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CHEM2D: A TWO-DIMENSIONAL, THREE-PHASE, NINE-COMPONENT CHEMICAL FLOOD SIMULATOR
Volume III: CHEM2D Appendices and Phase Behavior Calculation Program

By
John R. Fanchi

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MASTER

Keplinger & Associates, Inc.
Tulsa, Oklahoma

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CHEM2D:

A TWO-DIMENSIONAL, THREE-PHASE, NINE-COMPONENT CHEMICAL FLOOD SIMULATOR

VOLUME III: CHEM2D APPENDICES AND PHASE BEHAVIOR CALCULATION PROGRAM

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VOLUME III: APPENDICES AND PHASE BEHAVIOR CALCULATION PROGRAM

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APPENDIX A. Cation Exchange*

A cation exchange model presented by Hirasaki (1982) is applied and extended to multiple phases. This model calculates the transport of sodium and calcium through porous media in the presence of clays and surfactant. The exchange of cation with both clays and the micelles is assumed to be entirely due to electrostatic association. The cation exchange is modelled as follows:

Calcium C_6 and sodium C_9 exchange by mass action**

$$\frac{\bar{C}_9^2}{\bar{C}_6} = \beta^c Q_v \frac{(C_{9\ell}^0)^2}{C_{6\ell}^0} \quad \text{for clay} \tag{A.1}$$

$$\frac{(C_{9\ell}^s)^2}{C_{6\ell}^s} = \beta^s C_{3\ell} \frac{(C_{9\ell}^0)^2}{C_{6\ell}^0} \quad \text{for micelles} \tag{A.2}$$

$$\ell = 1,2,3$$

where Q_v is cation exchange capacity, and the superscripts 0, s represent free ions and ions associated with surfactant (counter-ions on micelle). It is assumed that the adsorbed surfactant ($\hat{C}_3$) associates sodium ($\hat{C}_9^s$) and calcium ($\hat{C}_9^s$) in the same way as the micelles, e.g.

$$\frac{\hat{C}_9^s}{\hat{C}_6^s} = \frac{C_{9\ell}^s}{C_{6\ell}^s} \tag{A.3}$$

* Except for minor editorial changes, this Appendix is a reproduction of C. H. Hong's Ph.D. Dissertation, Section 5.10 (1982).

** All concentrations are expressed in milliequivalents/gram for the cation exchange calculations. The concentrations are converted to volume fractions when the cation exchange calculations are completed.

From electrical neutrality, we obtain the following equations

$$C^s_{6\ell} + C^s_{9\ell} = C_{3\ell} \tag{A.4}$$

$$C^0_{6\ell} + C^0_{9\ell} = C_{5\ell} \tag{A.5}$$

$$\hat{C}^s_6 + \hat{C}^s_9 = \hat{C}_3 \tag{A.6}$$

$$\bar{C}_6 + \bar{C}_9 = Q_v \tag{A.7}$$

$$\ell = 1,2,3$$

The material balance equation for calcium C_6 is

$$\tilde{C}_6 = \sum_{\ell=1}^{3} S_\ell C_{6\ell} + \bar{C}_6 + \hat{C}^s_6 = \sum_{\ell=1}^{3} S_\ell (C^0_{6\ell} + C^s_{6\ell}) + \bar{C}_6 + \hat{C}^s_6 \tag{A.8}$$

We also assume

$$C_{53} = \left(\frac{C_5}{C_1}\right) C_{13} \tag{A.9}$$

$$C^0_{61} = \left(\frac{C^0_{63}}{C_{13}}\right) C_{11} \tag{A.10}$$

$$C^0_{62} = \left(\frac{C^0_{63}}{C_{13}}\right) C_{12} \tag{A.11}$$

$$C^s_{61} = \left(\frac{C^s_{63}}{C_{13}}\right) C_{31} \tag{A.12}$$

$$C_{62}^{s} = \left(\frac{C_{63}^{s}}{C_{33}}\right) C_{32} \tag{A.13}$$

$$\hat{C}_{6}^{s} = \left(\frac{C_{63}^{s}}{C_{33}}\right) \hat{C}_{3} \tag{A.14}$$

Given S_1, S_2, S_3, C_{53}, C_{11}, C_{12}, C_{13}, C_{31}, C_{32}, C_{33}, $\hat{C}_3$ from the old time step value, we calculate C_{63}^{0}, $\bar{C}_6$, $\hat{C}_{63}^{s}$, C_{63}^{s} for the new time step as follows.

A function of C_{63}^{0} is defined as

$$F(C_{63}^{0}) = \sum_{\ell=1}^{3} S_{\ell}(C_{6\ell}^{0} + C_{6\ell}^{s}) + \bar{C}_6 + \hat{C}_6^{s} - \tilde{C}_{6N} \tag{A.15}$$

where C_{6N} is the new time step value just calculated by the convection-diffusion equations (explicit solution). C_6 and C_6^s are calculated by equations (A.1) through (A.7)

$$\bar{C}_6 = \tfrac{1}{2}\left(2Q_s + R_{96}^{c} - \sqrt{(R_{96}^{c})^2 + 4R_{96}^{c}\, Q_v}\right) \tag{A.16}$$

where

$$R_{96}^{c} = \beta^{c} Q_v \frac{(C_{53} - C_{63}^{0})^2}{C_{63}^{0}} \tag{A.17}$$

$$C_{63}^{s} = \tfrac{1}{2}\left(2C_{33} + R_{96}^{s} - \sqrt{(R_{96}^{s})^2 + 4R_{96}^{s}\, C_{33}}\right) \tag{A.18}$$

where

$$R_{96}^{s} = \beta^{s} C_{33} \frac{(C_{33} - C_{63}^{0})^2}{C_{63}^{0}} \tag{A.19}$$

The Newton-Raphson iteration method is used to solve the nonlinear equation

$$F(C_{63}^{0}) = 0 \tag{A.20}$$

We then calculate $C_{6\ell}$, $C_{9\ell}$, $\bar{C}_6$, $\bar{C}_9$, $\hat{C}_6$, and $\hat{C}_9$ at the new time step by equations (A.1) through (A.3).

The iteration converges when $F(C_{63}^{0})$ is less than a specified tolerance where $C_{3\ell}$, S_ℓ, $\hat{C}_3$ are considered known. However, strictly speaking, the phase behavior routine should be in the loop because the new value of $C_{6\ell}$ obviously strongly affects $C_{3\ell}$, S_ℓ, $\hat{C}_3$. One could iterate, calling one routine, then the other, successively until they converge. This is not done at present.

APPENDIX B.1. Calculation of Phase Diagrams*

We can qualitatively depict the phase diagram as shown in Figure B.1. All features vary in a continuous way with an effective ionic strength ("salinity"), C_{SE}. This includes specifically the binodal curve, tie lines, plait points (left P_L and right P_R) and invariant point, M. We make the basic assumption that the binodal curve is the same function of C_{SE} for all three types of diagrams, so that all that distinguishes the Type III diagrams is the three phase triangle located by the Point M, and the left and right node tie lines.

The basic idea is to model the diagrams with modified Hand equations, which in turn are based upon the observation that the phase boundary (binodal curve) and distribution curve (tie lines) plot as straight lines on log plots as shown on Figure B.2.

For either Type II(-) or Type II(+) we have only two phases below the binodal curve. The two basic equations are

$$\frac{C_{3\ell}}{C_{2\ell}} = A\left(\frac{C_{3\ell}}{C_{1\ell}}\right)^B \qquad (B.1)$$

$$\ell = 1,2$$

$$\frac{C_{32}}{C_{22}} = E\left(\frac{C_{31}}{C_{11}}\right)^F \qquad (B.2)$$

These are equations for the binodal curve and distribution curve, respectively. The parameters A, B, E, and F must be estimated as a function of C_{SE} as discussed below. We also know that

* Except for minor editorial changes, this Appendix is a reproduction of C. H. Hong's Ph.D. Dissertation, Appendix F (1982).

$$C_{11} + C_{21} + C_{31} = 1 \tag{B.3}$$

$$C_{12} + C_{22} + C_{32} = 1 \tag{B.4}$$

Equation (B.1) applies to either phase 1 or phase 2, i.e., either to the left or right of the plait point. Thus, we have five equations in six unknowns (the $C_{k\ell}$, $k = 1,2,3$, $\ell = 1,2$). So we have one degree of freedom, as expected. We can take any one concentration, such as C_{21}, and give it values between 0 and 1 and sweep out the phase diagram. We do this explicitly later, but for now we take a ratio defined below as our one degree of freedom.

$$\text{Let} \quad R^{\ell}_{ij} = C_{i\ell}/C_{j\ell} \tag{B.5}$$

Let R^1_{31} be taken as independent. The following set of equations then yield the $C_{k\ell}$ without iteration:

$$R^1_{32} = A(R^1_{31})^B \tag{B.6}$$

$$C_{11} = \frac{R^1_{32}}{R^1_{31} + R^1_{31}R^1_{32} + R^1_{32}} \tag{B.7}$$

$$C_{21} = 1 - (R^1_{31} + 1)C_{11} \tag{B.8}$$

$$C_{31} = 1 - C_{11} - C_{21} \tag{B.9}$$

$$R_{32} = C(R^1_{31})^F \tag{B.10}$$

$$C_{12} = \frac{R^2_{32}}{R^2_{31} + R^2_{31}R^2_{32} + R^2_{32}} \tag{B.11}$$

$$C_{22} = 1 - (R^2_{31} + 1)C_{12} \tag{B.12}$$

$$C_{32} = 1 - C_{12} - C_{22} \tag{B.13}$$

R^1_{31} varies between zero and infinity.

B.1.1. Parameter Estimation

The basic input is the set of three parameters C_{3MAX0}, C_{3MAX1}, and C_{3MAX2}. These are physically the maximum in the binodal curve (the "height" of the two phase region) at C_{SE} = 0, 1, and 2, respectively. These are values easily visualized and obtained from even limited phase data and do not vary widely from case to case, so reasonable values can be assumed in the absence of any data (caution: some data are needed to support the assumption that the system fits the qualitative trends depicted, so having some data is highly desirable). The values do matter, however, because the extent of the single phase region directly affects the degree of miscibility. Thus, once again, some data are highly desirable.

We now use this interpolation scheme for A:

$$A_0 = \left(\frac{2\ C_{3MAX0}}{1 - C_{3MAX0}}\right)^2 \tag{B.14}$$

$$A_1 = \left(\frac{2\ C_{3MAX1}}{1 - C_{3MAX1}}\right)^2 \tag{B.15}$$

$$A_2 = \left(\frac{2\ C_{3MAX2}}{1 - C_{3MAX2}}\right)^2 \tag{B.16}$$

$$A = A_0 + (A_1 - A_0)\ C_{SE} \qquad C_{SE} \leq 1 \tag{B.17}$$

$$A = A_1 + (A_2 - A_1)(C_{SE} - 1) \qquad C_{SE} \geq 1 \tag{B.18}$$

Recall that C_{SE} is in optimal salinity units (effective salinity divided by optimal effective salinity).

We assume B and F are constants. The most flexible scheme allows B and F to be arbitrary. However, many times the binodal curve is known but the tie lines are not. Thus, we can get B, but not F, from the data available. In such cases, we will take F = -1/B by analogy with those

cases where we do have data, since this relationship tends to hold approximately. Furthermore, many times we do not have enough data to even estimate B properly. In such cases, we take B = -1. This gives a symmetrical binodal curve. The deviation of most actual curves from this symmetry is probably not significant. The type of phase diagram (II(-), III, II(+)) and the extent of the single phase region are the most important factors. It seems unlikely that the detailed shape of the curve is significant. Also, recall that since we are dealing with pseudo-ternary diagrams, the curves themselves shift around depending on the exact overall composition (especially with respect to alcohol), so it makes no sense at all to try to describe them in great detail with high precision, even in the rare circumstances when we have the large amount of data required to do so.

Let us return to parameter estimation. We still need E. We estimate E from the location of the plait point. This is done once again because it is a method easy to visualize and apply, and it has a direct physical meaning. Since equations (B.1) and (B.2) must apply at the plait point, denoted by subscript p, we have

$$\frac{C_{3p}}{C_{2p}} = E\left(\frac{C_{3p}}{C_{1p}}\right)^F \tag{B.19}$$

$$\frac{C_{3p}}{C_{2p}} = A\left(\frac{C_{3p}}{C_{1p}}\right)^B \tag{B.20}$$

$$C_{1p} + C_{2p} + C_{3p} = 1 \tag{B.21}$$

Given A, B, and F from above, these equations can be used to calculate E as a function of C_{2p}. For the special case of B = -1 and F = +1, we calculate all the phase concentrations ($C_{k\ell}$) explicitly. From Equation (B.1) we solve for C_{31} ($\ell = 1$)

$$C_{31} = \tfrac{1}{2}\left(-AC_{21} + \sqrt{(AC_{21})^2 + 4AC_{21}(1 - C_{21})}\right) \tag{B.22}$$

and

$$C_{11} = 1 - C_{21} - C_{31} \tag{B.23}$$

From equation (B.19), we calculate

$$E = C_{1p}/C_{2p} \tag{B.24}$$

where

$$C_{3p} = \tfrac{1}{2}\left(-AC_{2p} + \sqrt{(AC_{2p})^2 + 4AC_{2p}(1 - C_{2p})}\right) \tag{B.24a}$$

and

$$C_{1p} = 1 - C_{2p} - C_{3p} \tag{B.24b}$$

Note that C_{2p} is an input parameter.

From equation (B.2), we have

$$C_{32} = h\ C_{22} \tag{B.25}$$

where

$$h = EC_{31}/C_{11} \tag{B.26}$$

is known. Substituting this into equation (B.1) with j = 1 and solving for C_{22}

$$C_{22} = \frac{A}{h^2 + Ah + A} \tag{B.27}$$

then

$$C_{32} = h\ C_{22} \tag{B.28}$$

and

$$C_{12} = 1 - C_{22} - C_{32} \tag{B.29}$$

We now know all $C_{k\ell}$.

The only difference between Type II(-) and II(+) is that for II(-) we input C_{2PR} and for II(+) C_{2PL}. The limits on II(-) are $0 \le C_{SE} \le C_{SEL}$ and on II(+) are $C_{SEU} \le C_{SE} \le 2$.

In summary, for II(-), we increment C_{SE} up to C_{SEL} and for each C_{SE} we increment C_{21} from 0 to C_{2PR}. The input parameters are C_{3MAX0}, C_{3MAX1}, and C^*_{2PR}. The C_{ij} are calculated from equations (B.22) through (B.29). For II(+), we increment C_{SE} from C_{SEU} to 2.0, and for each C_{SE}, we increment C_{21} from 0 to C^*_{2PL}. The $C_{k\ell}$ are calculated from the same equations as before.

B.1.2. Type III

For Type III, we must calculate the left node and the right node separately. First, we calculate the invariant point (M) as a function of C_{SE} from

$$C_{2M} = \frac{C_{SE} - C_{SEL}}{C_{SEU} - C_{SEL}} \tag{B.30}$$

$$C_{3M} = \tfrac{1}{2}\left(-AC_{2M} + \sqrt{(AC_{2M})^2 + 4AC_{2M}(1 - C_{2M})}\right) \tag{B.31}$$

$$C_{1M} = 1 - C_{2M} - C_{3M} \tag{B.32}$$

B.1.2.1. Left Node

The plait point must vary between zero and the II(-) value C^*_{2PL}. By interpolation

$$C_{2PL} = C^*_{2PL} + \frac{C^*_{2PL}}{C_{SEU} - C_{SEL}} (C_{SE} - C_{SEU}) \quad . \tag{B.33}$$

We now do a coordinate rotation as shown in Figure B.3. This enables us to apply the Hand equation in the new coordinate system as

$$\frac{C'_{32}}{C'_{22}} = E \; \frac{C'_{31}}{C'_{11}} \tag{B.34}$$

where

$$C'_{2\ell} = C_{2\ell} \sec \theta \tag{B.35}$$

$$C'_{3\ell} = C_{3\ell} - C_{2\ell} \tan \theta \tag{B.36}$$

$$C'_{1\ell} = 1 - C'_{2\ell} - C'_{3\ell} \tag{B.37}$$

Define two parameters α and β as

$$\beta = \sec \theta = \sqrt{C_2^2 + C_{3M}^2}/C_{2M} \tag{B.38}$$

$$\alpha = \tan \theta = C_{3M}/C_{2M} \tag{B.39}$$

Again taking F = 1, we calculate E explicitly from

$$E = C'_{1p}/C'_{2p} = \frac{1 - (\beta - \alpha)C_{2p} - C_{3p}}{\beta C_{2p}} \tag{B.40}$$

where

$$C_{2P} = C_{2p1}$$

and C_{1p} and C_{3p} are given by equations (B.24a) and (B.24b) as before. We calculate C_{31} and C_{11} as before and solve equation (B.34) for C_{22}

$$C_{22} = \frac{A}{h'^2 + Ah' + A} \tag{B.41}$$

where

$$h' = \frac{\beta E C'_{31}}{C'_{11}} + \alpha \tag{B.42}$$

and then

$$C_{32} = h' \, C_{22} \tag{B.43}$$

$$C_{12} = 1 - C_{22} - C_{32} \tag{B.44}$$

We now know all $C_{k\ell}$ for the left node. We increment C_{21} from zero to C_{2PL} for each C_{SE} as before.

B.1.2.2 Right Node

The process is almost the same as for the left node except we calculate C_{2PR} from

$$C_{2PR} = C^*_{2PR} + \frac{1 - C^*_{2PR}}{C_{SEU} - C_{SEL}} (C_{SE} - C_{SEL}) \tag{B.45}$$

We first calculate C_{32} from

$$C_{32} = \tfrac{1}{2} \left(-AC_{12} + \sqrt{(AC_{12})^2 + 4AC_{12}(1 - C_{12})}\right) \tag{B.46}$$

and

$$C_{22} = 1 - C_{12} - C_{32} \tag{B.47}$$

Note that C_{12} is incremented rather than C_{21} (this is simply more convenient).

Let

$$h' \equiv \frac{\beta C'_{32}}{E\ C'_{11}} + \alpha \tag{B.48}$$

then

$$C_{11} = \frac{A}{h'^2 + Ah' + A} \tag{B.49}$$

$$C_{31} = h'\ C_{11} \tag{B.50}$$

$$C_{21} = 1 - C_{11} - C_{31} \tag{B.51}$$

where

$$\alpha = C_{3M}/C_{1M} \tag{B.52}$$

$$\beta = \sqrt{C_{3M}^2 + C_{1M}^2}\,/C_{1M} \tag{B.53}$$

$$C'_{1\ell} = \beta C_{1\ell} \tag{B.54}$$

$$C'_{3\ell} = C_{3\ell} - \alpha C_{1\ell} \tag{B.55}$$

$$C'_{2\ell} = 1 - C'_{1\ell} - C'_{3\ell} \tag{B.56}$$

$$E = C'_{1p}/C'_{2p} \tag{B.57}$$

and C'_{1p} and C'_{2p} are calculated using equations (B.54) to (B.56) and (B.24a) and (B.24b). We now know all $C_{k\ell}$ for the right node.

B.2. Summary of Calculation Procedure

I. Given: C_{3MAX1}, C_{3MAX0}, C_{3MAX2} = height of binodal curve when C_{SE} = 1, 0, and 2

C_{SEL}, C_{SEU} = minimum and maximum effective salinities for Type III

C^*_{2PR}, C^*_{2PL} = oil coordinate of plait point in Type II(-) and Type II(+) regions

Seven input parameters

II. For $C_{SE} < C_{SEL}$: Type II(-)

1. Calculate parameter A from (B.17)
2. Calculate C^*_{3PR} and C^*_{1PR} from (B.24a) and (B.24b) using C^*_{2PR}
3. Calculate E from (B.24) and C^*_{1PR} and C^*_{2PR}
4. Pick C_{21}, calculate C_{31} and C_{11} from (B.22) and (B.23)
5. Calculate h from (B.26)
6. Calculate C_{22}, C_{32}, C_{12} from (B.27) through (B.29)

III. For $C_{SE} > C_{SEU}$: Type II(+)

1. Calculate parameter A from (B.18)
2. Calculate C^*_{3PL} and C^*_{1PL} from (B.24a) and (B.24b) using C^*_{2PL}
3. Calculate E from (B.24) and C^*_{1PL} and C^*_{3PL}
4. Pick C_{21}, calculate C_{31} and C_{11} from (B.22) and (B.23)
5. Calculate h from (B.26)
6. Calculate C_{22}, C_{32}, C_{12} from (B.27) through (B.29)

IV. For $C_{SEL} < C_{SE} < C_{SEU}$: Type III

1. Calculate C_{2M} from (B.30)
2. Calculate A from (B.17) or (B.18)
3. Calculate C_{3M} and C_{1M} from (B.31) and (B.32)
4. Left Node - Type II(+)
   a. Calculate α and β from (B.38) and (B.39)
   b. Calculate C_{2PL} from (B.33)
   c. Calculate C_{3PL} and C_{1PL} from (B.24a) and (B.24b) using C_{2PL}
   d. Calculate E from (B.40)
   e. Pick C_{21}, calculate C_{31} and C_{11} from (B.22) and (B.23)
   f. Calculate h' from (B.42)
   g. Calculate C_{32}, C_{12}, and C_{22} from (B.41) through (B.44)
5. Right Node - Type II(-)
   a. Calculate α and β from (B.52) and (B.53)
   b. Calculate C_{2PR} from (B.45)
   c. Calculate C_{3PR} and C_{1PR} from (B.24a) and (B.24b) using C_{2PR}
   d. Calculate E from (B.40)
   e. Pick C_{12}, calculate C_{32} and C_{22} from (B.46) and (B.47)
   f. Calculate h' from (B.48)
   g. Calculate C_{31}, C_{11}, C_{21} from (B.49) through (B.51)

FIGURE B.1: Ternary Phase Diagrams

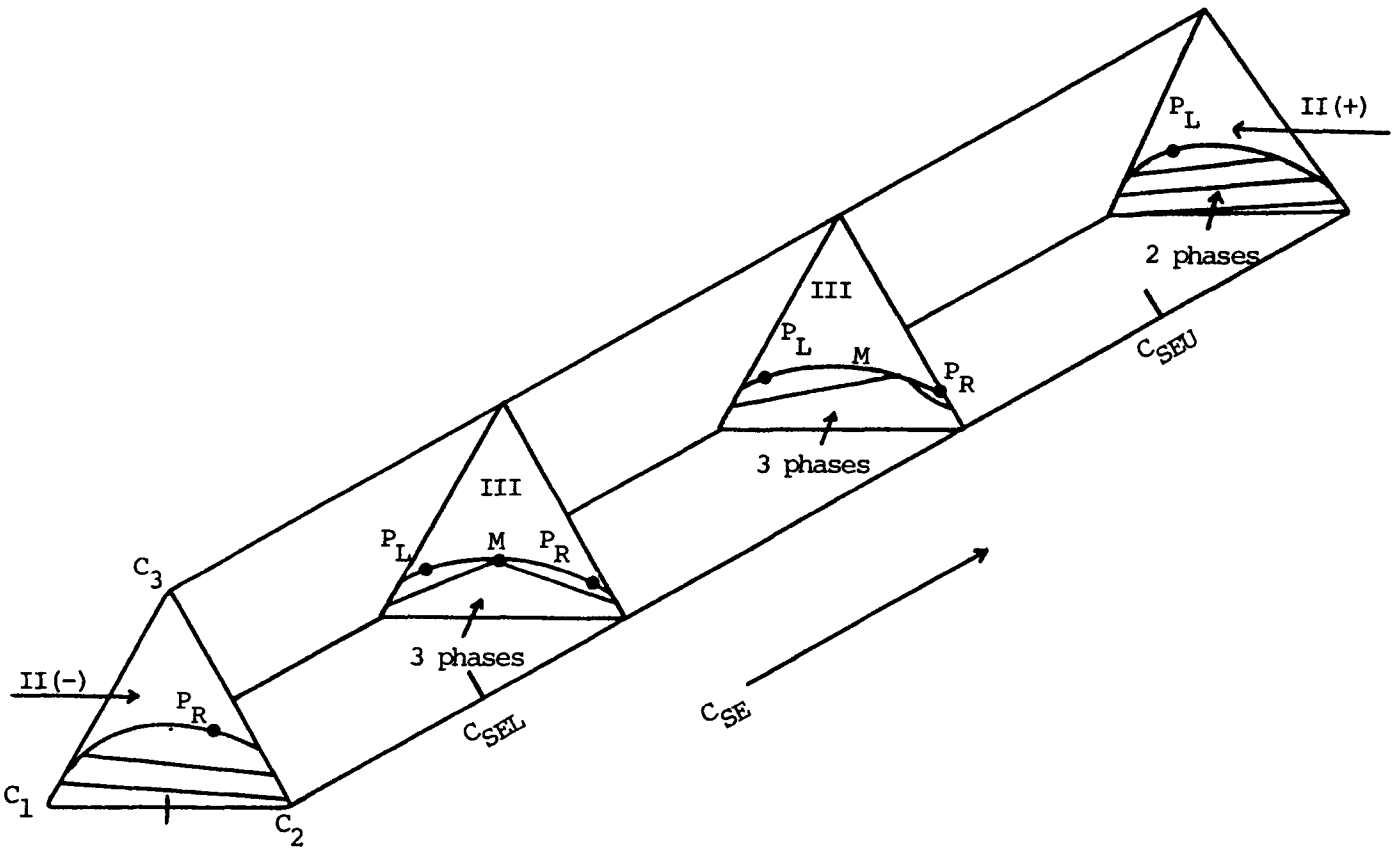


FIGURE B.2: Hand Plot

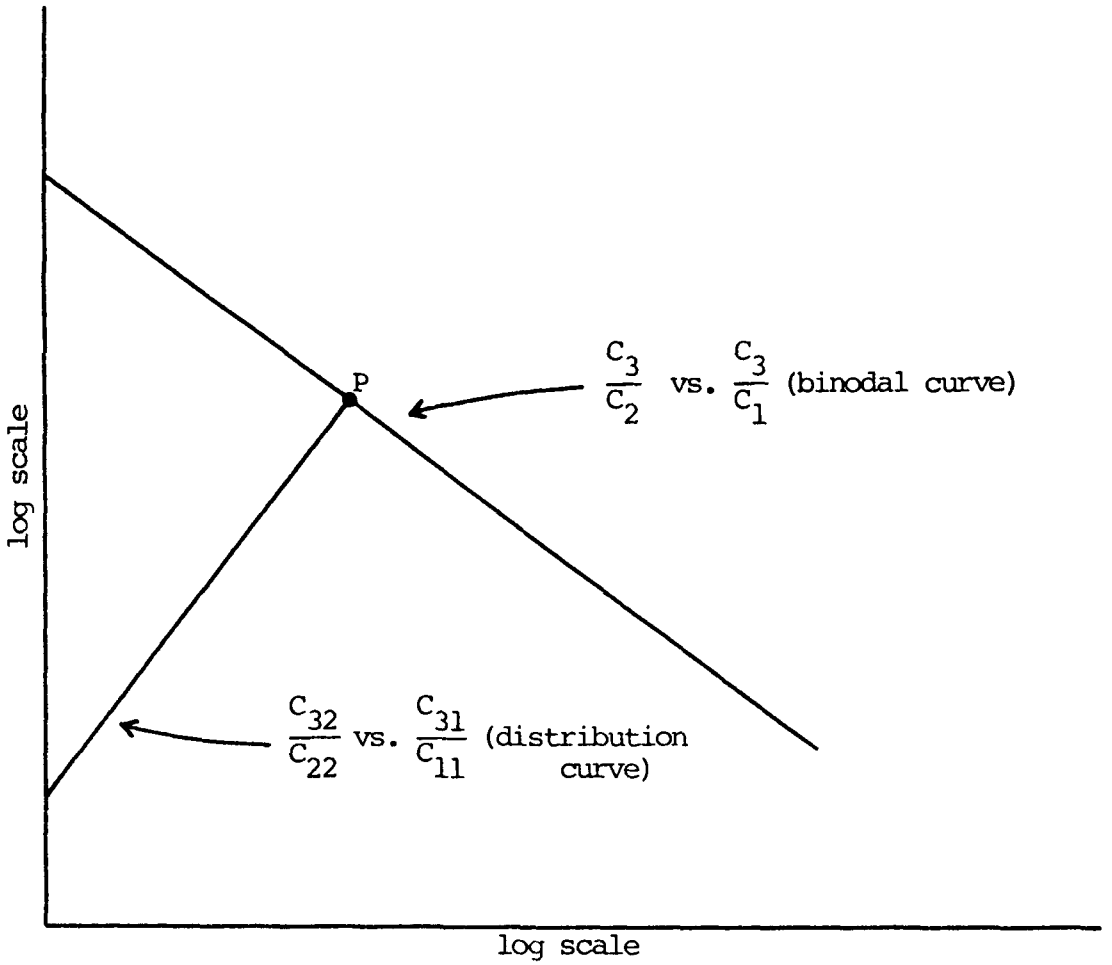
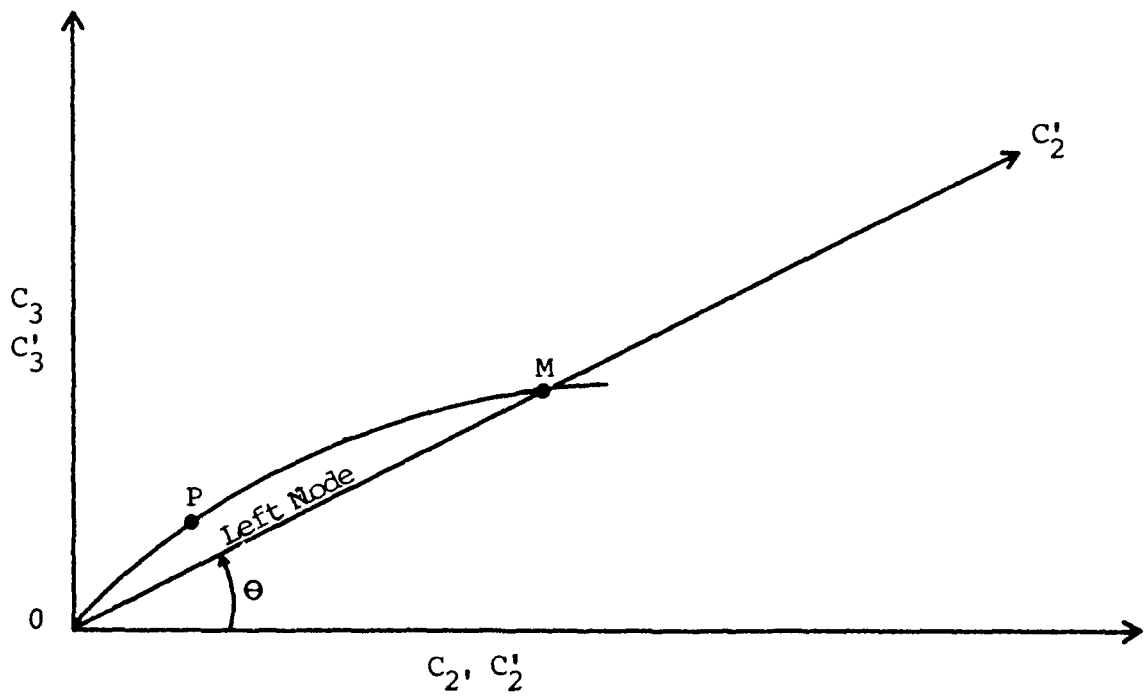


FIGURE B.3: Coordinate Rotation



APPENDIX C: PHASE: A Ternary Phase Calculation Program

A short FORTRAN program called PHASE has been written to provide the CHEM2D user with a tool for looking directly at the phase behavior of a system. PHASE is the phase behavior calculation of CHEM2D coupled with a driving program for generating ternary phase behavior input data and for outputting tabular results.

PHASE can be used to compute:

1. phase concentrations and saturations as a function of effective salinity and total component concentrations; and
2. phase saturations (relative volumes) as a function of effective salinity for a fixed set of total component concentrations.

The latter capability is particularly useful for preparing phase volume versus effective salinity diagrams (Figure C.1).

Any CHEM2D data set may be run with PHASE (on a DEC 2060, TOPS 20 operating system or other compatible configuration) without modification *if*:

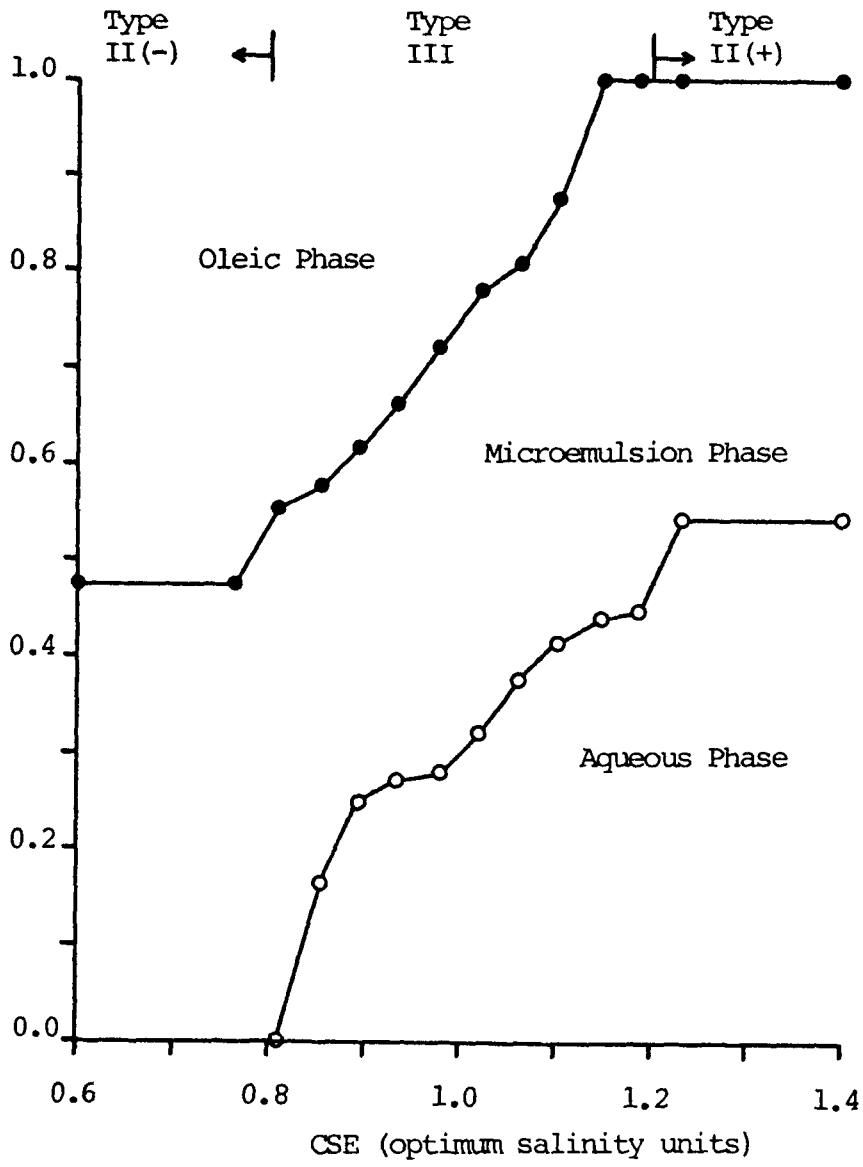
1. the first five columns of the title card for the Phase Behavior Data section (see Volume II of this report) are P H A S E; and
2. no other title card of the CHEM2D input data set begins with the five letters P H A S E.

Other data required by PHASE are input interactively.

The FORTRAN code for the program PHASE is reproduced in Section C.1. An example run is reproduced in its entirety in Section C.2. All underlined values are input by the user during an interactive session. For Type II(-) systems the aqueous phase saturation of the output represents the microemulsion phase of Figure C.1, while for Type II(+) systems the microemulsion phase of Figure C.1 is represented by the oleic phase saturation.

FIGURE C.1: Phase Volume vs. Effective Salinity

Total Water Concentration = 0.475
Total Oil Concentration = 0.475
Total Surfactant Concentration = 0.050



```
C
C       PHASE  PHASE BEHAVIOR CALCULATION PROGRAM
C       JOHN R  FANCHI
C       OCTOBER, 1983
C
        COMMON /HH1/ CTOT(11,11,9),C(121,9,3),CSE(11,11),S(11,11,3)
        COMMON /HH2/ CSEL,CSEU,C2PLC,C2PRC,A11,A12,A21,A22,B1,B2,B3,(
       1G3,F1,F2,F3,G11,G12,G13,G21,G22,G23,XIFTW,CSEOPT
        COMMON /HH3/ IJ1,I,J,NP,NPHASE(11,11),XIFT1,XIFT2,XIFT3,ALPH/
       1,SR1,SR2,SR3
        COMMON /HH4/ A,B,G,F,IFX,XR,XL
        COMMON /HH7/ IERROR
        DOUBLE PRECISION INDAT,OUTDAT
        DIMENSION PRIVAR(11,11),TITLE(48),CSEO(7)
        DATA LINSUM/0/
        DATA ICOUNT,FC/0,1 0/
        DATA NX,NY,N/1,1,3/
C       OPEN FILES FOR I/O ON DEC 2060, KCS, HOUSTON
        WRITE ( 5,3)
      3 FORMAT(1X,'ENTER INPUT DATA FILE NAME .    ',$)
        READ(5,5) INDAT
      5 FORMAT(A10)
        OPEN(UNIT=20,DEVICE='DSK',MODE='ASCII',ACCESS='SEQIN',
       & FILE=INDAT,DISPOSE='SAVE')
        WRITE ( 5,7)
      7 FORMAT(1X,'ENTER OUTPUT DATA FILE NAME .    ',$)
        READ(5,5) OUTDAT
        OPEN(UNIT=21,DEVICE='DSK',MODE='ASCII',ACCESS='SEQOUT',
       & FILE=OUTDAT,DISPOSE='SAVE')
C       END OF OPEN FILES
        WRITE ( 5,2001)
   2001 FORMAT(//T30,69('*'),/T30,'*',T98,'*',/T30,'*',T98,'*')
        WRITE ( 5,2002)
   2002 FORMAT(T30,'*',T61,' PHASE ',T98,'*',/T30,'*',T50,
       & 'TERNARY PHASE CALCULATION',T98,
       & '*',/T30,'*',T58,'(VERSION 1 0)',T98,'*')
        WRITE ( 5,2003)
   2003 FORMAT(T30,'*',T98,'*',/T30,'*',T98,'*',/T30,69('*'),///)
C       TITLE OF INPUT DATA SET
C
        WRITE(5,2010)
   2010 FORMAT(1X,'TERNARY PHASE CALC OR PHASE VOLUME?',
       & /,1X,'ENTER 0 FOR TERNARY PHASE CALC,',
       & /,1X 'ENTER 1 FOR PHASE VOLUME ',$)
        READ(5,*) ICODE
     10 CONTINUE
C
        READ (20,1090) (TITLE(I),I=1,16)
        IF(TITLE(1) NE 5HPHASE) GO TO 10
C
C       PHASE BEHAVIOR DATA
```

```
C
      READ (20,*) CSELI,CSEUI,CSEOPT
      READ (20,*) C2PLC,C2PRC
      READ (20,*) C3MAXO,C3MAX1,C3MAX2
      READ (20,*) B1,B2,B3
      READ (20,*) F1,F2,F3
C
      AAO=((2.*C3MAXO)/(1.-C3MAXO))**2
      AA1=((2.*C3MAX1)/(1.-C3MAX1))**2
      AA2=((2.*C3MAX2)/(1.-C3MAX2))**2
      A21=AAO
      A22=(AA1-AAO)
      A11=2.*AA1-AA2
      A12=(AA2-AA1)
      WRITE ( 5,1340)
      WRITE ( 5,1350)
      WRITE ( 5,1360) CSELI,CSEUI,CSEOPT
      WRITE ( 5,1380)
      WRITE ( 5,1360) C2PLC,C2PRC
      WRITE ( 5,1390)
      WRITE ( 5,1360) C3MAXO,C3MAX1,C3MAX2
      WRITE ( 5,1400)
      WRITE ( 5,1360) B1,B2,B3
      WRITE ( 5,1410)
      WRITE ( 5,1360) F1,F2,F3
      CSEL=CSELI
      CSEU=CSEUI
C
C
C     ------------------------------------------------------------
C     SET INITIAL VALUE
C     ------------------------------------------------------------
C
      IF(ICODE.NE.0) GO TO 2105
      CSEO(1)=0 5*CSEL
      CSEO(2)=0.95*CSEL
      CSEO(3)=1 0-0.95*(1 0-CSEL)
      CSEO(4)=1.0
      CSEO(5)=1.0+0.95*(CSEU-1 0)
      CSEO(6)=1.05*CSEU
      CSEO(7)=1.5*CSEU
C
      DO 1040 INDEX=1,7
      C3MAX=C3MAX1
      IF(INDEX.LT.3) C3MAX=C3MAXO
      IF(INDEX.GT.5) C3MAX=C3MAX2
  170 DO 190 J=1,NY
      DO 190 I=1,NX
      WRITE(5,1034) CSEO(INDEX)
 1034 FORMAT(/,5X,120('*'),/,10X,'CSE =',F10.6,/)
```

```
C
      DO 190 INDTOT=1,4
      CTOT(I,J,3)=(INDTOT)*0.25*C3MAX
      WRITE(5,1036)
      DO 190 JNDTOT=1,9
      WRITE(5,1038)
 1038 FORMAT(/,7X,'  K    CTOT(K)     C(K,1)     C(K,2)     C(K,3)
     & '    S(K)')
      CTOT(I,J,1)=0.1*JNDTOT
      IF((CTOT(I,J,3)+CTOT(I,J,1)).GT.1.0) CTOT(I,J,1)=1.-CTOT(I,
      CTOT(I,J,2)=1.-CTOT(I,J,1)-CTOT(I,J,3)
C
         CSE(I,J)=CSEO(INDEX)*CSEOPT
         DO 180 L=1,3
         DO 180 K=1,9
  180    C(IJ1,K,L)=0.
      CALL PHCOMP
      DO  25 K=1,3
      WRITE(5,26) K, CTOT(I,J,K),(C(IJ1,K,L),L=1,3),S(I,J,K)
   26 FORMAT(5X,I5,6F10.6)
   25 CONTINUE
  190 CONTINUE
 1036 FORMAT(/,5X,120('.'),/)
C
 1040 CONTINUE
      GO TO 2004
C
C
C       PHASE VOLUME CALC
C
C
 2105 CONTINUE
      I=1
      J=1
      WRITE(5,2110)
 2110 FORMAT(/1X,'ENTER TOTAL WATER CONC (FR) ',$)
      READ(5,*) CTOT(I,J,1)
      WRITE(5,2120)
 2120 FORMAT(1X,'ENTER TOTAL OIL CONC (FR) ',$)
      READ(5,*) CTOT(I,J,2)
      CTOT(I,J,3)=1.-CTOT(I,J,1)-CTOT(I,J,2)
      WRITE(5,2130) CTOT(I,J,3)
 2130 FORMAT(1X,'TOTAL SURF CONC (FR) =',F10.6)
      DO 3000 JVOL=1,20
      DCSE=CSEU-CSEL
      CSE(I,J)=CSEOPT+CSEOPT*DCSE*(1.-(20-JVOL)*2./19.)
      CALL PHCOMP
      WRITE(5,2150)
 2150 FORMAT(/,7X,'  K    CTOT(K)     C(K,1)     C(K,2)     C(K,3)
     & '    S(K)     CSE(OSU)')
```

```
      DO 3025 K=1,3
      CSEOUT=CSE(I,J)/CSEOPT
      WRITE(5,26) K,CTOT(I,J,K),(C(IJ1,K,L),L=1,3),S(I,J,K),CSEOU
 3025 CONTINUE
 3000 CONTINUE
      WRITE(5,3110)
 3110 FORMAT(//1X,'ANOTHER PHASE VOLUME CALC? (Y/N) ',$)
      READ(5,3120) PVCALC
 3120 FORMAT(A5)
      IF(PVCALC.EQ.5HN    .OR.PVCALC.EQ.5HNO   ) GO TO 2004
      GO TO 2105
 2004 WRITE(5,2005)
 2005 FORMAT(//,50('*'),T55,'RUN TERMINATED',T73,50('*'),//)
C      CLOSE I/O FILES FOR DEC 20/60
      CLOSE(UNIT=20)
      CLOSE(UNIT=21)
C      END OF CLOSE FILES
      STOP
C
 1090 FORMAT(16A5)
 1095 FORMAT (16A5)
 1340 FORMAT(///,5X,'PARAMETERS FOR PHASE DIAGRAM')
 1350 FORMAT(/,8X,'CSELI',7X,'CSEUI',6X,'CSEOPT')
 1360 FORMAT (5X,10G12.4)
 1370 FORMAT (8X,I3,9X,I3,4X,5G12.4)
 1380 FORMAT (/,8X,  5HC2PLC,7X,  5HC2PRC)
 1390 FORMAT (/,8X,  6HC3MAX0,6X,  6HC3MAX1,6X,  6HC3MAX2)
 1400 FORMAT (/,10X,  2HB1,10X,  2HB2,10X,  2HB3)
 1410 FORMAT (/,10X,  2HF1,10X,  2HF2,10X,  2HF3)
 1920 FORMAT (//,5X,  8HSALINITY)
 1930 FORMAT (//,5X, 32HTOTAL CONCENTRATION OF COMPONENT,I3)
 1940 FORMAT (//,5X, 26HCONCENTRATION OF COMPONENT,I3,  9H IN PHA
C
      END
```

```
C.        .. .  . .  .. .  . .....  .... ....  . . . . .PH
      SUBROUTINE PHCOMP
C
C     ------------------------------------------------------------------
C
C     THIS SUBROUTINE IS USED TO FIND THE PHASE ENVIRONMENT AND
C     TO CALCULATE THE PHASE COMPOSITIONS AND SATURATIONS
C
C     ------------------------------------------------------------------
C
      COMMON /HH1/ CTOT(11,11,9),C(121,9,3),CSE(11,11),S(11,11,3)
      COMMON /HH2/ CSEL,CSEU,C2PLC,C2PRC,A11,A12,A21,A22,B1,B2,B3,
     1G3,F1,F2,F3,G11,G12,G13,G21,G22,G23,XIFTW,CSEOPT
      COMMON /HH3/ IJ1,I,J,NP,NPHASE(11,11),XIFT1,XIFT2,XIFT3,ALPH
     1,SR1,SR2,SR3
      COMMON /HH4/ A,B,G,F,IFX,XR,XL
      COMMON /HH7/ IERROR
C
      IJ1=1
      I=1
      J=1
C
      IF (CTOT(I,J,7).GE.1.0E-8) RSA=CTOT(I,J,3)/CTOT(I,J,7)
C
C     COMBINE SURFACTANT AND ALCOHOL TOGETHER AS COMPONENT THREE
C
      CTOT(I,J,3)=CTOT(I,J,3)+CTOT(I,J,7)
C
C      EFFECTIVE SALINITY CSE(I,J) IS CONVERTED TO OPTIMAL SALINI
C      UNITS BY DIVIDING BY OPTIMAL SALINITY CSEOPT IN SUB PHCOMP
C      CSEOPT IS IN VOL FRAC UNITS.
C
      IF ((CSE(I,J)/CSEOPT).LT.CSEU) GO TO 80
C
C     TYPE II(+) BEHAVIOR  HIGH SALINITY
C
      A1=A11+A12*(CSE(I,J)/CSEOPT)
      IF (CTOT(I,J,2).LT.0.0010) GO TO 60
      R32=CTOT(I,J,3)/CTOT(I,J,2)
      R31=(R32/A1)**(1.0/B1)
      C(IJ1,1,2)=R32/(R32+R32*R31+R31)
      C(IJ1,2,2)=1.0-(R31+1.0)*C(IJ1,1,2)
      C(IJ1,3,2)=1.0-C(IJ1,1,2)-C(IJ1,2,2)
      IF (C(IJ1,3,2).LT.CTOT(I,J,3)) GO TO 60
      NPHASE(I,J)=2
      NP=1
      IF (ABS(C2PLC).GT.00001 AND ABS(F1).GT..00001) GO TO 20
      C(IJ1,1,1)=1.0
      C(IJ1,2,1)=0.0
      C(IJ1,3,1)=0.0
      GO TO 30
```

```
   20 A=A1
      B=B1
      F=F1
      C3PLC= 5*(-A*C2PLC+((A*C2PLC)**2+4.*A*C2PLC*(1 -C2PLC))**.5.
      G=(1 -C3PLC-C2PLC)/C2PLC
C
C     CALCULATE R31 ,R32 AT PLAIT POINT
C
      XR=C3PLC/C2PLC-.0000001
      XL=.0000001
C
C     CALCULATE THE CONCENTRATIONS OF COMPONENTS OF TWO PHASES
C
      CALL TIELIN
      IF (IERROR.EQ 1) RETURN
   30 DO 40 K=1,9
   40 C(IJ1,K,3)=0.0
      DO 50 K=5,9
      DO 50 L=1,2
   50 C(IJ1,K,L)=CTOT(I,J,K)*C(IJ1,1,L)/CTOT(I,J,1)
      S(I,J,1)=(CTOT(I,J,1)-C(IJ1,1,2))/(C(IJ1,1,1)-C(IJ1,1,2))
      S(I,J,2)=1.-S(I,J,1)
      S(I,J,3)=0.0
      GO TO 350
   60 NPHASE(I,J)=1
      DO 70 K=1,9
         C(IJ1,K,1)=CTOT(I,J,K)
         C(IJ1,K,2)=0.
   70 C(IJ1,K,3)=0.
      S(I,J,1)=1.
      S(I,J,2)=0.
      S(I,J,3)=0.
      GO TO 350
   80 IF ((CSE(I,J)/CSEOPT).GT.CSEL) GO TO 150
C
C     TYPE II(-) BEHAVIOR  LOW SALINITY
C
      A2=A21+A22*(CSE(I,J)/CSEOPT)
      R31=CTOT(I,J,3)/CTOT(I,J,1)
      R32=A2*R31**B2
      C(IJ1,1,1)=R32/(R32+R32*R31+R31)
      C(IJ1,2,1)=1 0-(R31+1.0)*C(IJ1,1,1)
      C(IJ1,3,1)=1.0-C(IJ1,1,1)-C(IJ1,2,1)
      IF (C(IJ1,3,1) LT CTOT(I,J,3)) GO TO 130
      NPHASE(I,J)=2
      NP=2
      IF (ABS(C2PRC) LT 1.0 AND ABS(F2) GT  000001) GO TO 90
      C(IJ1,1,2)=0.0
      C(IJ1,2,2)=1 0
      C(IJ1,3,2)=0.0
```

```
      GO TO 100
   90 A=A21+A22*(CSE(I,J)/CSEOPT)
      B=B2
      F=F2
      C3PRC=.5*(-A*C2PRC+((A*C2PRC)**2+4.*A*C2PRC*(1.-C2PRC))**.!
      G=(1.-C3PRC-C2PRC)/C2PRC
      XR=G*R31**F
      XL=.0000001
C
C     CALCULATE THE CONCENTRATIONS OF COMPONENTS OF TWO PHASES
C
      CALL TIELIN
  100 DO 110 K=1,9
  110 C(IJ1,K,3)=0.0
      DO 120 K=5,9
      DO 120 L=1,2
  120 C(IJ1,K,L)=CTOT(I,J,K)*C(IJ1,1,L)/CTOT(I,J,1)
      S(I,J,1)=(CTOT(I,J,1)-C(IJ1,1,2))/(C(IJ1,1,1)-C(IJ1,1,2))
      S(I,J,2)=1.-S(I,J,1)
      S(I,J,3)=0.
      GO TO 350
  130 NPHASE(I,J)=1
      DO 140 K=1,9
         C(IJ1,K,2)=0.0
         C(IJ1,K,1)=CTOT(I,J,K)
  140 C(IJ1,K,3)=0.
      S(I,J,1)=1.0
      S(I,J,2)=0.0
      S(I,J,3)=0.0
      GO TO 350
C
C     TYPE III BEHAVIOR: INTERMEDIATE SALINITY
C
  150 C2M=((CSE(I,J)/CSEOPT)-CSEL)/(CSEU-CSEL)
      IF ((CSE(I,J)/CSEOPT)-.5*(CSEU+CSEL)) 160,160,170
  160 A3=A21+A22*(CSE(I,J)/CSEOPT)
      GO TO 180
  170 A3=A11+A12*(CSE(I,J)/CSEOPT)
  180 A=A3
      B=B3
      F=F3
      C3M= 5*(-A*C2M+((A*C2M)**2+4.*A*C2M*(1.-C2M))**.5)
      C1M=1.-C2M-C3M
      IF (C2M.LT.1.0E-10) C2M=1.0E-10
      IF (C1M.LT.1.0E-10) C1M=1.0E-10
      IF (CTOT(I,J,2).GT.C2M) GO TO 250
C
C     TEST FOR THREE PHASES
C
      IF (CTOT(I,J,3).LT C3M*CTOT(I,J,2)/C2M) GO TO 300
```

```
C
C     PHASES 1 AND 2 -- LEFT NODE AND ONE PHASE REGION
C
      IF (CTOT(I,J,2).LE 0.001) GO TO 230
      NPHASE(I,J)=2
      NP=1
      R32=CTOT(I,J,3)/CTOT(I,J,2)
      R31=(R32/A3)**(1.0/B3)
      C(IJ1,1,2)=R32/(R32+R32*R31+R31)
      C(IJ1,2,2)=1.0-(R31+1.0)*C(IJ1,1,2)
      C(IJ1,3,2)=1.0-C(IJ1,1,2)-C(IJ1,2,2)
      IF (C(IJ1,3,2).LT.CTOT(I,J,3)) GO TO 230
      IF (ABS(C2PLC).GT.1.0E-10) GO TO 190
      C(IJ1,1,1)=1.0
      C(IJ1,2,1)=0.0
      C(IJ1,3,1)=0.0
      GO TO 200
  190 C2PL=C2PLC+((CSE(I,J)/CSEOPT)-CSEU)*C2PLC/(CSEU-CSEL)
      C3PL=.5*(-A*C2PL+((A*C2PL)**2+4.*A*C2PL*(1.-C2PL))**.5)
      C1PL=1.-C2PL-C3PL
      ALPHA=C3M/C2M
      BETA=SQRT(C2M**2+C3M**2)/C2M
      G=(1.+(ALPHA-BETA)*C2PL-C3PL)/(BETA*C2PL)
      XR=C3PL/C1PL-.0000001
      XL=.0000001
      CALL TIELIN
      IF (IERROR.EQ.1) RETURN
  200 DO 210 K=1,9
  210 C(IJ1,K,3)=0.0
      IF (CTOT(I,J,3).GT.C(IJ1,3,2)) GO TO 230
      DO 220 K=5,9
      DO 220 L=1,2
  220 C(IJ1,K,L)=CTOT(I,J,K)*C(IJ1,1,L)/CTOT(I,J,1)
      S(I,J,1)=(CTOT(I,J,1)-C(IJ1,1,2))/(C(IJ1,1,1)-C(IJ1,1,2))
      S(I,J,2)=1.0-S(I,J,1)
      S(I,J,3)=0.0
      GO TO 350
C
C     SINGLE PHASE
C
  230 NPHASE(I,J)=1
      DO 240 K=1,9
         C(IJ1,K,2)=0.
         C(IJ1,K,3)=0.
  240 C(IJ1,K,1)=CTOT(I,J,K)
      S(I,J,1)=1.0
      S(I,J,2)=0.0
      S(I,J,3)=0.0
      GO TO 350
  250 IF (CTOT(I,J,3).LT C3M*CTOT(I,J,1)/C1M) GO TO 300
```

```
C
C     PHASES 1 AND 2 -- RIGHT NODE AND ONE PHASE REGION
C
      NPHASE(I,J)=2
      NP=2
      R31=CTOT(I,J,3)/CTOT(I,J,1)
      R32=A3*R31**B3
      C(IJ1,1,1)=R32/(R32+R32*R31+R31)
      C(IJ1,2,1)=1.0-(R31+1.0)*C(IJ1,1,1)
      C(IJ1,3,1)=1.0-C(IJ1,1,1)-C(IJ1,2,1)
      IF (CTOT(I,J,3).GT.C(IJ1,3,1)) GO TO 230
      IF (ABS(C2PRC).LT.1.) GO TO 260
      C(IJ1,1,2)=0.0
      C(IJ1,2,2)=1.0
      C(IJ1,3,2)=0.0
      GO TO 270
  260 C2PR=C2PRC+(1.-C2PRC)*((CSE(I,J)/CSEOPT)-CSEL)/(CSEU-CSEL)
      C3PR=.5*(-A*C2PR+((A*C2PR)**2+4.*A*C2PR*(1.-C2PR))**.5)
      C1PR=1.-C2PR-C3PR
      ALPHA=C3M/C1M
      BETA=SQRT(C3M**2+C1M**2)/C1M
      G=BETA*C1PR/(1.+(ALPHA-BETA)*C1PR-C3PR)
      XR=G*R31**F-.0000001
      XL=.0000001
      CALL TIELIN
      IF (IERROR.EQ.1) RETURN
  270 DO 280 K=1,9
  280 C(IJ1,K,3)=0.0
      DO 290 K=5,9
      DO 290 L=1,2
  290 C(IJ1,K,L)=CTOT(I,J,K)*C(IJ1,1,L)/CTOT(I,J,1)
      S(I,J,2)=(CTOT(I,J,2)-C(IJ1,2,1))/(C(IJ1,2,2)-C(IJ1,2,1))
      S(I,J,1)=1.0-S(I,J,2)
      S(I,J,3)=0.0
      GO TO 350
C
C     THREE PHASES
C
  300 NPHASE(I,J)=3
      C(IJ1,1,1)=1.0
      C(IJ1,2,1)=0.0
      C(IJ1,3,1)=0.0
      C(IJ1,1,2)=0.0
      C(IJ1,2,2)=1.0
      C(IJ1,3,2)=0.0
      C(IJ1,1,3)=C1M
      C(IJ1,2,3)=C2M
      C(IJ1,3,3)=C3M
      DO 310 L=1,3
      DO 310 K=5,9
```

```
  310 C(IJ1,K,L)=CTOT(I,J,K)*C(IJ1,1,L)/CTOT(I,J,1)
      S(I,J,2)=((CTOT(I,J,1)-C(IJ1,1,3))*C(IJ1,2,3)+(1.0-C(IJ1,1,3))
     & *(CTOT(I,J,2)-C(IJ1,2,3)))/(1.0-C(IJ1,1,3)-C(IJ1,2,3))
      S(I,J,1)=((CTOT(I,J,1)-C(IJ1,1,3))*(1.0-C(IJ1,2,3))+(CTOT(I,J,2)
     & -C(IJ1,2,3))*C(IJ1,1,3))/(1 0-C(IJ1,1,3)-C(IJ1,2,3))
      DO 315 L=1,2
      IF(S(I,J,L).LT.0.0) S(I,J,L)=0.0
      IF(S(I,J,L).GT.1.0) S(I,J,L)=1.0
  315 CONTINUE
      S(I,J,3)=1.-S(I,J,1)-S(I,J,2)
      GO TO 350
  316 CONTINUE
  350 CONTINUE
      RETURN
C
      END
```

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```
C     ..  ...  ....  ..  .....  ...  .  .......  ..  .....  .....TIELIN
      SUBROUTINE TIELIN
C
C     ------------------------------------------------------------------
C
C     USING HALF INTERVAL METHOD TO FIND  THE CORRECT ANSWER
C     OF C31/C21
C
C     ------------------------------------------------------------------
C
      COMMON /HH1/ CTOT(11,11,9),C(121,9,3),CSE(11,11),S(11,11,3)
      COMMON /HH4/ A,B,G,F,IFX,XR,XL
      COMMON /HH7/ IERROR
      EPS=0.0001
      IFX=0
      CALL TRY (XR,FXR)
      IF (IERROR.EQ.1) RETURN
      CALL TRY (XL,FXL)
      IF (IERROR.EQ.1) RETURN
   10 APP=(XL+XR)/2.
      CALL TRY (APP,FXAPP)
      IF (IERROR.EQ.1) RETURN
      IF (FXAPP*FXL) 20,40,30
   20 XR=APP
      FXR=FXAPP
      IF (ABS(XR-XL).LE.EPS) GO TO 40
      GO TO 10
   30 XL=APP
      FXL=FXAPP
      IF (ABS(XR-XL).LE.EPS) GO TO 40
      GO TO 10
   40 CONTINUE
      RETURN
C
      END
```

```
C                 ..... . .. . .. . . . . .... .. . ..TRY
      SUBROUTINE TRY (X,FX)
C
C     ------------------------------------------------------------------
C
C     USING EQUATION OF DISTRIBUTION CURVE AND EQUATION OF BINODAL
C     CURVE TO CALCULATE PHASE COMPOSITIONS
C
C     ------------------------------------------------------------------
C
      COMMON /HH1/ CTOT(11,11,9),C(121,9,3),CSE(11,11),S(11,11,3)
      COMMON /HH3/ IJ1,I,J,NP,NPHASE(11,11),XIFT1,XIFT2,XIFT3,ALPHA,B
     1,SR1,SR2,SR3
      COMMON /HH4/ A,B,G,F,IFX,XR,XL
      COMMON /HH7/ IERROR
      IFX=IFX+1
      IF (IFX.LE.100) GO TO 10
      IERROR=1
      WRITE ( 5,30) X,FX
      RETURN
   10 IF (NP.EQ.2) GO TO 20
C
C     C     Y=R32(1) X=R31(1) W=R32(2) Z=R31(2)
C     C     LEFT NODE
C
      Y=A*X**B
      C(IJ1,2,1)=X/(X+X*Y+Y)
      C(IJ1,3,1)=C(IJ1,2,1)*Y
      C(IJ1,1,1)=1.-C(IJ1,2,1)-C(IJ1,3,1)
      P=G*((C(IJ1,3,1)-C(IJ1,2,1)*ALPHA)/(1.-C(IJ1,3,1)+C(IJ1,2,1)*(A
     1A-BETA)))**F
      W=BETA*P + ALPHA
      IF(W LE 0 0) GO TO 11
      Z=(W/A)**(1./B)
      C(IJ1,2,2)=Z/(Z+Z*W+W)
      C(IJ1,3,2)=C(IJ1,2,2)*W
      C(IJ1,1,2)=1 -C(IJ1,2,2)-C(IJ1,3,2)
      GO TO 15
C
   11 CONTINUE
      C(IJ1,2,2)=1.
      C(IJ1,3,2)=0.
      C(IJ1,1,2)=0.
C
   15 FX=(C(IJ1,3,2)-CTOT(I,J,3))*(C(IJ1,2,1)-CTOT(I,J,2))-(C(IJ1,3,1
     1TOT(I,J,3))*(C(IJ1,2,2)-CTOT(I,J,2))
      RETURN
C
C     CALCUTE THE CONC  OF WATER, OIL, SURFACTANT IN EACH PHASE
C     AT RIGHT NODE (TYPE III, II(-)) PHASE BEHAVIOR
C     X=R32(2) Y=R31(2) W=R32(1) Z=R31(1)
```

```
C
   20 Y=(X/A)**(1./B)
      C(IJ1,2,2)=Y/(X+Y*X+Y)
      C(IJ1,3,2)=C(IJ1,2,2)*X
      C(IJ1,1,2)=1.-C(IJ1,2,2)-C(IJ1,3,2)
      P=((C(IJ1,3,2)-ALPHA*C(IJ1,1,2))/G/(1.+C(IJ1,1,2)*(ALPHA-BETA)
     1J1,3,2)))**(1./F)
      Z=BETA*P + ALPHA
      IF(Z.LE.0.0) GO TO 21
      W=A*(Z**B)
      C(IJ1,2,1)=Z/(Z+Z*W+W)
      C(IJ1,3,1)=C(IJ1,2,1)*W
      C(IJ1,1,1)=1.-C(IJ1,2,1)-C(IJ1,3,1)
      GO TO 25
C
   21 CONTINUE
      C(IJ1,1,1)=1.0
      C(IJ1,2,1)=0.
      C(IJ1,3,1)=0.
C
   25 FX=(C(IJ1,3,2)-CTOT(I,J,3))*(C(IJ1,2,1)-CTOT(I,J,2))-(C(IJ1,3,1
     1TOT(I,J,3))*(C(IJ1,2,2)-CTOT(I,J,2))
C
      RETURN
C
   30 FORMAT (1X,  8HIERROR=1,//,  4HR32=,E16.5,  3HFX=,E16.5)
C
      END
```

```
RUN PHASE
ENTER INPUT DATA FILE NAME ... CHMC12
ENTER OUTPUT DATA FILE NAME ... OUT

                    ***********************************************************************
                    *                                                                     *
                    *                                                                     *
                    *                          PHASE:                                     *
                    *                 TERNARY PHASE CALCULATION                           *
                    *                        (VERSION 1.0)                                *
                    *                                                                     *
                    *                                                                     *
                    ***********************************************************************


TERNARY PHASE CALC OR PHASE VOLUME?
ENTER 0 FOR TERNARY PHASE CALC;
ENTER 1 FOR PHASE VOLUME:1


    PARAMETERS FOR PHASE DIAGRAM

      CSELI        CSEUI       CSEOPT
     0.8000        1.200       0.3640E-02

      C2PLC        C2PRC
     0.5000E-01   0.9500

      C3MAX0       C3MAX1       C3MAX2
     0.3000       0.1000       0.3000

        B1           B2           B3
     -1.000       -1.000       -1.000

        F1           F2           F3
      1.000        1.000        1.000

ENTER TOTAL WATER CONC (FR) 0.475
ENTER TOTAL OIL CONC (FR) 0.475
TOTAL SURF CONC (FR) =  0.050000

      K   CTOT(K)    C(K,1)    C(K,2)    C(K,3)     S(K)    CSE(OSU)
      1  0.475000  1.000000  0.000001  0.000000  0.474999  0.600000
      2  0.475000  0.000000  0.999395  0.000000  0.525001  0.600000
      3  0.050000  0.000000  0.000604  0.000000  0.000000  0.600000

      K   CTOT(K)    C(K,1)    C(K,2)    C(K,3)     S(K)    CSE(OSU)
      1  0.475000  1.000000  0.000001  0.000000  0.474999  0.642105
      2  0.475000  0.000000  0.999350  0.000000  0.525001  0.642105
      3  0.050000  0.000000  0.000649  0.000000  0.000000  0.642105

      K   CTOT(K)    C(K,1)    C(K,2)    C(K,3)     S(K)    CSE(OSU)
      1  0.475000  1.000000  0.000002  0.000000  0.474999  0.684211
      2  0.475000  0.000000  0.999246  0.000000  0.525001  0.684211
      3  0.050000  0.000000  0.000752  0.000000  0.000000  0.684211

      K   CTOT(K)    C(K,1)    C(K,2)    C(K,3)     S(K)    CSE(OSU)
      1  0.475000  1.000000  0.000003  0.000000  0.474999  0.726316
      2  0.475000  0.000000  0.999179  0.000000  0.525001  0.726316
      3  0.050000  0.000000  0.000818  0.000000  0.000000  0.726316
```

K	CTOT(K)	C(K,1)	C(K,2)	C(K,3)	S(K)	CSE(OSU)
1	0.475000	1.000000	0.000004	0.000000	0.474998	0.768421
2	0.475000	0.000000	0.999098	0.000000	0.525002	0.768421
3	0.050000	0.000000	0.000898	0.000000	0.000000	0.768421

K	CTOT(K)	C(K,1)	C(K,2)	C(K,3)	S(K)	CSE(OSU)
1	0.475000	0.857187	0.000001	0.000000	0.554097	0.810526
2	0.475000	0.052771	0.999682	0.000000	0.445901	0.810526
3	0.050000	0.090042	0.000317	0.000000	0.000000	0.810526

K	CTOT(K)	C(K,1)	C(K,2)	C(K,3)	S(K)	CSE(OSU)
1	0.475000	1.000000	0.000000	0.746858	0.167810	0.852632
2	0.475000	0.000000	1.000000	0.131579	0.420880	0.852632
3	0.050000	0.000000	0.000000	0.121563	0.411309	0.852632

K	CTOT(K)	C(K,1)	C(K,2)	C(K,3)	S(K)	CSE(OSU)
1	0.475000	1.000000	0.000000	0.628647	0.241322	0.894737
2	0.475000	0.000000	1.000000	0.236842	0.386962	0.894737
3	0.050000	0.000000	0.000000	0.134511	0.371717	0.894737

K	CTOT(K)	C(K,1)	C(K,2)	C(K,3)	S(K)	CSE(OSU)
1	0.475000	1.000000	0.000000	0.528462	0.270855	0.936842
2	0.475000	0.000000	1.000000	0.342105	0.342845	0.936842
3	0.050000	0.000000	0.000000	0.129433	0.386300	0.936842

K	CTOT(K)	C(K,1)	C(K,2)	C(K,3)	S(K)	CSE(OSU)
1	0.475000	1.000000	0.000000	0.410495	0.276591	0.978947
2	0.475000	0.000000	1.000000	0.447368	0.275526	0.978947
3	0.050000	0.000000	0.000000	0.112137	0.445884	0.978947

K	CTOT(K)	C(K,1)	C(K,2)	C(K,3)	S(K)	CSE(OSU)
1	0.475000	1.000000	0.000000	0.338167	0.320164	1.021053
2	0.475000	0.000000	1.000000	0.552632	0.221967	1.021053
3	0.050000	0.000000	0.000000	0.109202	0.457869	1.021053

K	CTOT(K)	C(K,1)	C(K,2)	C(K,3)	S(K)	CSE(OSU)
1	0.475000	1.000000	0.000000	0.224289	0.378947	1.063158
2	0.475000	0.000000	1.000000	0.657895	0.194128	1.063158
3	0.050000	0.000000	0.000000	0.117116	0.426926	1.063158

K	CTOT(K)	C(K,1)	C(K,2)	C(K,3)	S(K)	CSE(OSU)
1	0.475000	1.000000	0.000000	0.127923	0.416277	1.105263
2	0.475000	0.000000	1.000000	0.763158	0.124669	1.105263
3	0.050000	0.000000	0.000000	0.108920	0.459074	1.105263

K	CTOT(K)	C(K,1)	C(K,2)	C(K,3)	S(K)	CSE(OSU)
1	0.475000	0.999409	0.062682	0.000000	0.440168	1.147368
2	0.475000	0.000002	0.847917	0.000000	0.559832	1.147368
3	0.050000	0.000588	0.089400	0.000000	0.000000	1.147368

K	CTOT(K)	C(K,1)	C(K,2)	C(K,3)	S(K)	CSE(OSU)
1	0.475000	0.995494	0.050314	0.000000	0.449316	1.189474
2	0.475000	0.000108	0.861542	0.000000	0.550684	1.189474
3	0.050000	0.004375	0.088143	0.000000	0.000000	1.189474

K	CTOT(K)	C(K,1)	C(K,2)	C(K,3)	S(K)	CSE(OSU)
1	0.475000	0.050003	0.937988	0.000000	0.546704	1.231579
2	0.475000	0.857642	0.000630	0.000000	0.453096	1.231579
3	0.050000	0.094355	0.011332	0.000000	0.000000	1.231579

K	CTOT(K)	C(K,1)	C(K,2)	C(K,3)	S(K)	CSE(OSU)
1	0.475000	0.050003	0.987359	0.000000	0.546600	1.273684
2	0.475000	0.849665	0.000618	0.000000	0.453400	1.273684
3	0.050000	0.100332	0.012023	0.000000	0.000000	1.273684

```
K    CTOT(K)    C(K,1)    C(K,2)    C(K,3)     S(K)     CSE(OSU)
1   0.475000   0.050003  0.986750  0.000000  0.546305   1.315789
2   0.475000   0.844081  0.000609  0.000000  0.453695   1.315789
3   0.050000   0.105917  0.012641  0.000000  0.000000   1.315789

K    CTOT(K)    C(K,1)    C(K,2)    C(K,3)     S(K)     CSE(OSU)
1   0.475000   0.050003  0.985159  0.000000  0.546019   1.357895
2   0.475000   0.838827  0.000603  0.000000  0.453981   1.357895
3   0.050000   0.111170  0.013238  0.000000  0.000000   1.357895

K    CTOT(K)    C(K,1)    C(K,2)    C(K,3)     S(K)     CSE(OSU)
1   0.475000   0.050003  0.985584  0.000000  0.545740   1.400000
2   0.475000   0.833857  0.000599  0.000000  0.454260   1.400000
3   0.050000   0.116141  0.013817  0.000000  0.000000   1.400000

ANOTHER PHASE VOLUME (ALC? (Y/N) N

**** ****************************************    RUN TERMINATED    ****************************************

End of Execution
```