TERNARY LLE EXERCISE
TOLUENE-ACETONE-WATER EXTRACTION

EX1. Create a new job with the following component list:

1	TOLUENE	(41)
2	ACETONE	(140)
3	WATER	(62)

Define the K-value options as NRTL, NCOR, LLV.

Set the third parameters (alphas) in the BIP table to 0.2. Otherwise, the regression will use the parameters it finds in the BIP table.

Regress DECHEMA ternary LLE data at 30 deg C (EXHIBIT 5).

LLE TERNARY REGRESSION

Temp C	X1	X2	Y1	Y2
30.00	0.97555	0.20400E-01	0.10000E-03	0.50200E-02
30.00	0.95041	0.45000E-01	0.12000E-03	0.10800E-01
30.00	0.92183	0.72220E-01	0.12000E-03	0.16400E-01
30.00	0.85506	0.13290	0.17000E-03	0.30490E-01
30.00	0.75815	0.21699	0.26000E-03	0.50800E-01
30.00	0.59332	0.35259	0.49000E-03	0.83650E-01
30.00	0.445555	0.46248	0.10500E-02	0.12083
30.00	0.33598	0.54872	0.19800E-02	0.15366

EXHIBIT 5

Toluene / Acetone / Water
LLE

Define an LLVF module with the following data:

MODE	=	1
PAR 1	=	30 (temp, deg C)
PAR 2	=	1500 (pressure, mmHg)

NOTE: Any pressure above the bubble point pressure would be satisfactory.

Define an input stream as follows:

TEMP	=	30 deg C
PRESSURE	=	1500 mmHg
TOLUENE	=	0.2 moles
ACETONE	=	0.3 "
WATER	=	0.5 "

Execute the LLVF and compare the resulting tie line with the DECHEMA plot, EXHIBIT 6.

NOTE: The first liquid output stream from the LLVF is the LEFT phase in the DECHEMA data and plot.

Regress the same data again using smaller tolerances (.1e-6). Execute the LLVF and recheck the fit of the tie line. The fit should be substantially improved.

NOTE: The regression tolerances in CHEMCAD are set purposely "loose" to facilitate convergence and to give the user a feel for the prospective fit. It is generally good practice to reduce the tolerances and improve the data fit. At some tolerance level the error can no longer be reduced. You may have the best fit possible even though the error is not within the stated tolerances. Use plots and LLVF calculations to check the data fits.

EX2. Create a new job by copying the previous job. Enter the following DECHEMA parameters into the BIP table:

I	J	Bij	Bji	Alphaij
1	2	489.2	-301.51	.20
1	3	1318.8	2557.3	.20
2	3	377.45	210.6	.20

Check the convergence and validity of these parameters by regressing the same DECHEMA data as above while "clamping" the parameter values.

Execute the LLVF and check the fit of the tie line.

EX3. Create a new job by copying the previous job. Replace the LLVF with a liquid-liquid extractor module, EXTR, with the following data:

NUMBER OF STAGES	=	10
HEAVY (TOP) FEED STAGE	=	1
LIGHT (BOT) FEED STAGE	=	10
PRESSURE	=	1400 mmHg

Enter top (heavy) and bottom (light) feeds as follows:

	TOP	BOTTOM
Temperature, deg C	30	30
Pressure, mmHg	1500	1500
TOLUENE, mols	0	50
ACETONE "	0	50
WATER "	350	0

Execute the job and note the distribution of products. This example is used to demonstrate the extraction of acetone from toluene, using water as the extractant.

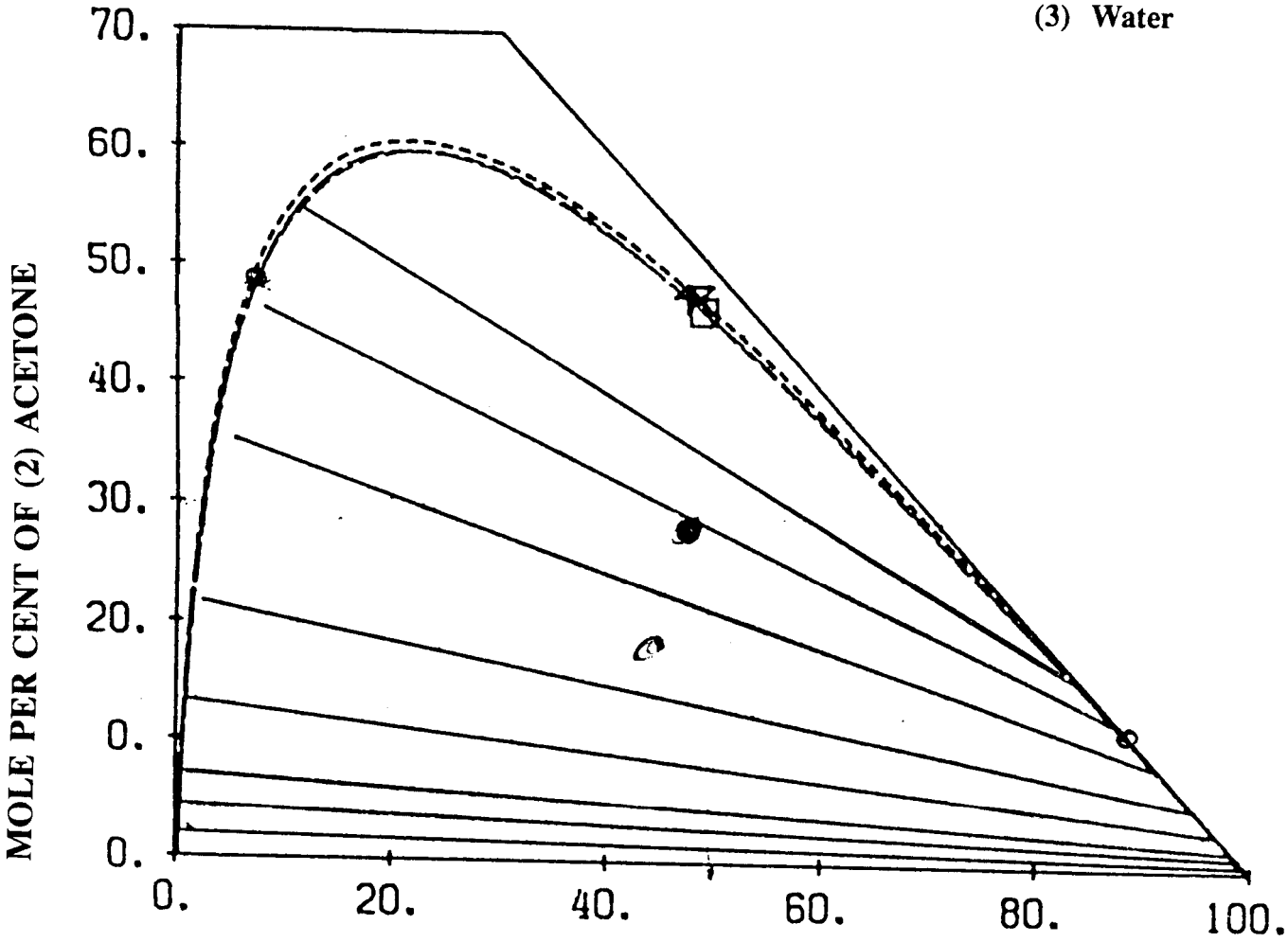
Plot the mole fraction profiles of the tower components using the PLOT PROFile command in TALK.

GENERAL OBSERVATIONS: LLE activity parameters will not extrapolate well beyond the temperature of the original data. LLE equilibrium is extremely temperature sensitive and large errors may result. On the other hand, VLE parameters will usually give good results over a moderate temperature range because the dominant temperature effect is on the vapor pressure of the pure components.

(1) Toluene

(2) Acetone

(3) Water



EXP. TIE LINE _____

CALC. BINODAL UNIQ (SP) _ _ NRTL(SP)- - - UNIQ(CO) -----

CALC.PLAIT P.

EXHIBIT 6

Toulene / Acetone / Water
LLE