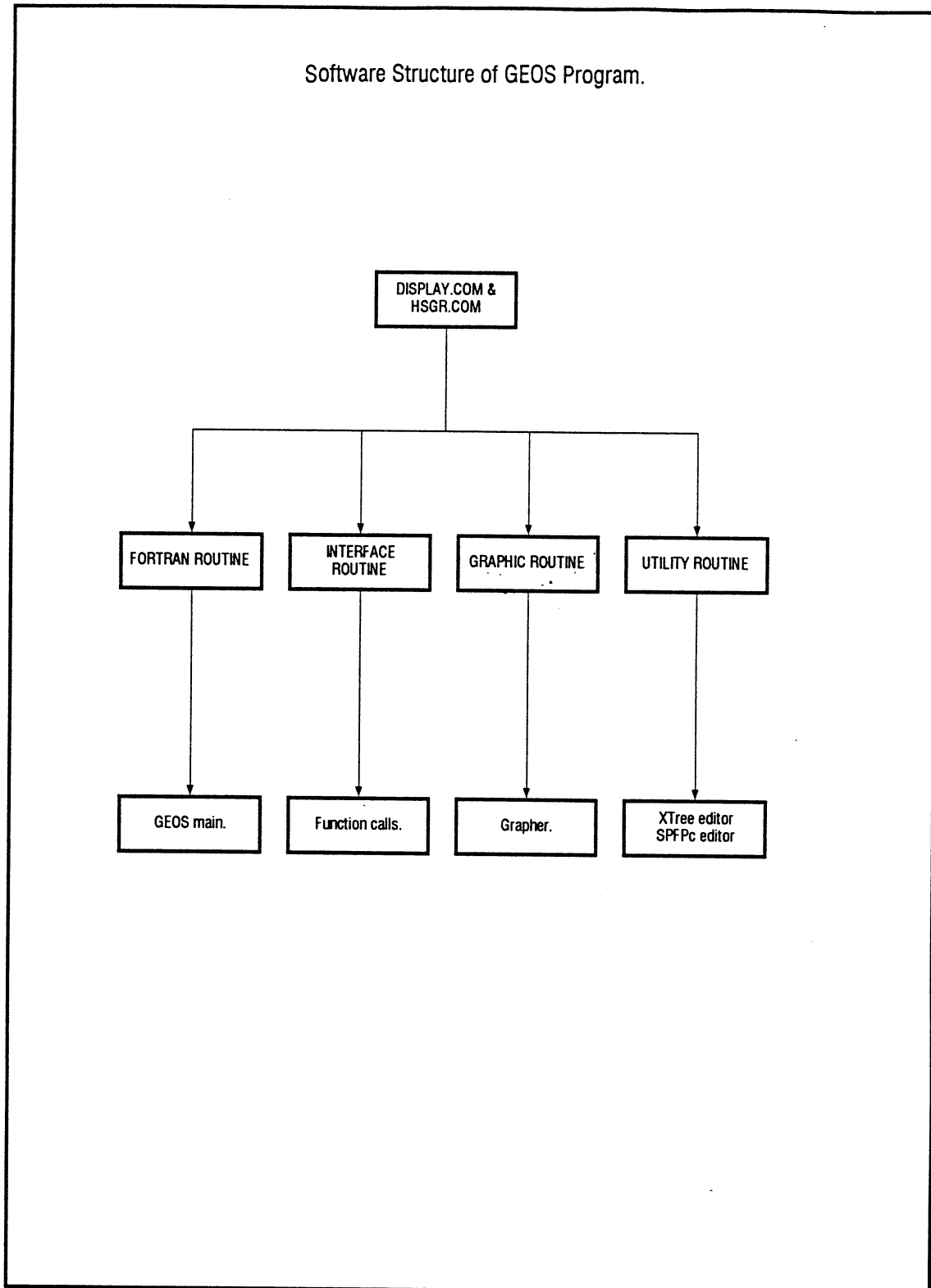


Figure 21. Software Structure of GEOS Program

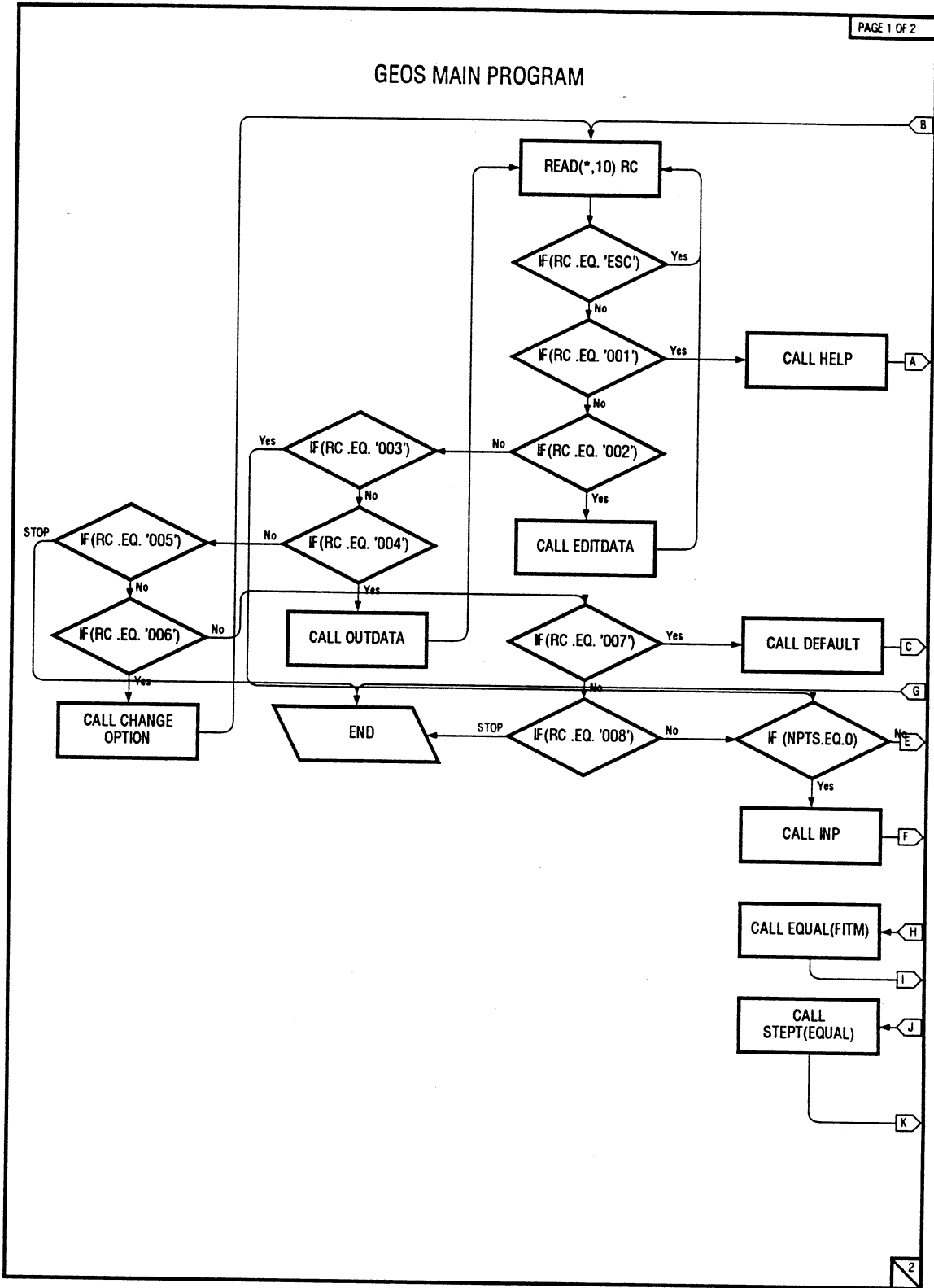


Figure 22. Flow Diagram for GEOS Main



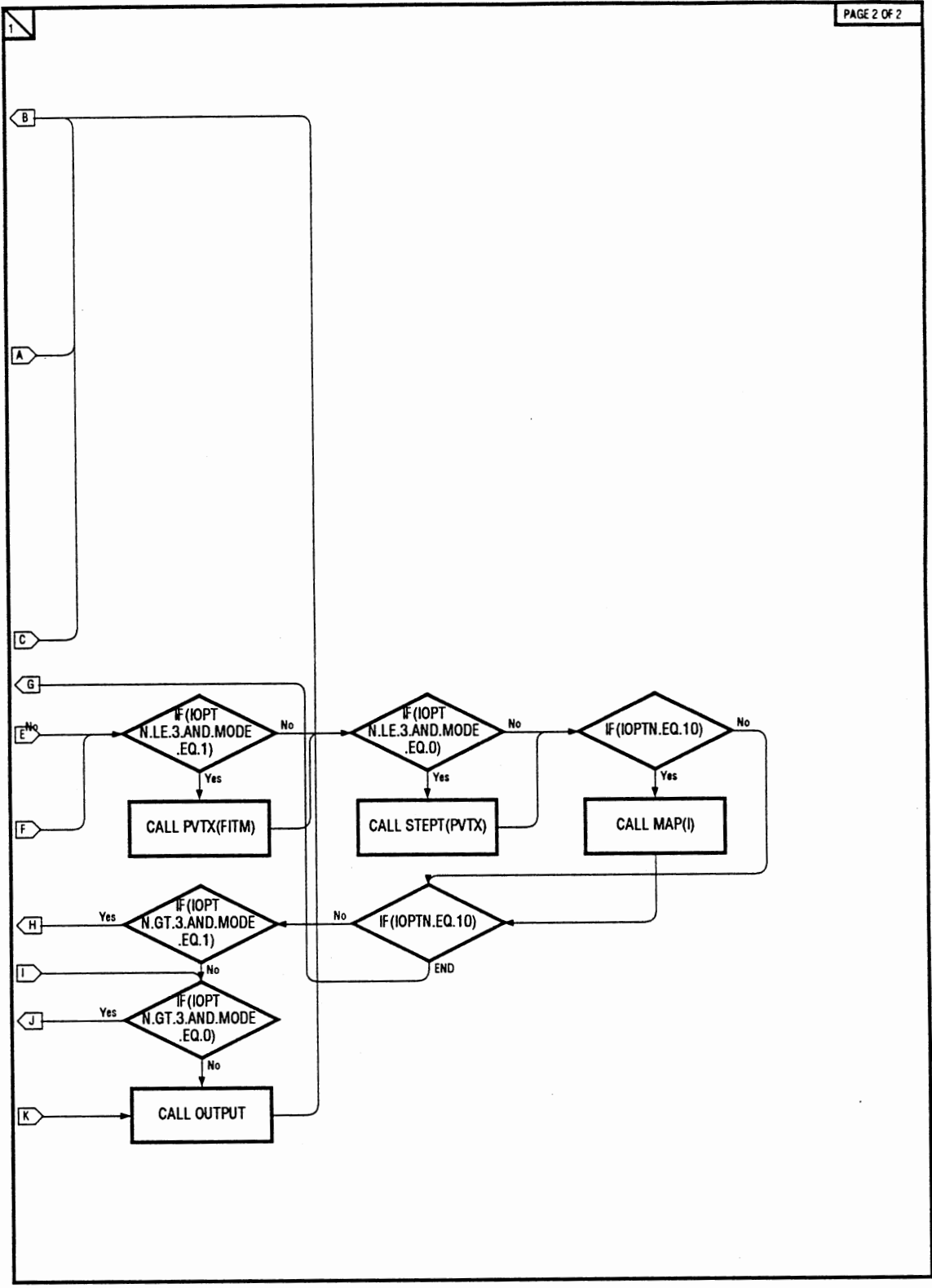


Figure 22. Continued

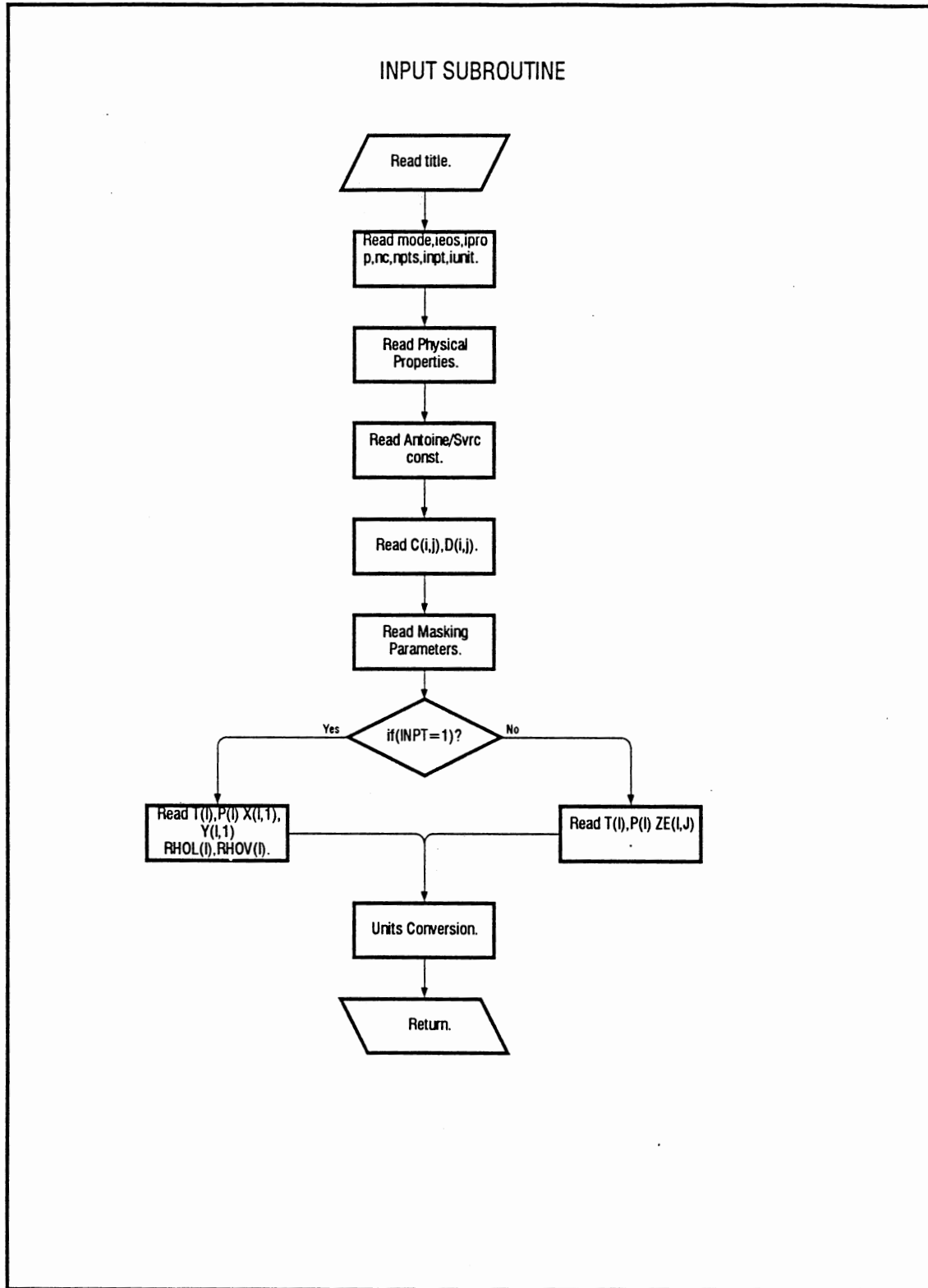


Figure 23. Flow Diagram for INPUT Subroutine

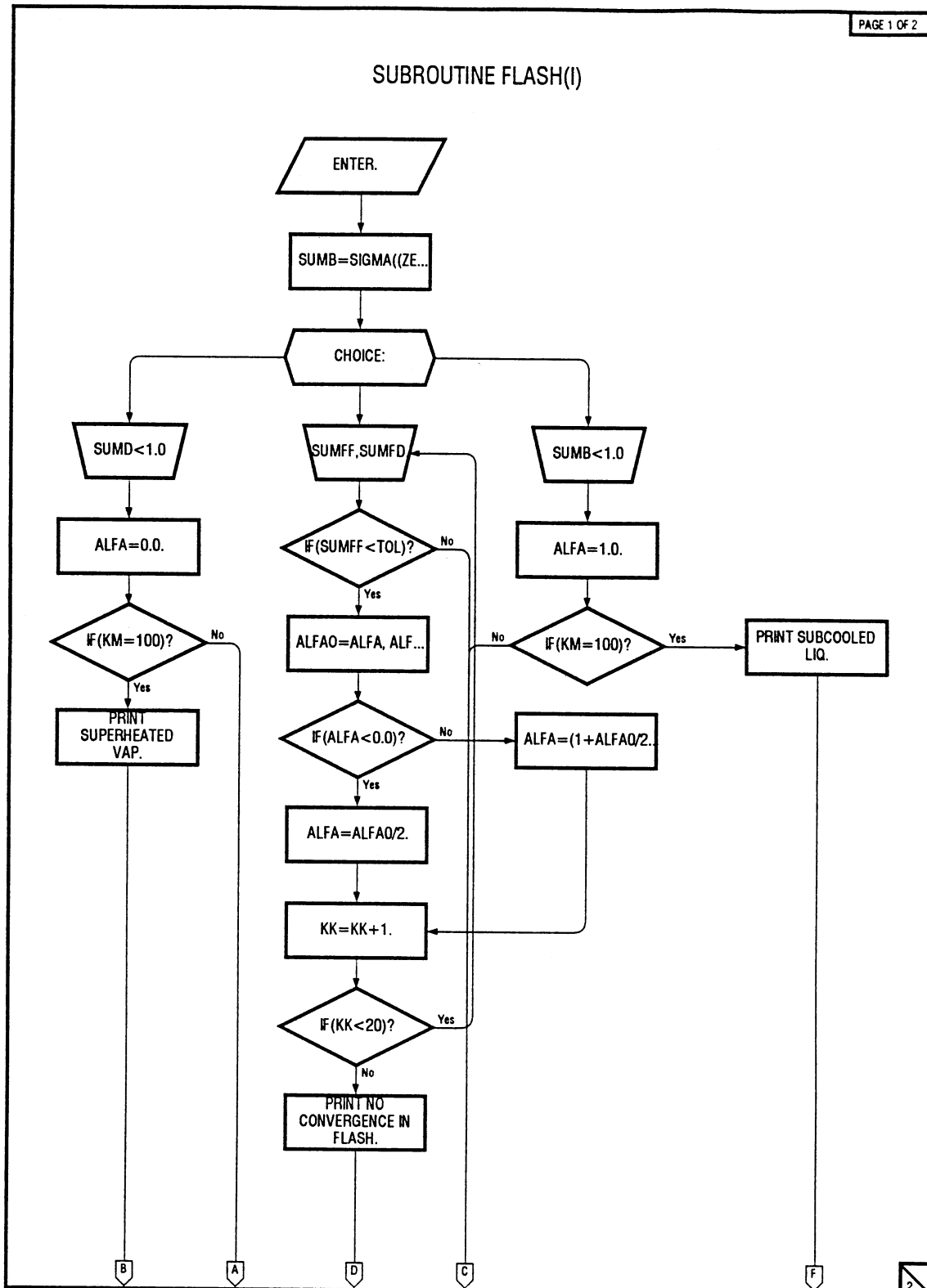


Figure 24. Flow Diagram for FLASH(I) Subroutine

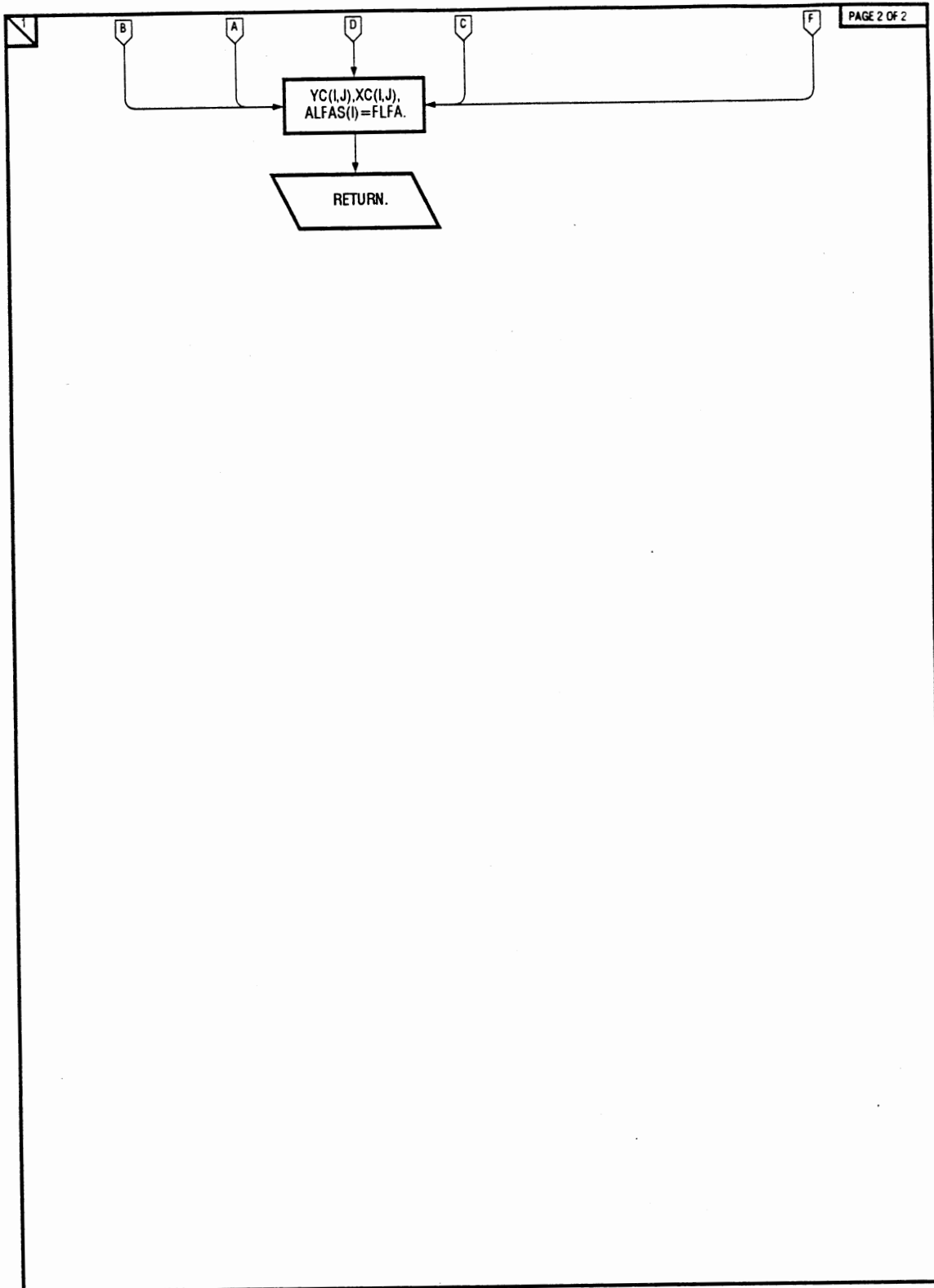


Figure 24. Continued

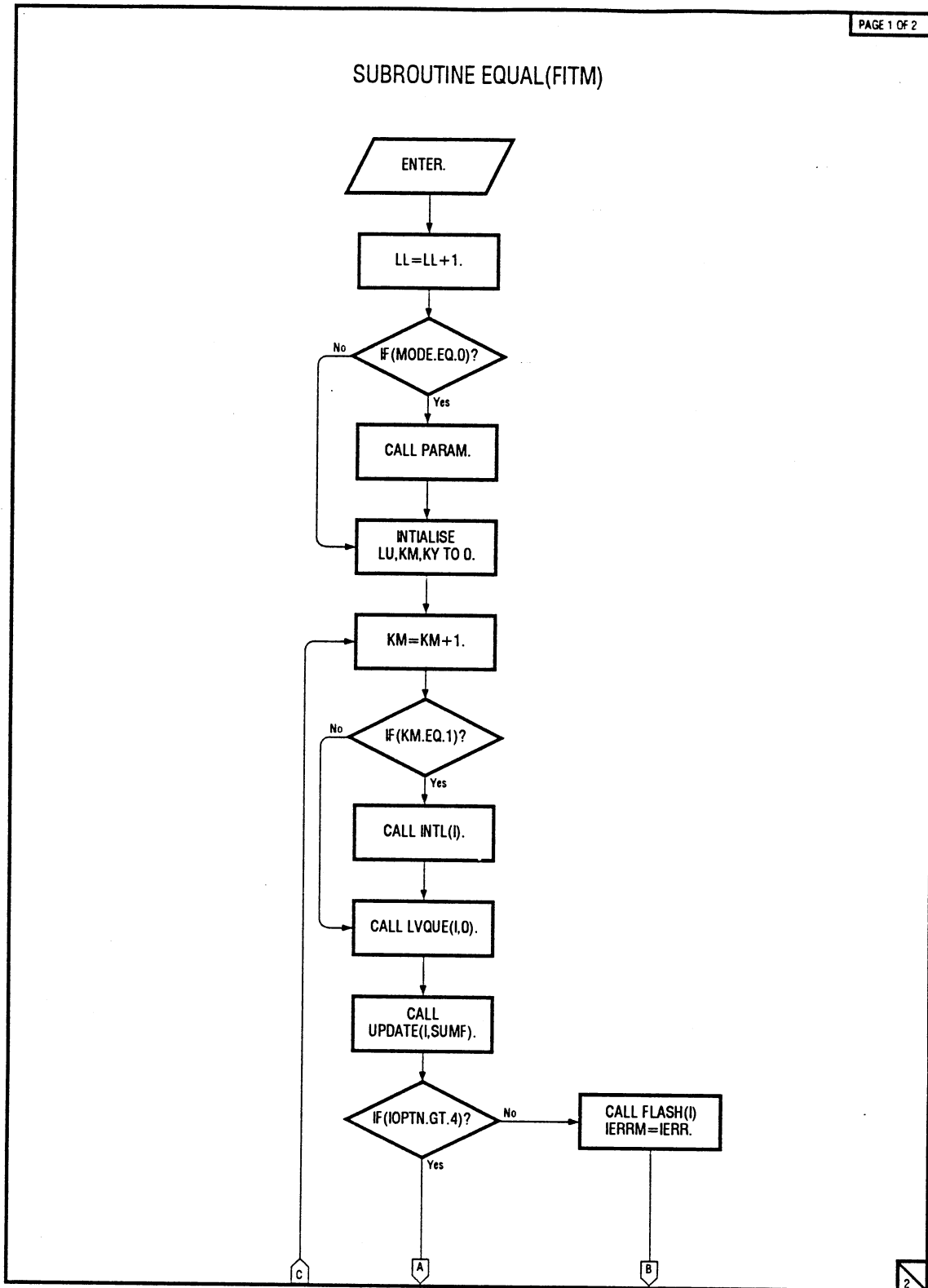


Figure 25. Flow Diagram For EQUAL(FITM) Subroutine

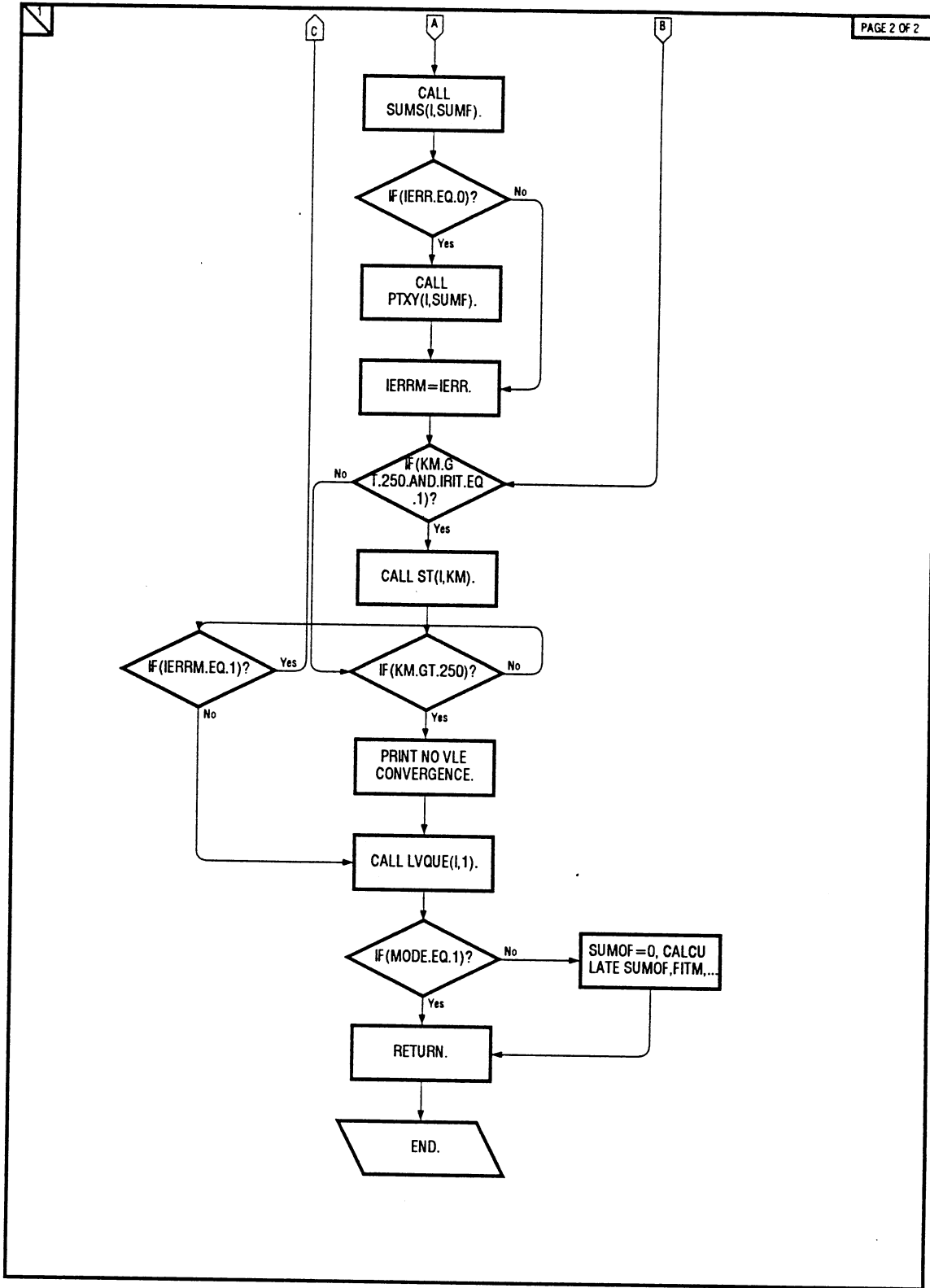


Figure 23. Continued

SUBROUTINE PTXY(I,SUMF)

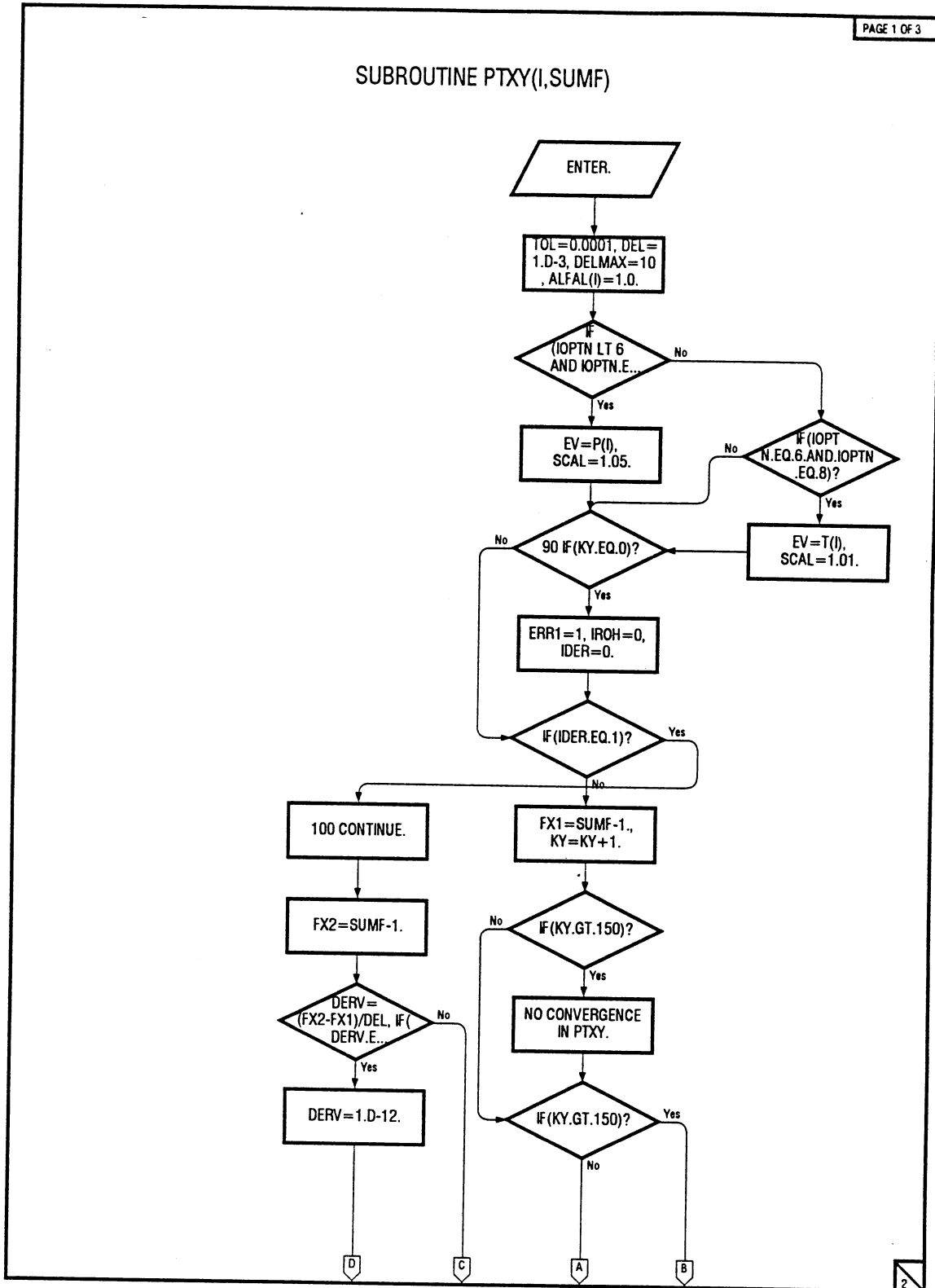


Figure 26. Flow Diagram for PTXY(I,SUMF) Subroutine

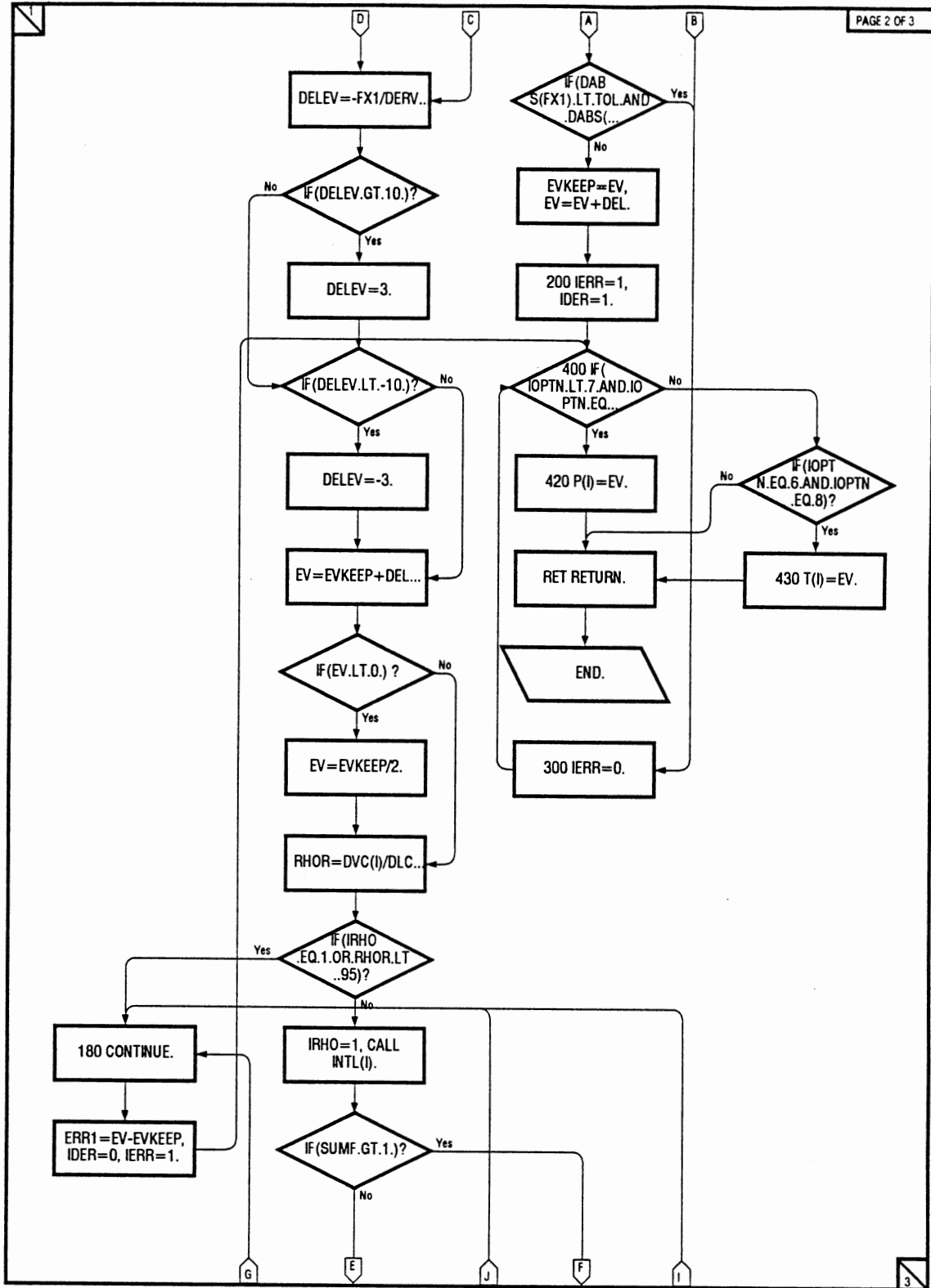


Figure 26. Continued



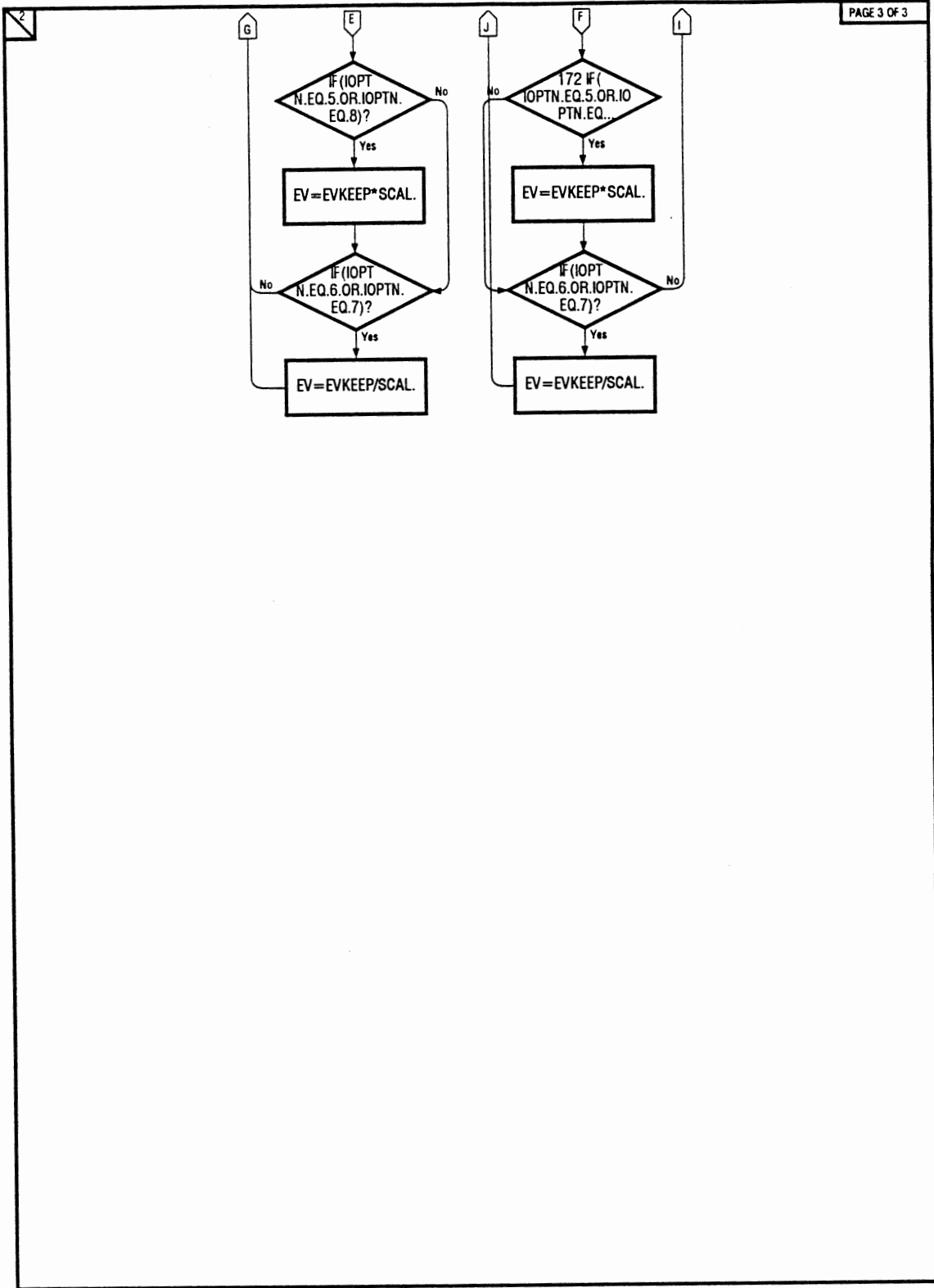


Figure 26. Continued

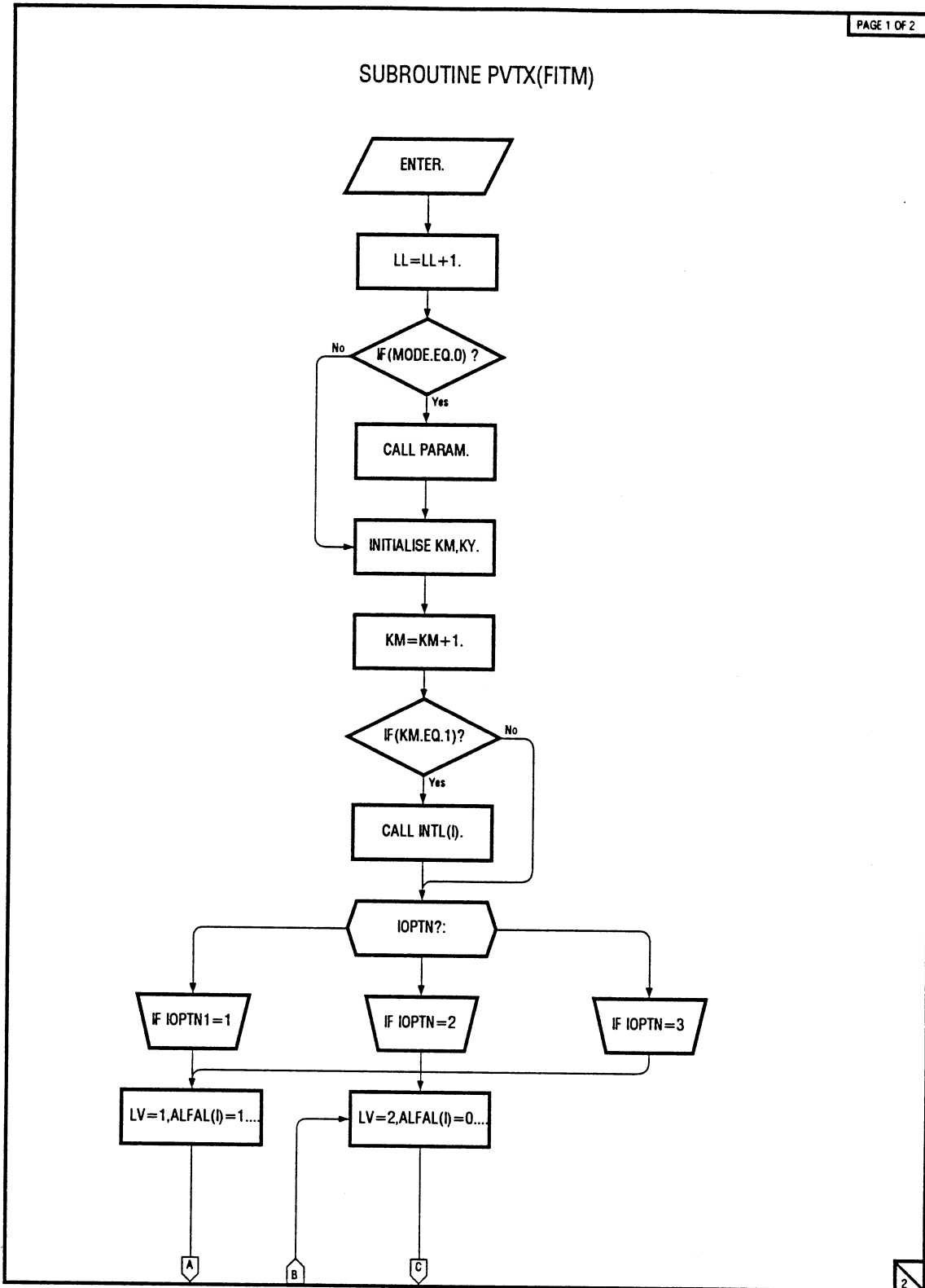


Figure 27. Flow Diagram for PVTX(FITM) Subroutine

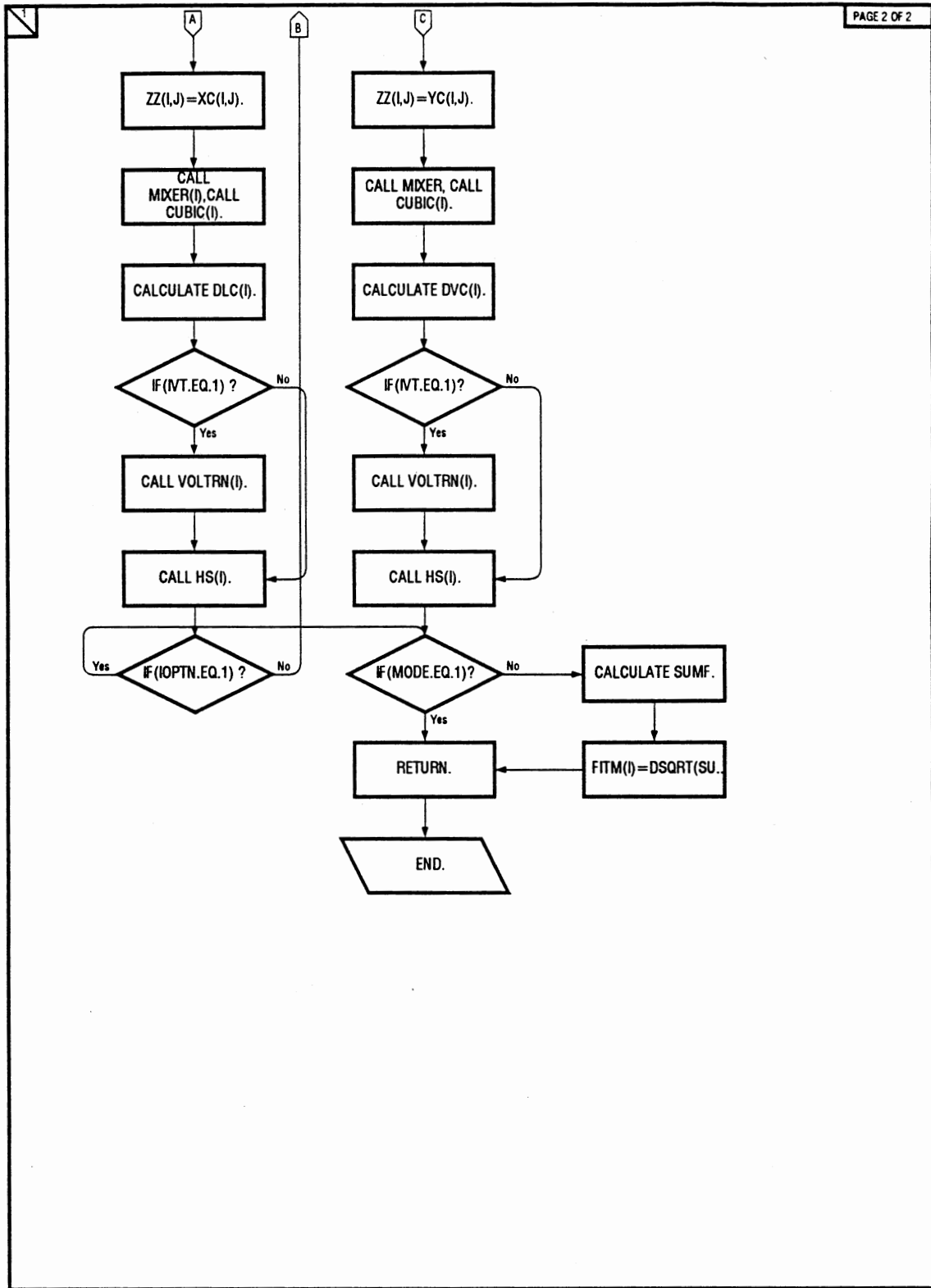


Figure 27. Continued

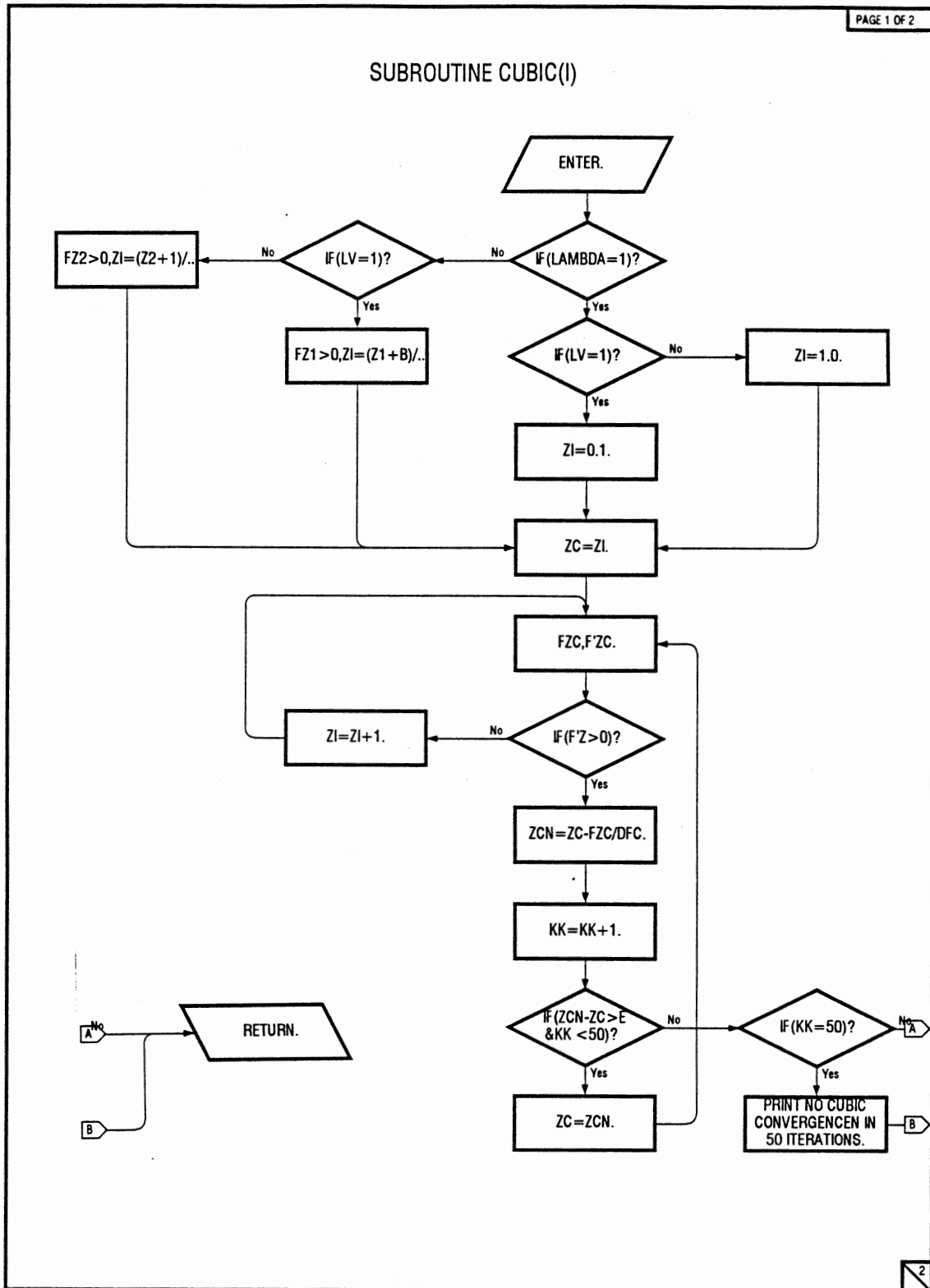


Figure 28. Flow Diagram for CUBIC(I) Subroutine

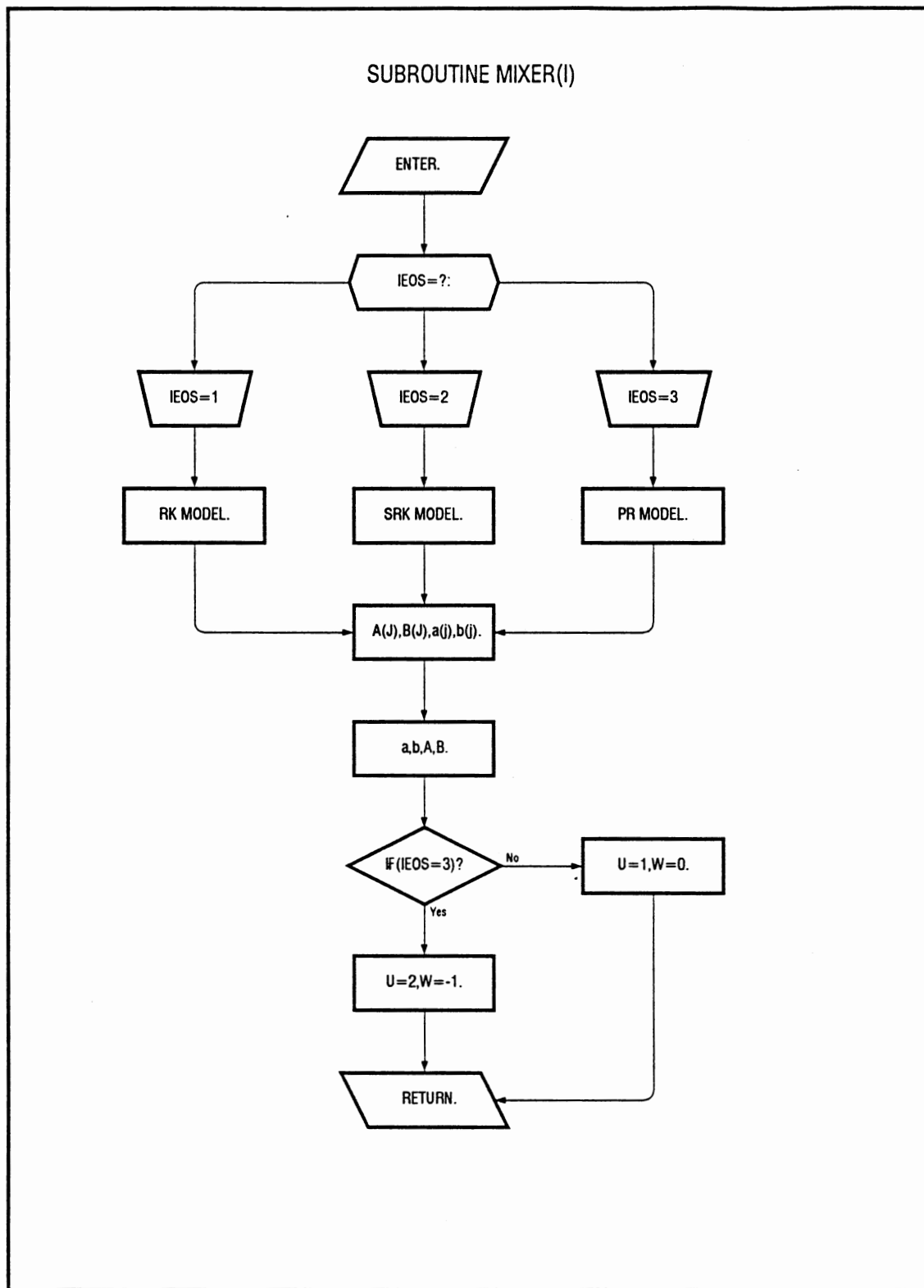


Figure 29. Flow Diagram for MIXER(I) Subroutine

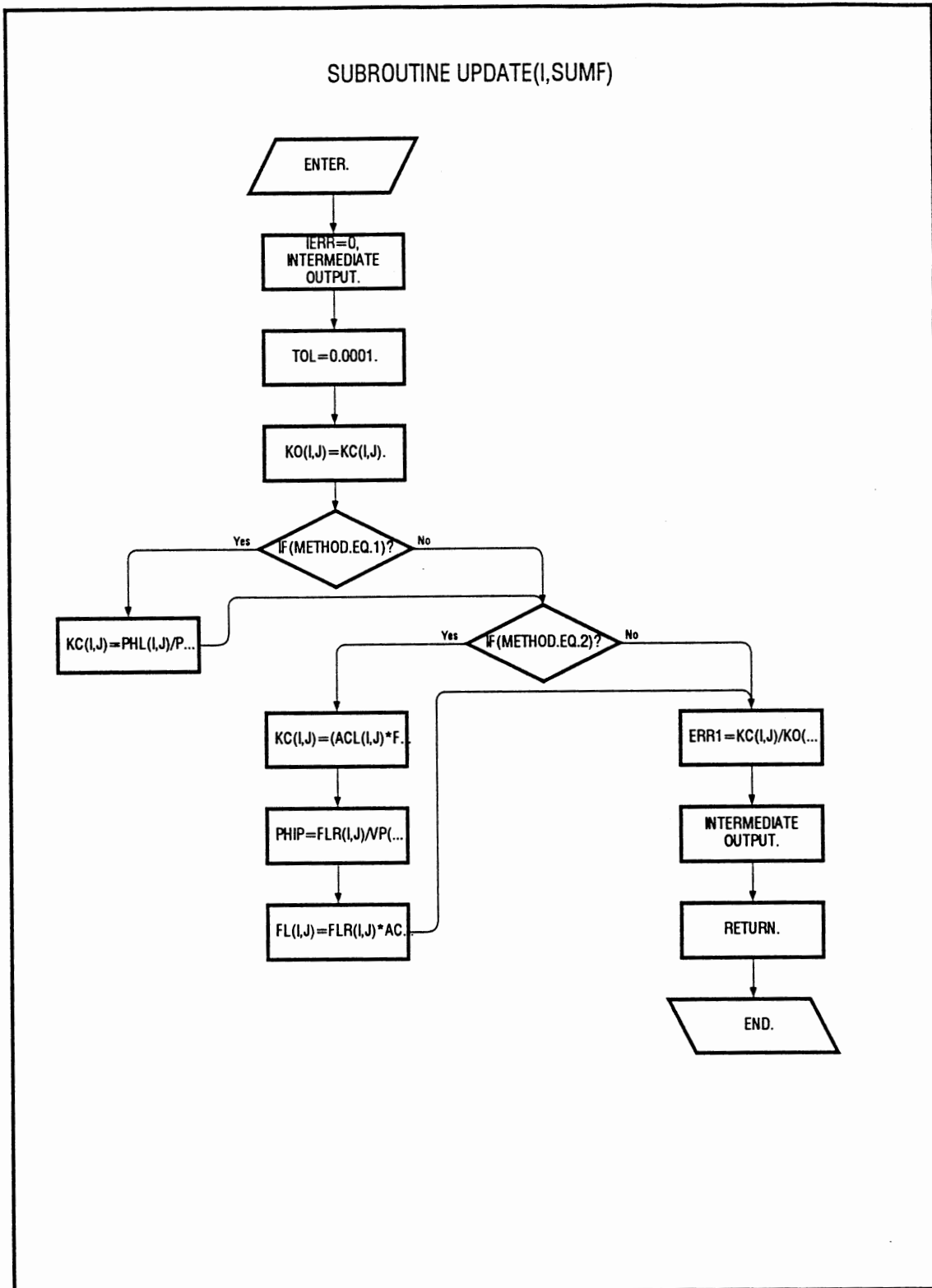


Figure 30. Flow Diagram for UPDATE(I,SUMF) Subroutine

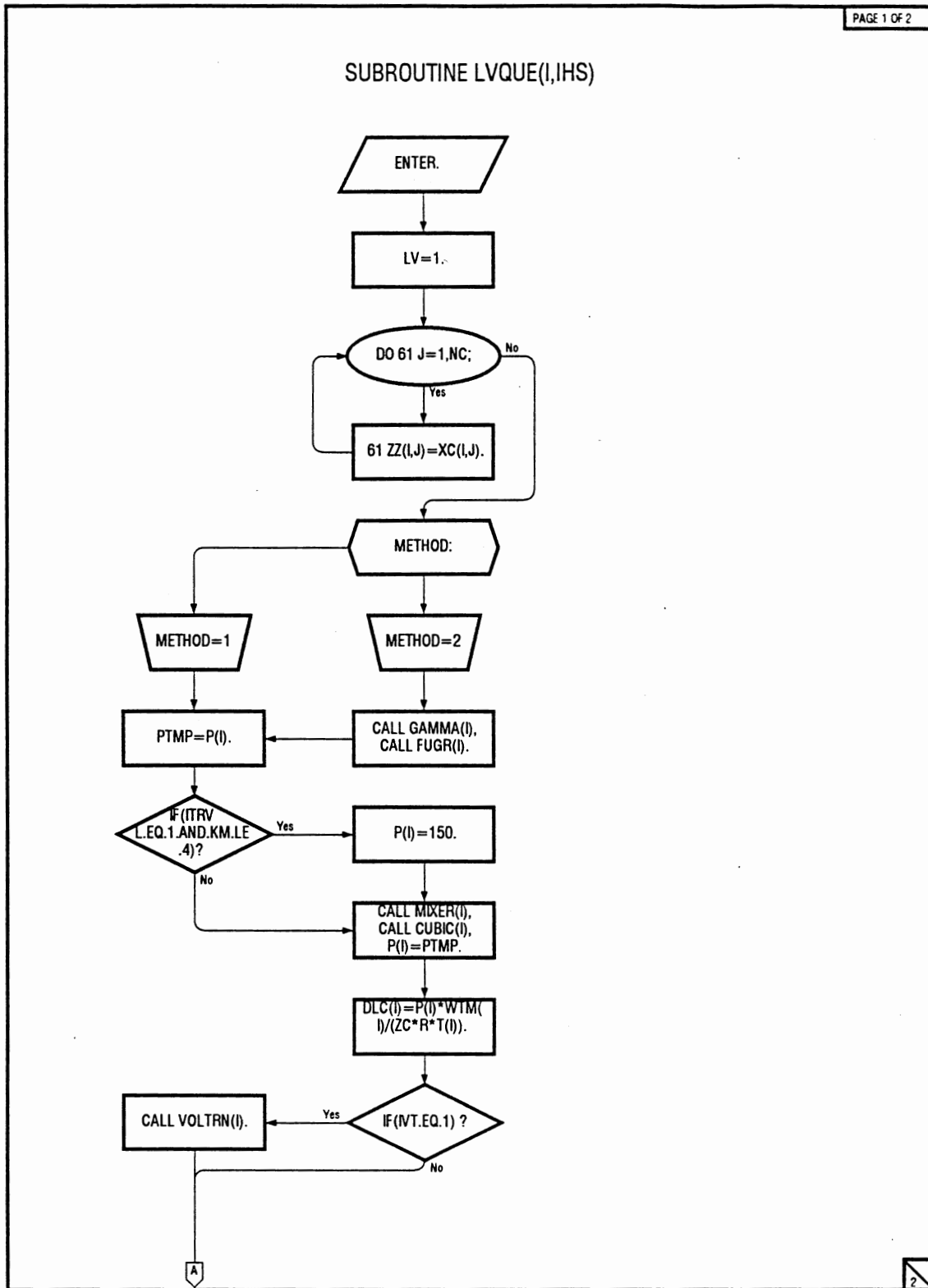


Figure 31. Flow Diagram for LVQUE(I,IHS) Subroutine

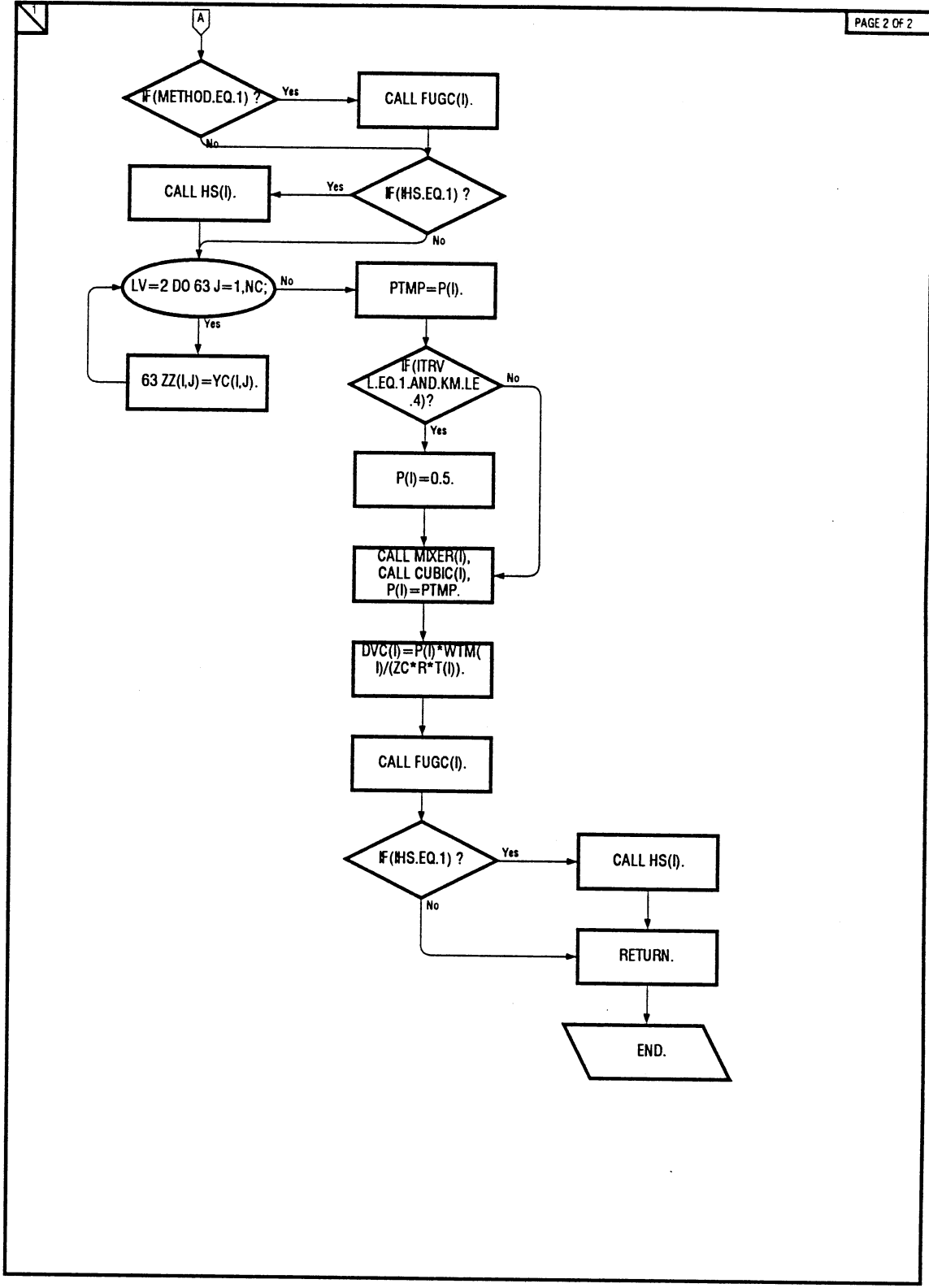


Figure 31. Continued



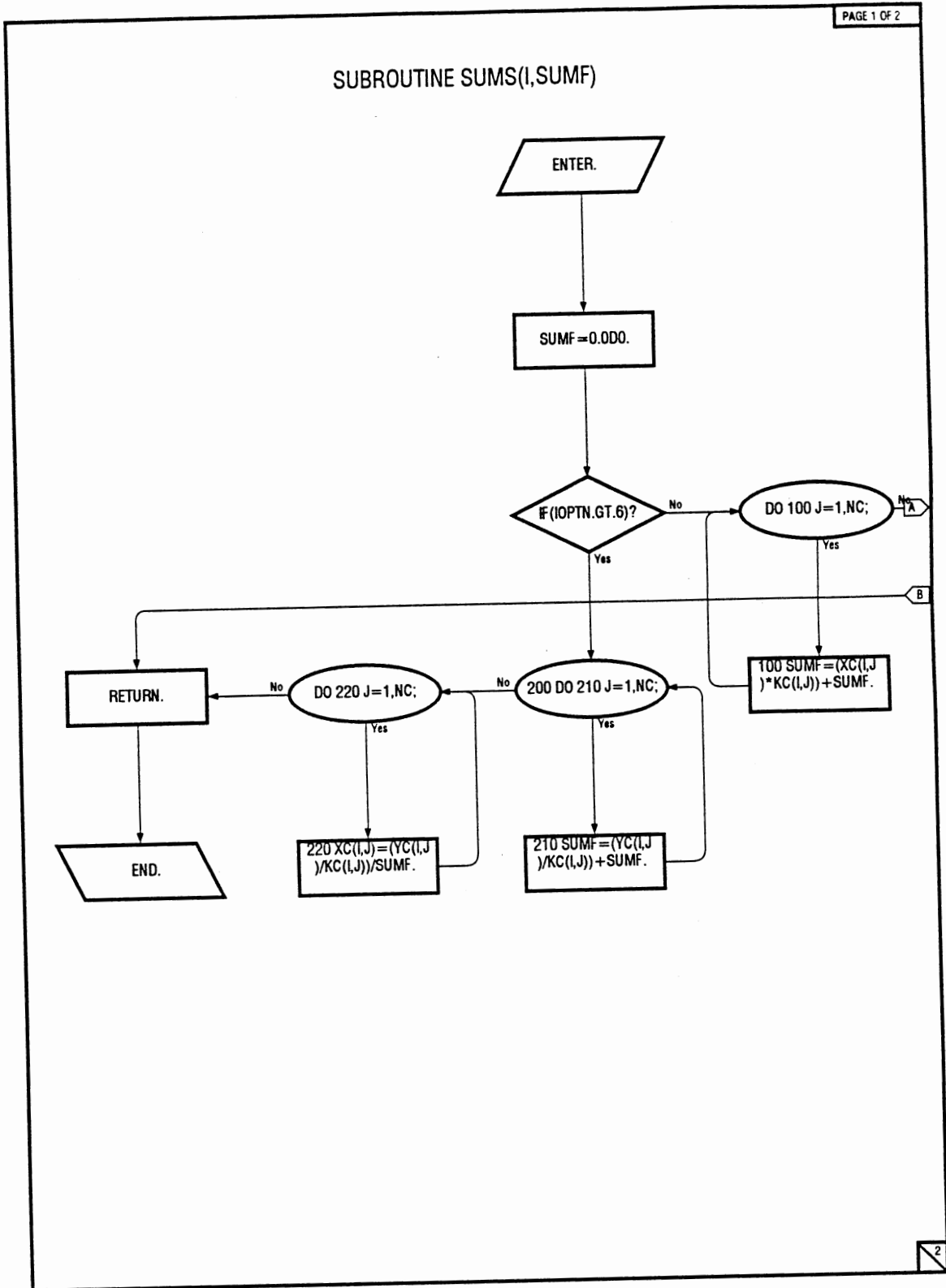


Figure 32. Flow Diagram for SUMS(I,SUMF) Subroutine

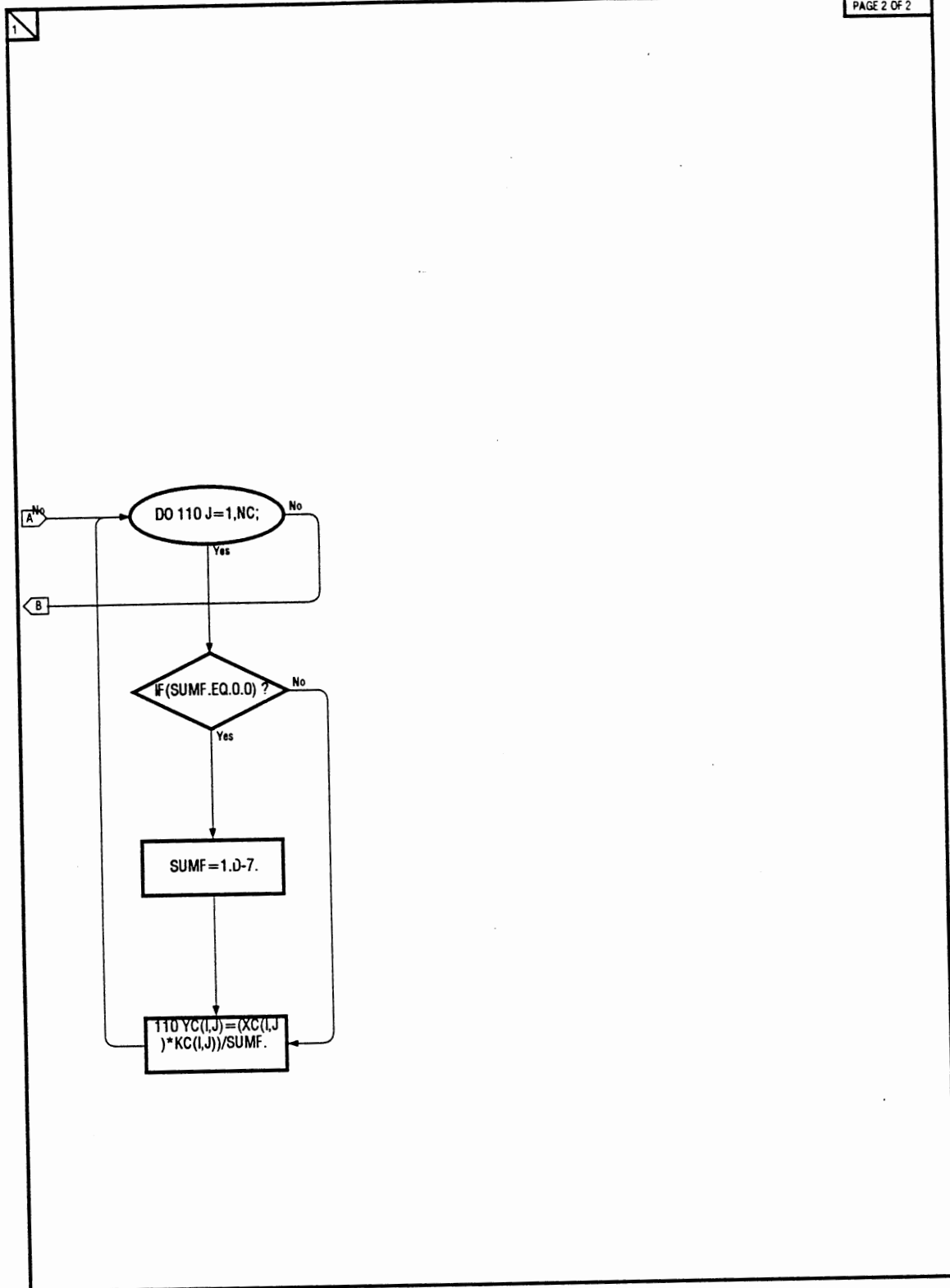


Figure 32. Continued

APPENDIX C

GRAPHIC PLOTS

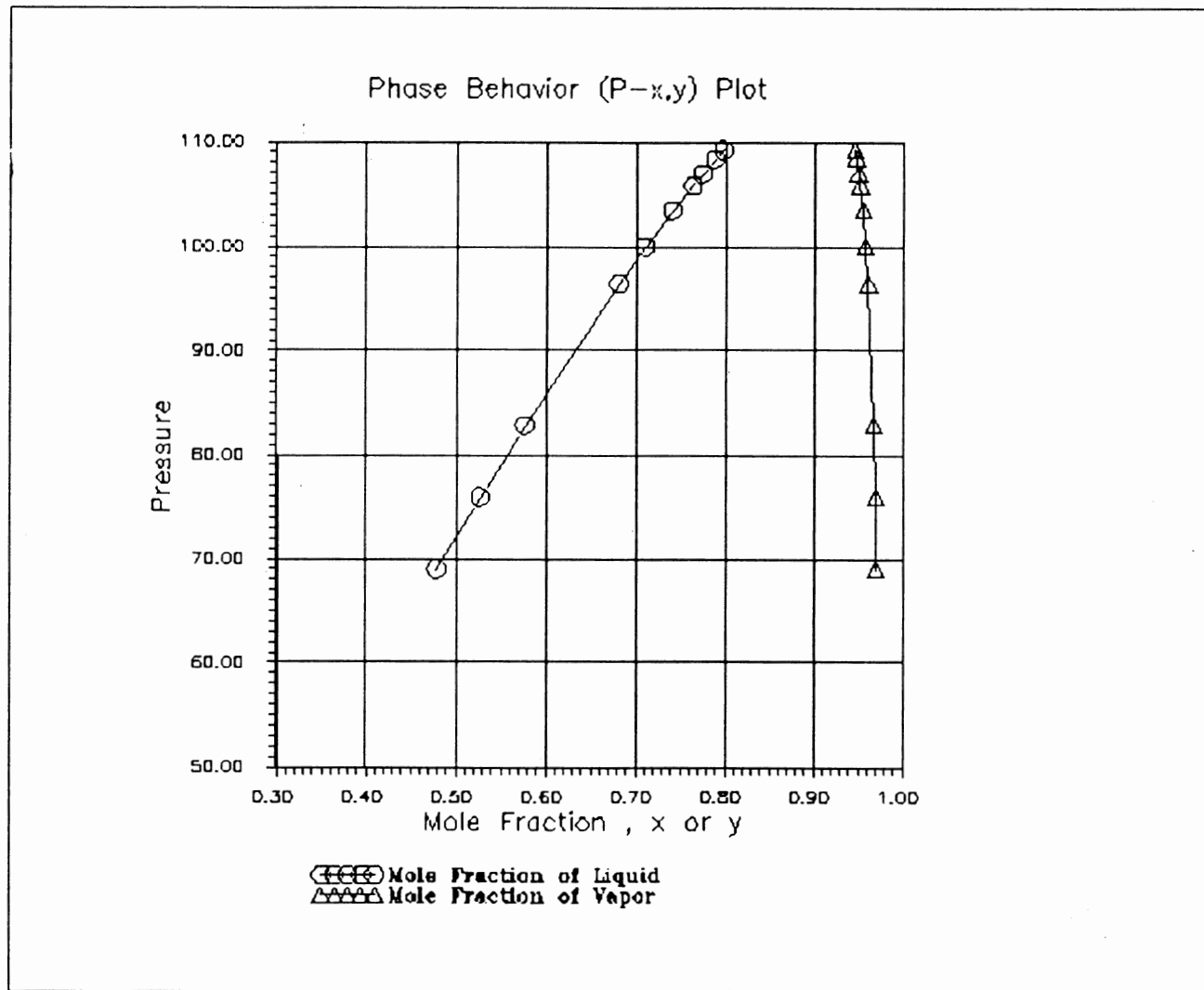


Figure 33. Pressure-Composition Plot  
for CO<sub>2</sub> + Benzene

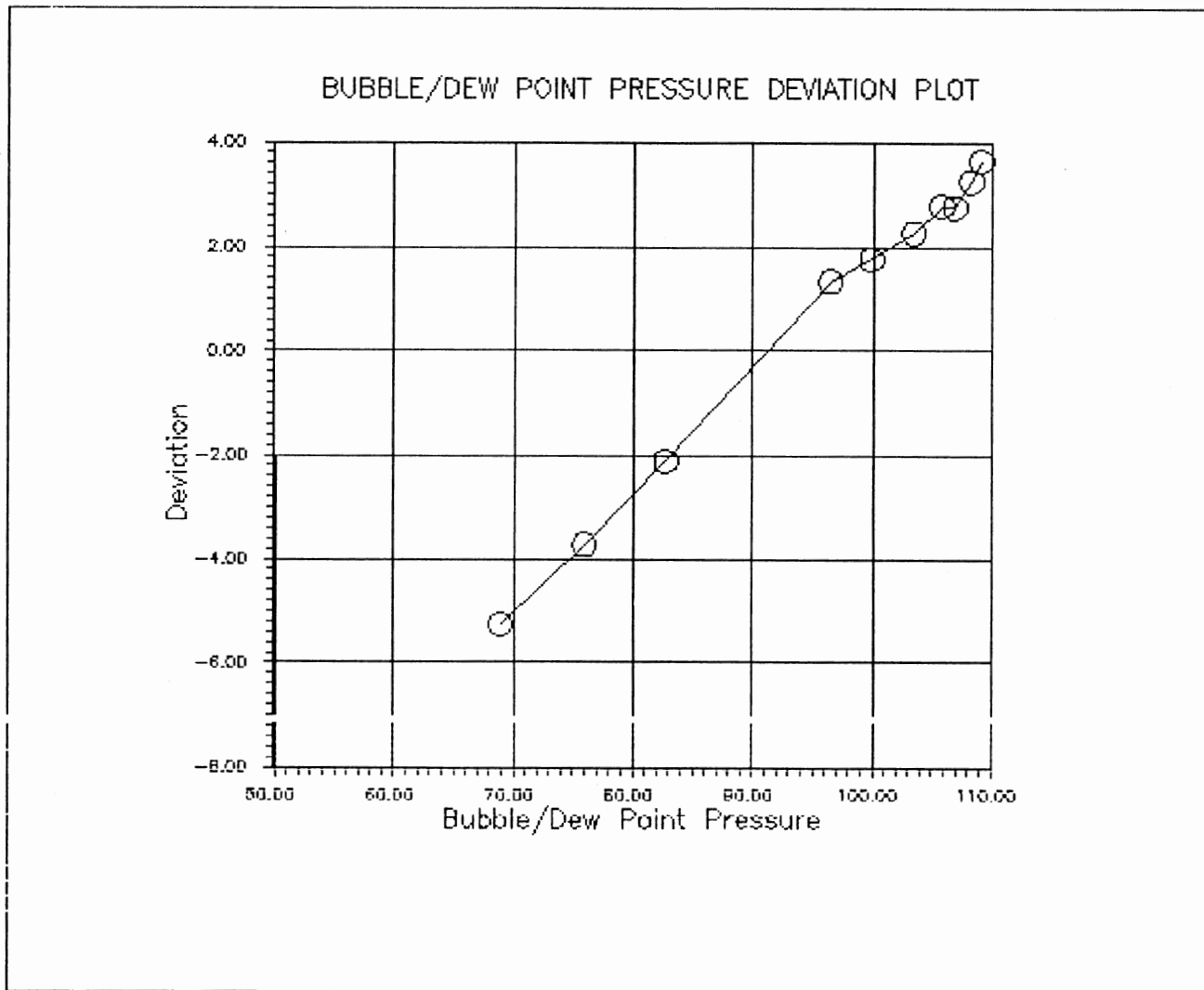


Figure 34. Bubble-Point Pressure Deviation Plot  
for CO<sub>2</sub> + Benzene

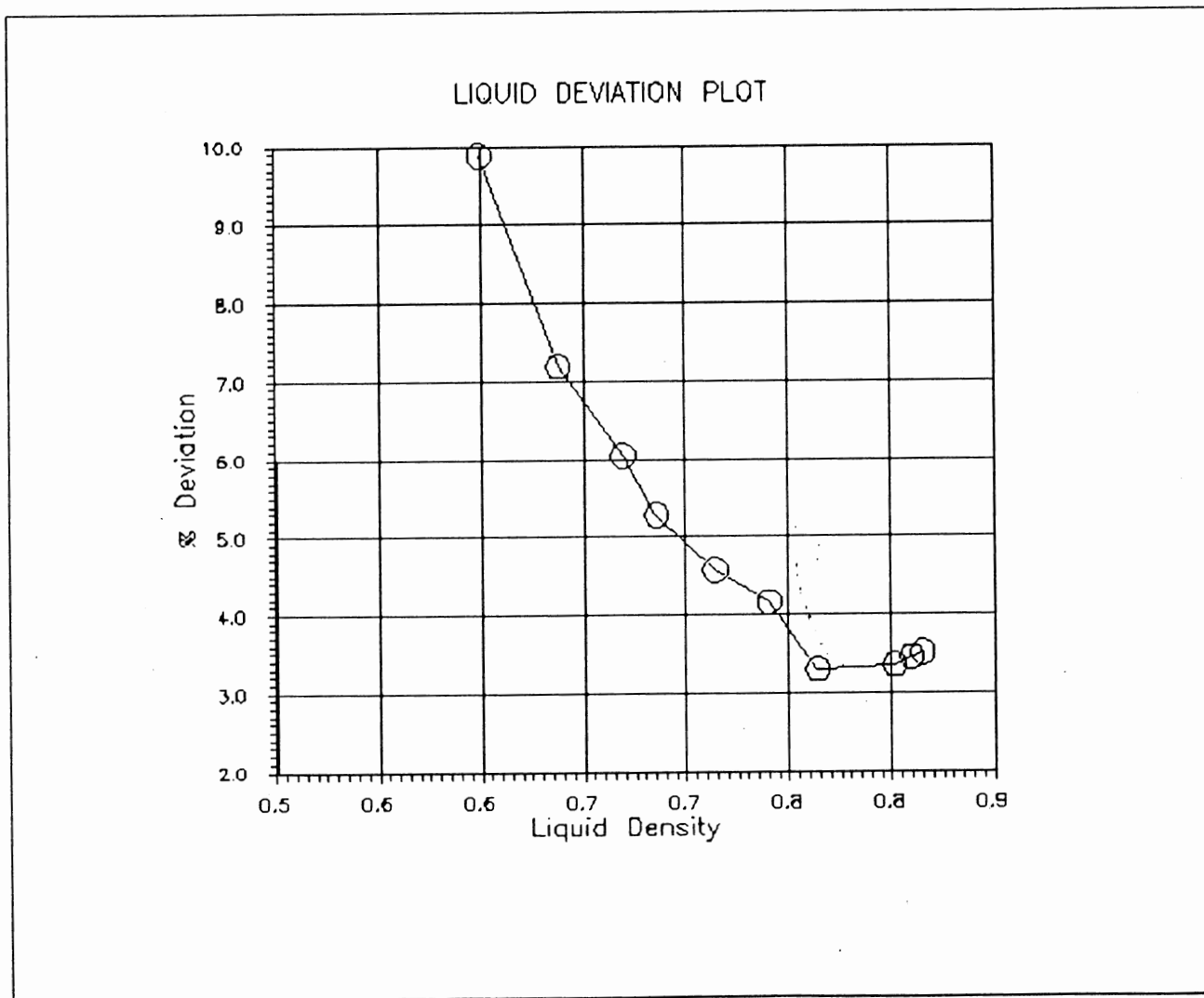


Figure 35. Liquid Density Deviation Plot  
for CO<sub>2</sub> + Benzene

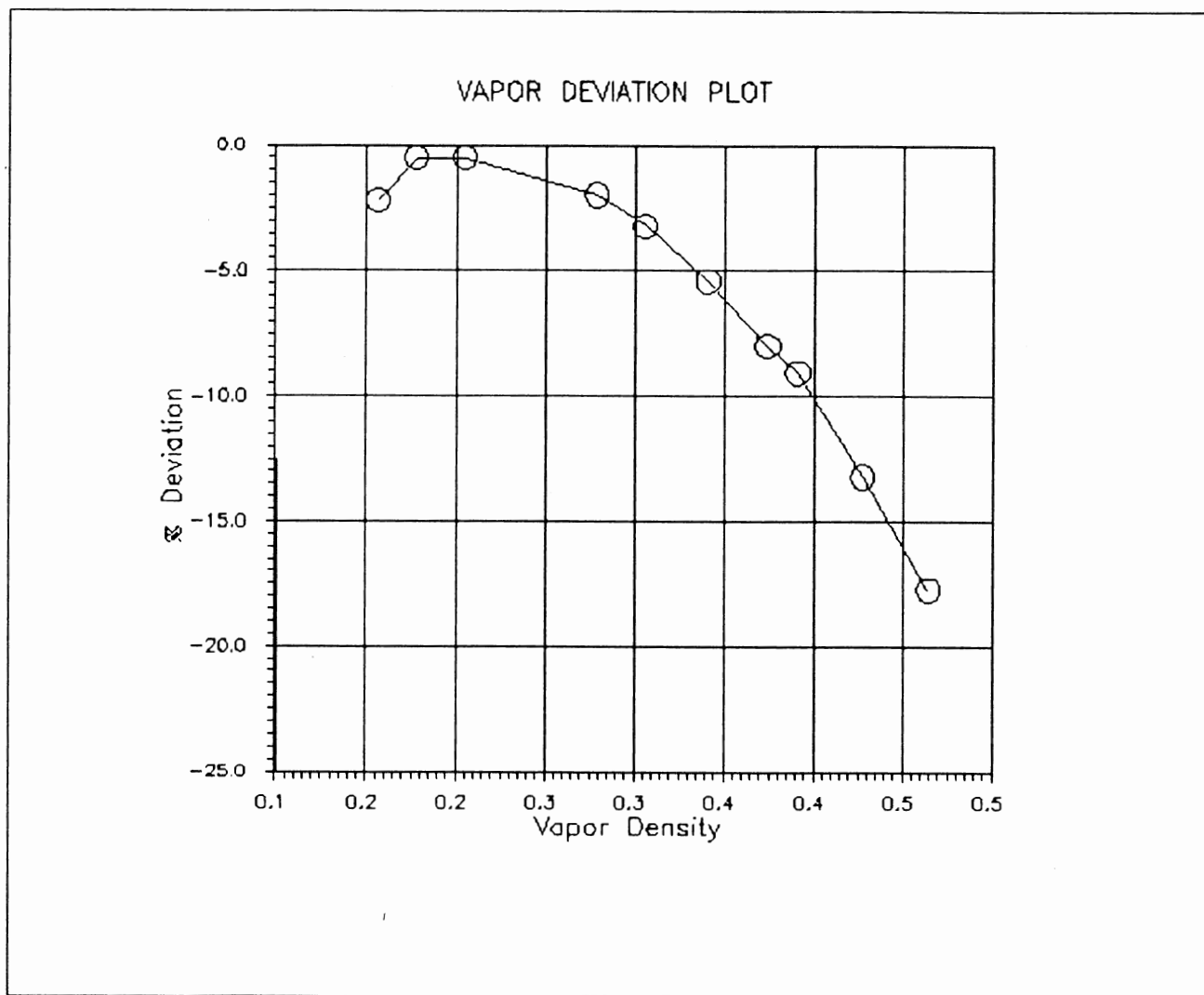


Figure 36. Vapor Density Deviation Plot for CO<sub>2</sub> + Benzene

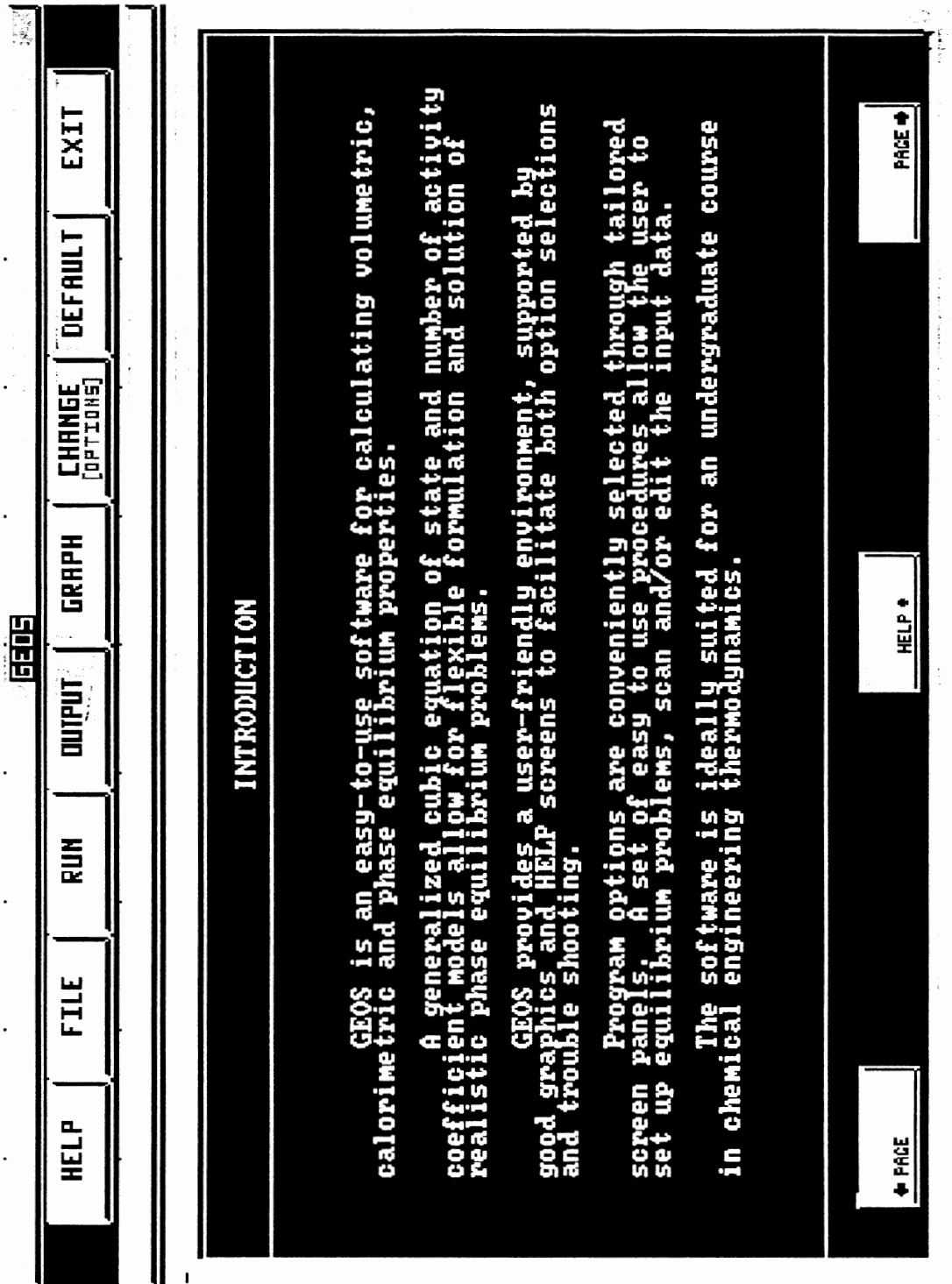


Figure 37. Sample HELP Screen 1



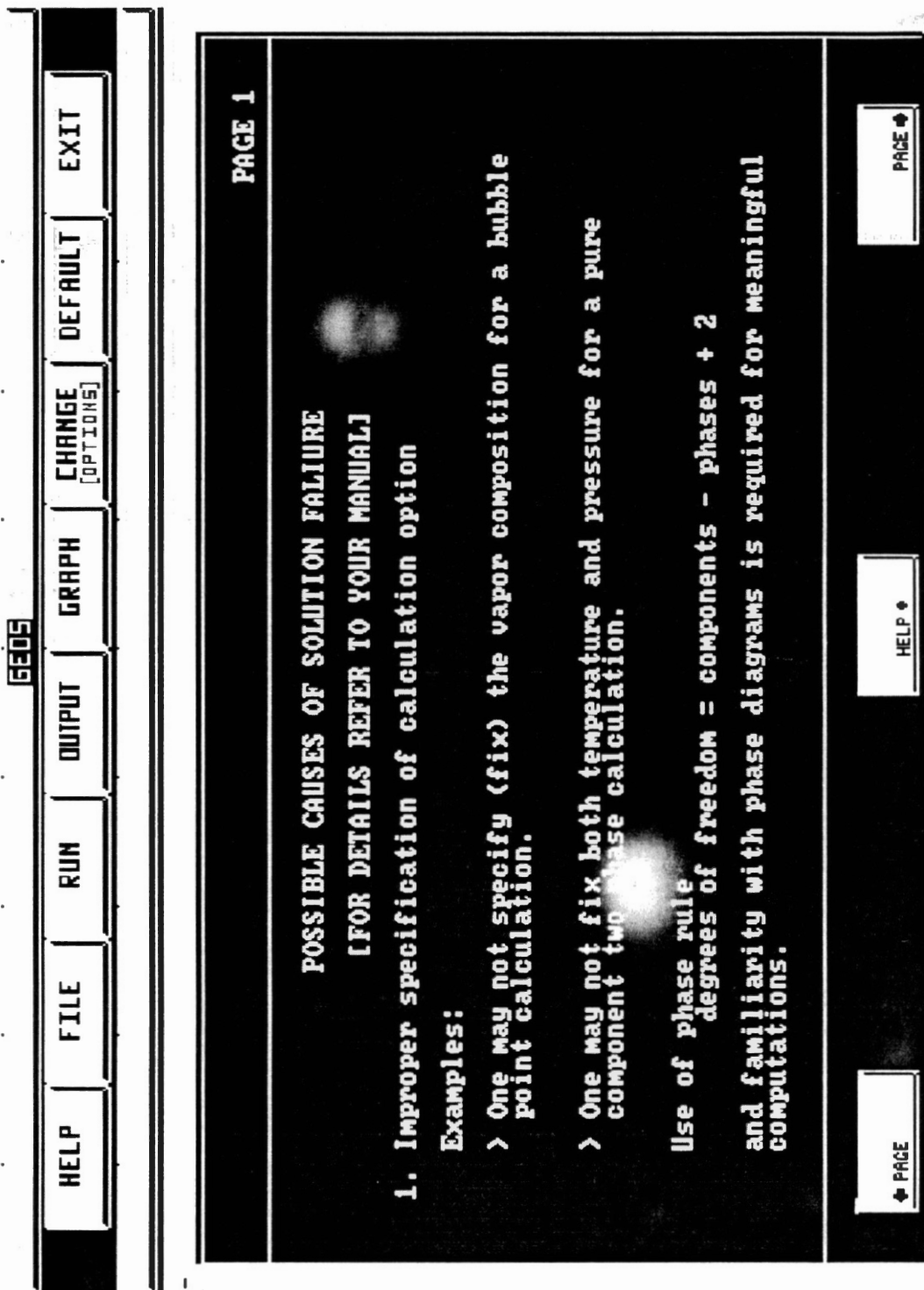


Figure 38. Sample HELP Screen 2

APPENDIX D

HARDWARE REQUIREMENTS

TABLE XII

## HARDWARE REQUIREMENTS

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**HARDWARE REQUIREMENTS FOR A PERSONAL COMPUTER**

---

1. DOS 5.0 OR later version
  2. 640 KB of Ram
  3. 64KB Extended Ram
  4. 80386 CPU @25Mhz
  5. 80387 Co-Processor
  6. VGA color monitor
  7. 20 MB Hard disk drive
  8. Mouse with driver software
  9. Printer
- 

640 kilobytes (KB) of random access memory (RAM) is required, since the executable code of the GEOS program requires the balance of the 614 KB RAM available after loading the disk operating system (DOS) files.

DOS 5.0 version or later is required since it has the facility for loading the support files of DOS into high memory. High memory (usually 64 KB) is the space in the RAM above the conventional 640 KB RAM area which can be utilized to load terminate-and-stay-resident (TSR) programs, where in the entire conventional memory can be utilized for the running of the main program and support DOS files.

64 KB of extended RAM is required to load the interface

support files DISPLAY.COM and HSGR.COM into high memory.

A 80386 central processing unit (CPU) computer is essential for the running of this program since other lower rated processors do not support access of the high memory, except for few of the 80286 CPU systems.

A 80387 Co-processor is required to speed up the optimization routines of the GEOS, which require a lot of number crunching.

A VGA color monitor is essential but not a must as this program will work in both the monochrome and color mode. Since all the interface screens have been developed in color, use of a VGA monitor will give full advantage of the facility and better presentation of the results.

Approximately 2.5MB of hard disk space is necessary to install the support files needed to run the GEOS program. It is possible to work from the floppy disk but then two high-density drives are needed to execute the program from one and use the other to write the output data.

Mouse is essential as this version of the software will not work without it. Also a printer is needed if one wants to take any graphic output from the GEOS interface program. This is achieved by loading the DOS utility GRAPHICS.COM.

APPENDIX E

INSTALLATION BATCH FILE

The source code of the batch file required to install this program is as follows:

```

ECHO OFF
cd\
%1:\
IF NOT EXIST %1:\%2 MD %2
CD %2
cls
copy %3:\*.axs %1:\%2
copy %3:\*.cat %1:\%2
copy %3:\*.cmd %1:\%2
copy %3:\*.cnf %1:\%2
copy %3:\*.dat %1:\%2
copy %3:\*.dlb %1:\%2
copy %3:\*.err %1:\%2
copy %3:\*.fat %1:\%2
copy %3:\*.grd %1:\%2
copy %3:\*.grf %1:\%2
copy %3:\*.lbr %1:\%2
copy %3:\*.lst %1:\%2
copy %3:\*.out %1:\%2
copy %3:\*.par %1:\%2
copy %3:\*.plt %1:\%2
copy %3:\*.prm %1:\%2
copy %3:\*.put %1:\%2
copy %3:\*.sym %1:\%2
copy %3:\*.tou %1:\%2
copy %3:\*.txt %1:\%2
copy %3:\*.exe %1:\%2

```

The syntax for the installation is to type

```
INSTALL C:\DIR B
```

where

```

INSTALL.... the batch file name INSTALL.BAT
C:\DIR .... C is the drive and DIR the path in
              which one wants the program to be
              installed.
B ..... the drive containing the
              installation disk.

```

VITAV

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