

--- Simulation Input File ---
-STMT-

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*XPSIM> ...generated by XpsimWin v.1.06 ...
*EXE-OPT> PAGELLEN=66

100  RUN ID=VLE-DEMO-1 CUSTOMER=STAFF PROJECT='REGRESSION TEST'
200  DESC  ETHANOL-WATER-MEAC  EQUILIBRIUM  REGRESSION  TEST
300  DIMENSION INPUT MET PRES=MMHG
*
*
400  Thermodynamic Data
*
*
500  METHOD METHOD=WILSON
600  COMP=ETHANOL PARA=58.68,,,,,,,,,,,,,,,,
700  COMP=WATER PARA=18.07,,,,,,,,,,,,,,,,
800  COMP=MEAC PARA=79.84
900  BINARY=ETHANOL,WATER KIJ=185.776,895.586,,,,,,,,,,,,,,,,
1000 BINARY=ETHANOL,MEAC KIJ=1265.686,-460.819,,,,,,,,,,,,,,,,
1100 BINARY=WATER,MEAC KIJ=1832.270,753.456
*
*
1200 System Data
*
*
1300 CHEMCOMP ETHANOL / WATER / MEAC
1400 THERMSET UID=M1
1500 METHODS AL=WILSON FV=IDEAL FL=IDEAL HV=IDEAL HL=WILSON
*
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1600 Experimental Data
*
*
1700 VLEREGRES METHOD=WILSON COMP=ETHANOL,WATER,MEAC
1800 CALC NITER=30
1900 DATA PRES(MMHG)=381. TEMP(C)=70.0 X=0.0857,0.9114,,,,,, +
    Y=0.3745,0.5382,,,,,,
2000 DATA PRES(MMHG)=415. TEMP(C)=70.0 X=0.1851,0.8120,,,,,, +
    Y=0.4905,0.4624,,,,,,
2100 DATA PRES(MMHG)=455. TEMP(C)=70.0 X=0.3889,0.6083,,,,,, +
    Y=0.5888,0.3809,,,,,,
2200 DATA PRES(MMHG)=507. TEMP(C)=70.0 X=0.5954,0.4003,,,,,, +
    Y=0.6817,0.2958,,,,,,
2300 DATA PRES(MMHG)=551. TEMP(C)=70.0 X=0.8005,0.1945,,,,,, +
    Y=0.8031,0.1774,,,,,,
2400 DATA PRES(MMHG)=402. TEMP(C)=70.0 X=0.0871,0.9073,,,,,, +
    Y=0.3511,0.5008,,,,,,
2500 DATA PRES(MMHG)=410. TEMP(C)=70.0 X=0.1870,0.8054,,,,,, +
    Y=0.5444,0.4357,,,,,,
2600 DATA PRES(MMHG)=416. TEMP(C)=70.0 X=0.3897,0.6019,,,,,, +
    Y=0.5658,0.3726,,,,,,
2700 DATA PRES(MMHG)=533. TEMP(C)=70.0 X=0.5959,0.3959,,,,,, +
    Y=0.6626,0.2924,,,,,,
2800 DATA PRES(MMHG)=556. TEMP(C)=70.0 X=0.8007,0.1905,,,,,, +
    Y=0.7927,0.1737,,,,,,
2900 DATA PRES(MMHG)=497. TEMP(C)=70.0 X=0.0929,0.8882,,,,,, +
    Y=0.2591,0.3800,,,,,,
3000 DATA PRES(MMHG)=501. TEMP(C)=70.0 X=0.1907,0.7866,,,,,, +
    Y=0.3730,0.3784,,,,,,
3100 DATA PRES(MMHG)=506. TEMP(C)=70.0 X=0.3936,0.5825,,,,,, +
    Y=0.5117,0.3392,,,,,,
3200 DATA PRES(MMHG)=543. TEMP(C)=70.0 X=0.5984,0.3750,,,,,, +
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* XPSIM, Vers. 1.07 *
* Cust/User " " *
* Proj/Problem " " *
* ... extended Process SIMulation ...*
* Job " " *
* Date MAR 05, 2009 *

* Simulation input - Continuation *
*-STMT-*
    Y=0.6181,0.2670,,,,,,,,
3300 DATA PRES(MMHG)=581. TEMP(C)=70.0 X=0.8031,0.1707,,,,,,,, +
    Y=0.7597,0.1496,,,,,,,,
3400 DATA PRES(MMHG)=555. TEMP(C)=70.0 X=0.1942,0.7678,,,,,,,, +
    Y=0.3274,0.3363,,,,,,,,
3500 DATA PRES(MMHG)=536. TEMP(C)=70.0 X=0.3967,0.5617,,,,,,,, +
    Y=0.4637,0.3189,,,,,,,,
3600 DATA PRES(MMHG)=543. TEMP(C)=70.0 X=0.6014,0.3561,,,,,,,, +
    Y=0.5888,0.2484,,,,,,,,
3700 DATA PRES(MMHG)=550. TEMP(C)=70.0 X=0.8044,0.1514,,,,,,,, +
    Y=0.7304,0.1326,,,,,,,,
3800 DATA PRES(MMHG)=778. TEMP(C)=70.0 X=0.1981,0.7179,,,,,,,, +
    Y=0.2333,0.2846,,,,,,,,
3900 DATA PRES(MMHG)=716. TEMP(C)=70.0 X=0.3995,0.5118,,,,,,,, +
    Y=0.3931,0.2709,,,,,,,,
4000 DATA PRES(MMHG)=610. TEMP(C)=70.0 X=0.6057,0.3051,,,,,,,, +
    Y=0.5270,0.2063,,,,,,,,
4100 DATA PRES(MMHG)=1078. TEMP(C)=70.0 X=0.2045,0.5153,,,,,,,, +
    Y=0.1329,0.2114,,,,,,,,
4200 DATA PRES(MMHG)=1001. TEMP(C)=70.0 X=0.4081,0.3082,,,,,,,, +
    Y=0.2604,0.1677,,,,,,,,
4300 DATA PRES(MMHG)=963. TEMP(C)=70.0 X=0.6137,0.1015,,,,,,,, +
    Y=0.3909,0.0737,,,,,,,,
4400 DATA PRES(MMHG)=1152. TEMP(C)=70.0 X=0.2066,0.3085,,,,,,,, +
    Y=0.1275,0.1645,,,,,,,,
4500 DATA PRES(MMHG)=1139. TEMP(C)=70.0 X=0.4105,0.1018,,,,,,,, +
    Y=0.2537,0.0713,,,,,,,,
4600 DATA PRES=760. TEMP=95.5 X=0.0180,,0.0000,,,,,,,, +
    Y=0.1790,,0.0000,,,,,,,,
4700 DATA PRES=760. TEMP=90.6 X=0.0540,,0.0000,,,,,,,, +
    Y=0.3375,,0.0000,,,,,,,,
4800 DATA PRES=760. TEMP=85.4 X=0.1240,,0.0000,,,,,,,, +
    Y=0.4700,,0.0000,,,,,,,,
4900 DATA PRES=760. TEMP=83.7 X=0.1760,,0.0000,,,,,,,, +
    Y=0.5140,,0.0000,,,,,,,,
5000 DATA PRES=760. TEMP=82.75 X=0.2300,,0.0000,,,,,,,, +
    Y=0.5420,,0.0000,,,,,,,,
5100 DATA PRES=760. TEMP=82.0 X=0.2880,,0.0000,,,,,,,, +
    Y=0.5700,,0.0000,,,,,,,,
5200 DATA PRES=760. TEMP=81.0 X=0.3850,,0.0000,,,,,,,, +
    Y=0.6120,,0.0000,,,,,,,,
5300 DATA PRES=760. TEMP=80.50 X=0.4400,,0.0000 Y=0.6330,,0.0000
5400 DATA PRES=760. TEMP=79.80 X=0.5140,,0.0000 Y=0.6570,,0.0000
5500 DATA PRES=760. TEMP=78.90 X=0.6730,,0.0000 Y=0.7375,,0.0000
5600 DATA PRES=760. TEMP=78.26 X=0.8400,,0.0000 Y=0.8500,,0.0000
5700 VARY BINARY=ETHANOL,WATER IDNO=1,2
5800 VARY BINARY=ETHANOL,MEAC IDNO=1,2
5900 VARY BINARY=WATER,MEAC IDNO=1,2
6000 ESTIMATE COMP=ETHANOL PARA=58.68
6100 ESTIMATE COMP=WATER PARA=18.07
6200 ESTIMATE COMP=MEAC PARA=79.84
6300 ESTIMATE BINARY=ETHANOL,WATER PARA=185.776,895.586
6400 ESTIMATE BINARY=ETHANOL,MEAC PARA=1265.686,-460.819
6500 ESTIMATE BINARY=WATER,MEAC PARA=1832.270,753.456
*
*
6600 Flowsheet Data
*
*
*
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extended Process SIMulation ...*
- INPUT -
- Simulation input - Continuation -
-STMT-
6700 STREAM=S1 TEMP=150. PRES=5000.
6800 COMP 0.30 / 0.40
*
6900 FLASH IN S1 OUT S2 UID=F1
*
*
7000 END
--- End of Simulation Input File ---

I) * PROBLEM GENERAL DATA *

- 1) * PROBLEM/PROJECT *
- ETHANOL-WATER-MEAC EQUILIBRIUM REGRESSION TEST
- 2) * UNITS OF MEASURE *
- Input system METRIC - Output system METRIC
- INPUT AND OUTPUT UNITS -
- | | | | |
|--------------|----------|--------------|------------|
| Time | - HR | Weight | - KG |
| Temperature | - CENT | Pressure | - MMHG |
| Energy/Duty | - M-KCAL | Work | - KW |
| Liq volums | - CUMT | Vap Volume | - CUMT |
| Viscosity | - CP | Thermal cond | - KCAL/HMC |
| Surface tens | - DYCM | Std Vap Vol | - N-CUMT |

Standard Vapor Volume is 23.64469 M3/KMOL
Reference Status - Temperature 15°C - Pressure 1 atm

Enthalpy is 0.0 for ideal gas at 298.15 K
Std entropy is for ideal gas at 298.15 K and 1 Atm

I.D) * USER'S SUPPLIED THERMODYNAMIC DATA *

1) * METHOD 'WILSON' *

No. of COMPONENT parameters 1
No. of BINARY parameters 2

* COMPONENT ETHANOL - '

1) 58.6800

INTERACTION/BINARY CONSTANTS WITH COMPONENT WATER - '

1) 185.776 2) 895.586

INTERACTION/BINARY CONSTANTS WITH COMPONENT MEAC - '

1) 1265.69 2) -460.819

* COMPONENT WATER - '

1) 18.0700

INTERACTION/BINARY CONSTANTS WITH COMPONENT MEAC - '

1) 1832.27 2) 753.456

* COMPONENT MEAC - '

1) 79.8400

II) * DEFINED COMPONENTS *

* No of Chemical Components 3
No of Hypothetical/Petroleum Components 0

No	1	2	3
CAS Registry no.	64-17-5	7732-18-5	79-20-9
Name	ETHANOL	WATER	METHYL ACETATE
Component Key	ETHANOL	WATER	MEAC
Type	LIBRARY	LIBRARY	LIBRARY
Class	ALCO	INOR	ESTE
Formula	C2H6O	H2O	C3H6O2
Molecular weight	46.069	18.020	74.080
Boiling point,CENT	78.29	100.00	56.87
Std spec. gravity	0.79265	1.00100	0.93931
Critical temp,CENT	240.77	374.15	233.75
Critical pres,MMHG	46031.189	165913.298	35440.341
Critical vol,CUMT	0.166918	0.056313	0.227940
Critical Z	0.239745	0.231459	0.255557
Acentric factor	0.644000	0.344000	0.323000
Lat. heat, KC/KMOL	9051.402	9724.411	7236.136
H form, KC/KMOL	-56084.062	-57759.487	-99526.658
G form, KC/KMOL	-76123.010	-71204.240	-121573.774
Std entr, KC/KML-C	67.21096	45.09392	73.94639

III) * PVT/THERMO/TRANSPORT PROPERTIES CALCULATION METHODS *

* CALCULATION SET 1 - M1 *

ACTIVITY coefficient

FUGACITY - Vapor

FUGACITY - Liquid

ENTHALPY - Vapor

ENTHALPY - Liquid

WILSON

IDEAL

IDEAL

IDEAL

WILSON

- WILSON

- IDEAL/LIBRARY

- IDEAL/LIBRARY

- IDEAL/LIBRARY

- WILSON

- LIMITS AND OPTIONS -

Temperature - Min -223.15 CENT - Max 1200.05 CENT

Pressure - Min 0.735559E-02 MMHG - Max 0.220668E+07 MMHG

Lowest significant composition 0.10000000E-19

Water K-values are calculated based on

'Vapor Pressure curve'

Water thermo-props are calculated based on

'Saturated conditions'

Water solubility in hydr phases calculated based on

'API solubility in HC mixtures'

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* XPSIM, Vers. 1.07 *
* Cust/User "STAFF" " *
* Proj/Problem "REGRESSION TEST" " *
* ... extended Process Simulation ...*
* Job "VLE-DEMO-1" *
* Date MAR 05, 2009 *

*** VAPOUR LIQUID EQUILIBRIUM DATA REGRESSION - SET NO. 1 ***

1) * SYSTEM COMPONENTS *
1) ETHANOL ETHANOL
2) WATER WATER
3) MEAC METHYL ACETATE

2) * CALCULATION OPTIONS *

Regression analysis is applied to
- PRESSURE
- TEMPERATURE
- LIQUID COMPOSITION
- VAPOUR COMPOSITION

The ABSOLUTE error function is minimized

Maximum changes per trial
- Temperature (ABSOLUTE) 2.0000 CENT
- Liquid composition (RELATIVE) 0.100000
- Parameter (RELATIVE) 0.10000

Relative perturbations for derivatives calculations
Parameters 0.010000
Liq fractions 0.005000
Temperature 0.001000

Maximum no of iterations 30
NON improvements 3
Calculation trace option PARTIAL

On bubble point calculation failure the point is RETAINED

3) * EQUILIBRIUM DATA & RELATED DEVIATIONS *

Next STD deviations apply to following data
- Temperature 0.1000 CENT - Pressure 7.3556 MMHG
- Liquid fraction 0.00100 ABSOLUTE - Vapor fraction 0.00100 ABSOLUTE

Point 1 - Temperature 70.0 C - Pressure 381. MMHG
Liquid Fraction Vapor Fraction
1) ETHANOL 0.085700 0.374500
2) WATER 0.911400 0.538200
3) MEAC 0.002900 0.087300

Point 2 - Temperature 70.0 C - Pressure 415. MMHG
Liquid Fraction Vapor Fraction
1) ETHANOL 0.185100 0.490500
2) WATER 0.812000 0.462400
3) MEAC 0.002900 0.047100

Point 3 - Temperature 70.0 C - Pressure 455. MMHG
Liquid Fraction Vapor Fraction
1) ETHANOL 0.388900 0.588800
2) WATER 0.608300 0.380900
3) MEAC 0.002800 0.030300

Point 4 - Temperature 70.0 C - Pressure 507. MMHG
Liquid Fraction Vapor Fraction
1) ETHANOL 0.595400 0.681700
2) WATER 0.400300 0.295800
3) MEAC 0.004300 0.022500

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(VLE DATA REGRESSION ANALYSIS - continuation)

Point	5	- Temperature	70.0 C	- Pressure	551. MMHG
		Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.800500		0.803100	
2)	WATER	0.194500		0.177400	
3)	MEAC	0.005000		0.019500	
Point	6	- Temperature	70.0 C	- Pressure	402. MMHG
		Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.087100		0.351100	
2)	WATER	0.907300		0.500800	
3)	MEAC	0.005600		0.148100	
Point	7	- Temperature	70.0 C	- Pressure	410. MMHG
		Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.187000		0.544400	
2)	WATER	0.805400		0.435700	
3)	MEAC	0.007600		0.019900	
Point	8	- Temperature	70.0 C	- Pressure	416. MMHG
		Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.389700		0.565800	
2)	WATER	0.601900		0.372600	
3)	MEAC	0.008400		0.061600	
Point	9	- Temperature	70.0 C	- Pressure	533. MMHG
		Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.595900		0.662600	
2)	WATER	0.395900		0.292400	
3)	MEAC	0.008200		0.045000	
Point	10	- Temperature	70.0 C	- Pressure	556. MMHG
		Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.800700		0.792700	
2)	WATER	0.190500		0.173700	
3)	MEAC	0.008800		0.033600	
Point	11	- Temperature	70.0 C	- Pressure	497. MMHG
		Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.092900		0.259100	
2)	WATER	0.888200		0.380000	
3)	MEAC	0.018900		0.360900	
Point	12	- Temperature	70.0 C	- Pressure	501. MMHG
		Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.190700		0.373000	
2)	WATER	0.786600		0.378400	
3)	MEAC	0.022700		0.248600	
Point	13	- Temperature	70.0 C	- Pressure	506. MMHG
		Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.393600		0.511700	
2)	WATER	0.582500		0.339200	
3)	MEAC	0.023900		0.149100	
Point	14	- Temperature	70.0 C	- Pressure	543. MMHG
		Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.598400		0.618100	
2)	WATER	0.375000		0.267000	
3)	MEAC	0.026600		0.114900	

(VLE DATA REGRESSION ANALYSIS - continuation)

Point 15	- Temperature	70.0 C	- Pressure	581. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.803100		0.759700
2)	WATER	0.170700		0.149600
3)	MEAC	0.026200		0.090700
Point 16	- Temperature	70.0 C	- Pressure	555. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.194200		0.327400
2)	WATER	0.767800		0.336300
3)	MEAC	0.038000		0.336300
Point 17	- Temperature	70.0 C	- Pressure	536. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.396700		0.463700
2)	WATER	0.561700		0.318900
3)	MEAC	0.041600		0.217400
Point 18	- Temperature	70.0 C	- Pressure	543. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.601400		0.588800
2)	WATER	0.356100		0.248400
3)	MEAC	0.042500		0.162800
Point 19	- Temperature	70.0 C	- Pressure	550. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.804400		0.730400
2)	WATER	0.151400		0.132600
3)	MEAC	0.044200		0.137000
Point 20	- Temperature	70.0 C	- Pressure	778. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.198100		0.233300
2)	WATER	0.717900		0.284600
3)	MEAC	0.084000		0.482100
Point 21	- Temperature	70.0 C	- Pressure	716. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.399500		0.393100
2)	WATER	0.511800		0.270900
3)	MEAC	0.088700		0.336000
Point 22	- Temperature	70.0 C	- Pressure	610. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.605700		0.527000
2)	WATER	0.305100		0.206300
3)	MEAC	0.089200		0.266700
Point 23	- Temperature	70.0 C	- Pressure	1078. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.204500		0.132900
2)	WATER	0.515300		0.211400
3)	MEAC	0.280200		0.655700
Point 24	- Temperature	70.0 C	- Pressure	1001. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.408100		0.260400
2)	WATER	0.308200		0.167700
3)	MEAC	0.283700		0.571900

(VLE DATA REGRESSION ANALYSIS - continuation)

Point 25	- Temperature	70.0 C	- Pressure	963. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.613700		0.390900
2)	WATER	0.101500		0.073700
3)	MEAC	0.284800		0.535400
Point 26	- Temperature	70.0 C	- Pressure	1152. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.206600		0.127500
2)	WATER	0.308500		0.164500
3)	MEAC	0.484900		0.708000
Point 27	- Temperature	70.0 C	- Pressure	1139. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.410500		0.253700
2)	WATER	0.101800		0.071300
3)	MEAC	0.487700		0.675000
Point 28	- Temperature	95.5 C	- Pressure	760. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.018000		0.179000
2)	WATER	0.982000		0.821000
3)	MEAC	0.000000		0.000000
Point 29	- Temperature	90.6 C	- Pressure	760. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.054000		0.337500
2)	WATER	0.946000		0.662500
3)	MEAC	0.000000		0.000000
Point 30	- Temperature	85.4 C	- Pressure	760. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.124000		0.470000
2)	WATER	0.876000		0.530000
3)	MEAC	0.000000		0.000000
Point 31	- Temperature	83.7 C	- Pressure	760. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.176000		0.514000
2)	WATER	0.824000		0.486000
3)	MEAC	0.000000		0.000000
Point 32	- Temperature	82.75 C	- Pressure	760. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.230000		0.542000
2)	WATER	0.770000		0.458000
3)	MEAC	0.000000		0.000000
Point 33	- Temperature	82.0 C	- Pressure	760. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.288000		0.570000
2)	WATER	0.712000		0.430000
3)	MEAC	0.000000		0.000000
Point 34	- Temperature	81.0 C	- Pressure	760. MMHG
	Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.385000		0.612000
2)	WATER	0.615000		0.388000
3)	MEAC	0.000000		0.000000

(VLE DATA REGRESSION ANALYSIS - continuation)

Point	35	- Temperature	80.50 C	- Pressure	760. MMHG
		Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.440000		0.633000	
2)	WATER	0.560000		0.367000	
3)	MEAC	0.000000		0.000000	
Point	36	- Temperature	79.80 C	- Pressure	760. MMHG
		Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.514000		0.657000	
2)	WATER	0.486000		0.343000	
3)	MEAC	0.000000		0.000000	
Point	37	- Temperature	78.90 C	- Pressure	760. MMHG
		Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.673000		0.737500	
2)	WATER	0.327000		0.262500	
3)	MEAC	0.000000		0.000000	
Point	38	- Temperature	78.26 C	- Pressure	760. MMHG
		Liquid Fraction		Vapor Fraction	
1)	ETHANOL	0.840000		0.850000	
2)	WATER	0.160000		0.150000	
3)	MEAC	0.000000		0.000000	

(VLE DATA REGRESSION ANALYSIS - continuation)

4) * METHOD INFORMATION & INITIAL ESTIMATES *

Regression analysis applied to
component/interaction parameters fo method WILSON

No of COMPONENT parameters 1
INTERACTION parameters 2

Optimized parameters are NOT RETAINED for subsequent calculations

- USER'S INITIAL ESTIMATES

Parameter estimates for component 1 - ETHANOL
1) 58.6800

Parameter estimates for component 2 - WATER
1) 18.0700

Parameter estimates for component 3 - MEAC
1) 79.8400

Interaction estimates for binary 1 ETHANOL - 2 WATER
1) 185.77600 2) 895.58600

Interaction estimates for binary 1 ETHANOL - 3 MEAC
1) 1265.6860 2) -460.81900

Interaction estimates for binary 2 WATER - 3 MEAC
1) 1832.2700 2) 753.45600

5) * PARAMETERS CHANGE SPECS *

Component/interaction parameters are VARIED as follow:

- 1 - Binary couple 1) ETHANOL - 2) WATER
Sequence Nos: 1 / 2 /
- 2 - Binary couple 1) ETHANOL - 3) MEAC
Sequence Nos: 1 / 2 /
- 3 - Binary couple 2) WATER - 3) MEAC
Sequence Nos: 1 / 2 /

*** STREAM 'S1' ***

- Temperature 150.000 CENT - Pressure 5000.0000 MMHG

		GLOBAL STREAM				-----	
* No *	Component	* - Mols	- Mol fr-	- Weight	- Wt fr-		
1	ETHANOL	0.300	0.428571	13.821	0.657230		
2	WATER	0.400	0.571429	7.208	0.342770		
* TOTAL *		0.700	1.000000	21.029	1.000000		
		KMOL		KG			

*** UNIT 1 - 'F1' - ' FLASH

--- Feed Streams ---

'S1'

- Product Streams -

'S2'

1) * CALCULATION TYPE *

Adiabatic flash

Temperature is variable

Pressure is fixed at lowest feed pressure

V) **** STREAM / UNITS DICTIONARY ****

1) STREAMS-UNITS CROSS-REFERENCE TABLE

No	Stream Id	Description/Service	Product of Unit	Feed of Unit(s)
1	S1			1 F1
2	S2		1 F1	

2) UNITS-STREAMS CROSS-REFERENCE TABLE

No	Unit	Unit Description	Feed Streams	Product Streams
1	F1		1 S1	2 S2

```
* XPSIM, Vers. 1.07 *
* Cust/User "STAFF" " *
* Proj/Problem "REGRESSION TEST" " *
* Date MAR 05, 2009 *

*... extended Process SIMulation ...*
* Job "VLE-DEMO-1" *

VI) **** RUN STATISTICS ****

* No of streams 2
  process operations 1
  topping structures 0
  control operations 0
  set operations 0

The calculation is NOT a RECYCLE PROBLEM
Calculation sequence defined by input sequence
```


* XPSIM, Vers. 1.07 * * Page 0017 *
* Cust/User "STAFF" " * extended Process SIMulation ...*
* Proj/Problem "REGRESSION TEST" " * - CALCULATION - * Job "VLE-DEMO-1" *
* Date MAR 05, 2009 *

*** REGRESSION ANALYSIS TRACE FOLLOWS ***

*** VLE DATA REGRESSION ANALYSIS - SET NO 1 ***

* At iter 0 - Weighted error sum 47075.6
X err sum 0.00000 Y err sum 45729.5
T err sum 0.00000 P err sum 1346.03

Point 1
* Temperature - Calc 70.000 CENT - Exp 70.000 CENT - dT 0.000 CENT
* Pressure - Calc 389.368 MMHG - Exp 380.999 MMHG
- dP 8.369 MMHG - dP/P 0.02197

Component	Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL	0.085700	0.085700	0.000000	0.0000	0.355241	0.374500	-.019259	-0.0514
2) WATER	0.911400	0.911400	0.000000	0.0000	0.559159	0.538200	0.020959	0.0389
3) METHYL ACETATE	0.002900	0.002900	0.000000	0.0000	0.085600	0.087300	-.001700	-0.0195

Point 2
* Temperature - Calc 70.000 CENT - Exp 70.000 CENT - dT 0.000 CENT
* Pressure - Calc 435.966 MMHG - Exp 414.999 MMHG
- dP 20.967 MMHG - dP/P 0.05052

Component	Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL	0.185100	0.185100	0.000000	0.0000	0.485371	0.490500	-.005129	-0.0105
2) WATER	0.812000	0.812000	0.000000	0.0000	0.470077	0.462400	0.007677	0.0166
3) METHYL ACETATE	0.002900	0.002900	0.000000	0.0000	0.044551	0.047100	-.002549	-0.0541

Point 3
* Temperature - Calc 70.000 CENT - Exp 70.000 CENT - dT 0.000 CENT
* Pressure - Calc 485.575 MMHG - Exp 454.999 MMHG
- dP 30.576 MMHG - dP/P 0.06720

Component	Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL	0.388900	0.388900	0.000000	0.0000	0.606560	0.588800	0.017760	0.0302
2) WATER	0.608300	0.608300	0.000000	0.0000	0.372240	0.380900	-.008660	-0.0227
3) METHYL ACETATE	0.002800	0.002800	0.000000	0.0000	0.021200	0.030300	-.009100	-0.3003

Point 4
* Temperature - Calc 70.000 CENT - Exp 70.000 CENT - dT 0.000 CENT
* Pressure - Calc 522.112 MMHG - Exp 506.999 MMHG
- dP 15.114 MMHG - dP/P 0.02981

Component	Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL	0.595400	0.595400	0.000000	0.0000	0.698984	0.681700	0.017284	0.0254
2) WATER	0.400300	0.400300	0.000000	0.0000	0.279642	0.295800	-.016158	-0.0546
3) METHYL ACETATE	0.004300	0.004300	0.000000	0.0000	0.021374	0.022500	-.001126	-0.0501

Point 5
* Temperature - Calc 70.000 CENT - Exp 70.000 CENT - dT 0.000 CENT
* Pressure - Calc 544.797 MMHG - Exp 550.999 MMHG
- dP -6.202 MMHG - dP/P -0.01126

Component	Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL	0.800500	0.800500	0.000000	0.0000	0.817584	0.803100	0.014484	0.0180
2) WATER	0.194500	0.194500	0.000000	0.0000	0.163401	0.177400	-.013999	-0.0789
3) METHYL ACETATE	0.005000	0.005000	0.000000	0.0000	0.019015	0.019500	-.000485	-0.0249

Point 6									
* Temperature - Calc		70.000	CENT	- Exp	70.000	CENT	- dT	0.000	CENT
* Pressure - Calc		416.618	MMHG	- Exp	401.999	MMHG			
- dP		14.620	MMHG	- dP/P	0.03637				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.087100	0.087100	0.000000	0.0000	0.329388	0.351100	-.021712	-0.0618
2) WATER		0.907300	0.907300	0.000000	0.0000	0.521530	0.500800	0.020730	0.0414
3) METHYL ACETATE		0.005600	0.005600	0.000000	0.0000	0.149082	0.148100	0.000982	0.0066
Point 7									
* Temperature - Calc		70.000	CENT	- Exp	70.000	CENT	- dT	0.000	CENT
* Pressure - Calc		462.473	MMHG	- Exp	409.999	MMHG			
- dP		52.474	MMHG	- dP/P	0.12799				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.187000	0.187000	0.000000	0.0000	0.451599	0.544400	-.092801	-0.1705
2) WATER		0.805400	0.805400	0.000000	0.0000	0.442011	0.435700	0.006311	0.0145
3) METHYL ACETATE		0.007600	0.007600	0.000000	0.0000	0.106390	0.019900	0.086490	4.3462
Point 8									
* Temperature - Calc		70.000	CENT	- Exp	70.000	CENT	- dT	0.000	CENT
* Pressure - Calc		502.353	MMHG	- Exp	415.999	MMHG			
- dP		86.354	MMHG	- dP/P	0.20758				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.389700	0.389700	0.000000	0.0000	0.580952	0.565800	0.015152	0.0268
2) WATER		0.601900	0.601900	0.000000	0.0000	0.358679	0.372600	-.013921	-0.0374
3) METHYL ACETATE		0.008400	0.008400	0.000000	0.0000	0.060370	0.061600	-.001230	-0.0200
Point 9									
* Temperature - Calc		70.000	CENT	- Exp	70.000	CENT	- dT	0.000	CENT
* Pressure - Calc		530.203	MMHG	- Exp	532.999	MMHG			
- dP		-2.796	MMHG	- dP/P	-0.00525				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.595900	0.595900	0.000000	0.0000	0.686171	0.662600	0.023571	0.0356
2) WATER		0.395900	0.395900	0.000000	0.0000	0.274016	0.292400	-.018384	-0.0629
3) METHYL ACETATE		0.008200	0.008200	0.000000	0.0000	0.039814	0.045000	-.005186	-0.1153
Point 10									
* Temperature - Calc		70.000	CENT	- Exp	70.000	CENT	- dT	0.000	CENT
* Pressure - Calc		550.755	MMHG	- Exp	555.999	MMHG			
- dP		-5.244	MMHG	- dP/P	-0.00943				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.800700	0.800700	0.000000	0.0000	0.807719	0.792700	0.015019	0.0189
2) WATER		0.190500	0.190500	0.000000	0.0000	0.159351	0.173700	-.014349	-0.0826
3) METHYL ACETATE		0.008800	0.008800	0.000000	0.0000	0.032931	0.033600	-.000669	-0.0199
Point 11									
* Temperature - Calc		70.000	CENT	- Exp	70.000	CENT	- dT	0.000	CENT
* Pressure - Calc		527.032	MMHG	- Exp	496.999	MMHG			
- dP		30.034	MMHG	- dP/P	0.06043				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.092900	0.092900	0.000000	0.0000	0.250457	0.259100	-.008643	-0.0334
2) WATER		0.888200	0.888200	0.000000	0.0000	0.408694	0.380000	0.028694	0.0755
3) METHYL ACETATE		0.018900	0.018900	0.000000	0.0000	0.340850	0.360900	-.020050	-0.0556

Point 12									
* Temperature - Calc		70.000	CENT	- Exp	70.000	CENT	- dT	0.000	CENT
* Pressure - Calc		536.741	MMHG	- Exp	500.999	MMHG			
- dP		35.742	MMHG	- dP/P	0.07134				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.190700	0.190700	0.000000	0.0000	0.372423	0.373000	- .000577	-0.0015
2) WATER		0.586600	0.786600	0.000000	0.0000	0.378317	0.378400	- .000083	-0.0002
3) METHYL ACETATE		0.022700	0.022700	0.000000	0.0000	0.249261	0.248600	0.000661	0.0027
Point 13									
* Temperature - Calc		70.000	CENT	- Exp	70.000	CENT	- dT	0.000	CENT
* Pressure - Calc		545.823	MMHG	- Exp	505.999	MMHG			
- dP		39.825	MMHG	- dP/P	0.07870				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.393600	0.393600	0.000000	0.0000	0.523188	0.511700	0.011488	0.0225
2) WATER		0.582500	0.582500	0.000000	0.0000	0.326742	0.339200	- .012458	-0.0367
3) METHYL ACETATE		0.023900	0.023900	0.000000	0.0000	0.150069	0.149100	0.000969	0.0065
Point 14									
* Temperature - Calc		70.000	CENT	- Exp	70.000	CENT	- dT	0.000	CENT
* Pressure - Calc		566.582	MMHG	- Exp	542.999	MMHG			
- dP		23.583	MMHG	- dP/P	0.04343				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.598400	0.598400	0.000000	0.0000	0.633456	0.618100	0.015356	0.0248
2) WATER		0.375000	0.375000	0.000000	0.0000	0.250131	0.267000	- .016869	-0.0632
3) METHYL ACETATE		0.026600	0.026600	0.000000	0.0000	0.116413	0.114900	0.001513	0.0132
Point 15									
* Temperature - Calc		70.000	CENT	- Exp	70.000	CENT	- dT	0.000	CENT
* Pressure - Calc		577.123	MMHG	- Exp	580.998	MMHG			
- dP		-3.875	MMHG	- dP/P	-0.00667				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.803100	0.803100	0.000000	0.0000	0.768019	0.759700	0.008319	0.0110
2) WATER		0.170700	0.170700	0.000000	0.0000	0.140725	0.149600	- .008875	-0.0593
3) METHYL ACETATE		0.026200	0.026200	0.000000	0.0000	0.091256	0.090700	0.000556	0.0061
Point 16									
* Temperature - Calc		70.000	CENT	- Exp	70.000	CENT	- dT	0.000	CENT
* Pressure - Calc		599.243	MMHG	- Exp	554.999	MMHG			
- dP		44.245	MMHG	- dP/P	0.07972				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.194200	0.194200	0.000000	0.0000	0.320787	0.327400	- .006613	-0.0202
2) WATER		0.767800	0.767800	0.000000	0.0000	0.336660	0.336300	0.000360	0.0011
3) METHYL ACETATE		0.038000	0.038000	0.000000	0.0000	0.342553	0.336300	0.006253	0.0186
Point 17									
* Temperature - Calc		70.000	CENT	- Exp	70.000	CENT	- dT	0.000	CENT
* Pressure - Calc		590.275	MMHG	- Exp	535.999	MMHG			
- dP		54.276	MMHG	- dP/P	0.10126				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.396700	0.396700	0.000000	0.0000	0.472393	0.463700	0.008693	0.0187
2) WATER		0.561700	0.561700	0.000000	0.0000	0.298753	0.318900	- .020147	-0.0632
3) METHYL ACETATE		0.041600	0.041600	0.000000	0.0000	0.228854	0.217400	0.011454	0.0527

Point 18									
* Temperature - Calc		70.000	CENT	-	Exp	70.000	CENT	-	dT 0.000 CENT
* Pressure - Calc		595.827	MMHG	-	Exp	542.999	MMHG		
- dP		52.828	MMHG	-	dP/P	0.09729			
--- Liquid fraction ---									
Component		Calc	Exp	dx	dx/X	Calc	Exp	fraction dY	dY/Y
1) ETHANOL		0.601400	0.601400	0.000000	0.0000	0.596694	0.588800	0.007894	0.0134
2) WATER		0.356100	0.356100	0.000000	0.0000	0.232035	0.248400	-0.016365	-0.0659
3) METHYL ACETATE		0.042500	0.042500	0.000000	0.0000	0.171271	0.162800	0.008471	0.0520
Point 19									
* Temperature - Calc		70.000	CENT	-	Exp	70.000	CENT	-	dT 0.000 CENT
* Pressure - Calc		602.732	MMHG	-	Exp	549.999	MMHG		
- dP		52.734	MMHG	-	dP/P	0.09588			
--- Liquid fraction ---									
Component		Calc	Exp	dx	dx/X	Calc	Exp	fraction dY	dY/Y
1) ETHANOL		0.804400	0.804400	0.000000	0.0000	0.732591	0.730400	0.002191	0.0030
2) WATER		0.151400	0.151400	0.000000	0.0000	0.123488	0.132600	-0.009112	-0.0687
3) METHYL ACETATE		0.044200	0.044200	0.000000	0.0000	0.143921	0.137000	0.006921	0.0505
Point 20									
* Temperature - Calc		70.000	CENT	-	Exp	70.000	CENT	-	dT 0.000 CENT
* Pressure - Calc		738.511	MMHG	-	Exp	777.998	MMHG		
- dP		-39.487	MMHG	-	dP/P	-0.05075			
--- Liquid fraction ---									
Component		Calc	Exp	dx	dx/X	Calc	Exp	fraction dY	dY/Y
1) ETHANOL		0.198100	0.198100	0.000000	0.0000	0.233115	0.233300	-0.000185	-0.0008
2) WATER		0.717900	0.717900	0.000000	0.0000	0.268978	0.284600	-0.015622	-0.0549
3) METHYL ACETATE		0.084000	0.084000	0.000000	0.0000	0.497907	0.482100	0.015807	0.0328
Point 21									
* Temperature - Calc		70.000	CENT	-	Exp	70.000	CENT	-	dT 0.000 CENT
* Pressure - Calc		688.866	MMHG	-	Exp	715.998	MMHG		
- dP		-27.133	MMHG	-	dP/P	-0.03789			
--- Liquid fraction ---									
Component		Calc	Exp	dx	dx/X	Calc	Exp	fraction dY	dY/Y
1) ETHANOL		0.399500	0.399500	0.000000	0.0000	0.381299	0.393100	-0.011801	-0.0300
2) WATER		0.511800	0.511800	0.000000	0.0000	0.248844	0.270900	-0.022056	-0.0814
3) METHYL ACETATE		0.088700	0.088700	0.000000	0.0000	0.369857	0.336000	0.033857	0.1008
Point 22									
* Temperature - Calc		70.000	CENT	-	Exp	70.000	CENT	-	dT 0.000 CENT
* Pressure - Calc		671.467	MMHG	-	Exp	609.998	MMHG		
- dP		61.469	MMHG	-	dP/P	0.10077			
--- Liquid fraction ---									
Component		Calc	Exp	dx	dx/X	Calc	Exp	fraction dY	dY/Y
1) ETHANOL		0.605700	0.605700	0.000000	0.0000	0.515866	0.527000	-0.011134	-0.0211
2) WATER		0.305100	0.305100	0.000000	0.0000	0.190647	0.206300	-0.015653	-0.0759
3) METHYL ACETATE		0.089200	0.089200	0.000000	0.0000	0.293488	0.266700	0.026788	0.1004
Point 23									
* Temperature - Calc		70.000	CENT	-	Exp	70.000	CENT	-	dT 0.000 CENT
* Pressure - Calc		995.964	MMHG	-	Exp	1077.997	MMHG		
- dP		-82.033	MMHG	-	dP/P	-0.07610			
--- Liquid fraction ---									
Component		Calc	Exp	dx	dx/X	Calc	Exp	fraction dY	dY/Y
1) ETHANOL		0.204500	0.204500	0.000000	0.0000	0.134403	0.132900	0.001503	0.0113
2) WATER		0.515300	0.515300	0.000000	0.0000	0.186007	0.211400	-0.025393	-0.1201
3) METHYL ACETATE		0.280200	0.280200	0.000000	0.0000	0.679590	0.655700	0.023890	0.0364

Point 24									
* Temperature - Calc		70.000	CENT	-	Exp	70.000	CENT	-	dT 0.000 CENT
* Pressure - Calc		928.641	MMHG	-	Exp	1000.997	MMHG		
- dP		-72.357	MMHG	-	dP/P	-0.07228			
--- Liquid fraction ---									
Component		Calc	Exp	dx	dx/X	Calc	Exp	fraction dY	dY/Y
1) ETHANOL		0.408100	0.408100	0.000000	0.0000	0.249486	0.260400	- .010914	-0.0419
2) WATER		0.308200	0.308200	0.000000	0.0000	0.152623	0.167700	- .015077	-0.0899
3) METHYL ACETATE		0.283700	0.283700	0.000000	0.0000	0.597891	0.571900	0.025991	0.0454
Point 25									
* Temperature - Calc		70.000	CENT	-	Exp	70.000	CENT	-	dT 0.000 CENT
* Pressure - Calc		880.714	MMHG	-	Exp	962.997	MMHG		
- dP		-82.284	MMHG	-	dP/P	-0.08545			
--- Liquid fraction ---									
Component		Calc	Exp	dx	dx/X	Calc	Exp	fraction dY	dY/Y
1) ETHANOL		0.613700	0.613700	0.000000	0.0000	0.381835	0.390900	- .009065	-0.0232
2) WATER		0.101500	0.101500	0.000000	0.0000	0.070366	0.073700	- .003334	-0.0452
3) METHYL ACETATE		0.284800	0.284800	0.000000	0.0000	0.547799	0.535400	0.012399	0.0232
Point 26									
* Temperature - Calc		70.000	CENT	-	Exp	70.000	CENT	-	dT 0.000 CENT
* Pressure - Calc		1100.098	MMHG	-	Exp	1151.997	MMHG		
- dP		-51.899	MMHG	-	dP/P	-0.04505			
--- Liquid fraction ---									
Component		Calc	Exp	dx	dx/X	Calc	Exp	fraction dY	dY/Y
1) ETHANOL		0.206600	0.206600	0.000000	0.0000	0.116069	0.127500	- .011431	-0.0897
2) WATER		0.308500	0.308500	0.000000	0.0000	0.145498	0.164500	- .001902	-0.1155
3) METHYL ACETATE		0.484900	0.484900	0.000000	0.0000	0.738433	0.708000	0.030433	0.0430
Point 27									
* Temperature - Calc		70.000	CENT	-	Exp	70.000	CENT	-	dT 0.000 CENT
* Pressure - Calc		1051.085	MMHG	-	Exp	1138.997	MMHG		
- dP		-87.912	MMHG	-	dP/P	-0.07718			
--- Liquid fraction ---									
Component		Calc	Exp	dx	dx/X	Calc	Exp	fraction dY	dY/Y
1) ETHANOL		0.410500	0.410500	0.000000	0.0000	0.226060	0.253700	- .027640	-0.1089
2) WATER		0.101800	0.101800	0.000000	0.0000	0.069368	0.071300	- .001932	-0.0271
3) METHYL ACETATE		0.487700	0.487700	0.000000	0.0000	0.704572	0.675000	0.029572	0.0438
Point 28									
* Temperature - Calc		95.500	CENT	-	Exp	95.500	CENT	-	dT 0.000 CENT
* Pressure - Calc		736.346	MMHG	-	Exp	759.998	MMHG		
- dP		-23.652	MMHG	-	dP/P	-0.03112			
--- Liquid fraction ---									
Component		Calc	Exp	dx	dx/X	Calc	Exp	fraction dY	dY/Y
1) ETHANOL		0.018000	0.018000	0.000000	0.0000	0.137936	0.179000	- .041064	-0.2294
2) WATER		0.982000	0.982000	0.000000	0.0000	0.862064	0.821000	0.041064	0.0500
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000
Point 29									
* Temperature - Calc		90.600	CENT	-	Exp	90.600	CENT	-	dT 0.000 CENT
* Pressure - Calc		727.825	MMHG	-	Exp	759.998	MMHG		
- dP		-32.173	MMHG	-	dP/P	-0.04233			
--- Liquid fraction ---									
Component		Calc	Exp	dx	dx/X	Calc	Exp	fraction dY	dY/Y
1) ETHANOL		0.054000	0.054000	0.000000	0.0000	0.294999	0.337500	- .042501	-0.1259
2) WATER		0.946000	0.946000	0.000000	0.0000	0.705001	0.662500	0.042501	0.0642
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000

Point 30									
* Temperature - Calc		85.400	CENT	-	Exp	85.400	CENT	-	dT 0.000 CENT
* Pressure - Calc		708.660	MMHG	-	Exp	759.998	MMHG		
- dP		-51.338	MMHG	-	dP/P	-0.06755			
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.124000	0.124000	0.000000	0.0000	0.435262	0.470000	-0.034738	-0.0739
2) WATER		0.876000	0.876000	0.000000	0.0000	0.564738	0.530000	0.034738	0.0655
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000
Point 31									
* Temperature - Calc		83.700	CENT	-	Exp	83.700	CENT	-	dT 0.000 CENT
* Pressure - Calc		711.409	MMHG	-	Exp	759.998	MMHG		
- dP		-48.589	MMHG	-	dP/P	-0.06393			
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.176000	0.176000	0.000000	0.0000	0.490153	0.514000	-0.023847	-0.0464
2) WATER		0.824000	0.824000	0.000000	0.0000	0.509847	0.486000	0.023847	0.0491
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000
Point 32									
* Temperature - Calc		82.750	CENT	-	Exp	82.750	CENT	-	dT 0.000 CENT
* Pressure - Calc		720.640	MMHG	-	Exp	759.998	MMHG		
- dP		-39.358	MMHG	-	dP/P	-0.05179			
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.230000	0.230000	0.000000	0.0000	0.530370	0.542000	-0.011630	-0.0215
2) WATER		0.770000	0.770000	0.000000	0.0000	0.469630	0.458000	0.011630	0.0254
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000
Point 33									
* Temperature - Calc		82.000	CENT	-	Exp	82.000	CENT	-	dT 0.000 CENT
* Pressure - Calc		728.543	MMHG	-	Exp	759.998	MMHG		
- dP		-31.455	MMHG	-	dP/P	-0.04139			
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.288000	0.288000	0.000000	0.0000	0.564577	0.570000	-0.005423	-0.0095
2) WATER		0.712000	0.712000	0.000000	0.0000	0.435423	0.430000	0.005423	0.0126
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000
Point 34									
* Temperature - Calc		81.000	CENT	-	Exp	81.000	CENT	-	dT 0.000 CENT
* Pressure - Calc		737.183	MMHG	-	Exp	759.998	MMHG		
- dP		-22.815	MMHG	-	dP/P	-0.03002			
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.385000	0.385000	0.000000	0.0000	0.612852	0.612000	0.000852	0.0014
2) WATER		0.615000	0.615000	0.000000	0.0000	0.387148	0.388000	-0.000852	-0.0022
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000
Point 35									
* Temperature - Calc		80.500	CENT	-	Exp	80.500	CENT	-	dT 0.000 CENT
* Pressure - Calc		740.077	MMHG	-	Exp	759.998	MMHG		
- dP		-19.921	MMHG	-	dP/P	-0.02621			
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.440000	0.440000	0.000000	0.0000	0.638436	0.633000	0.005436	0.0086
2) WATER		0.560000	0.560000	0.000000	0.0000	0.361564	0.367000	-0.005436	-0.0148
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000

Point 36									
* Temperature - Calc		79.800	CENT	- Exp	79.800	CENT	- dT	0.000	CENT
* Pressure - Calc		740.189	MMHG	- Exp	759.998	MMHG			
- dP		-19.809	MMHG	- dP/P	-0.02606				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.514000	0.514000	0.000000	0.0000	0.672963	0.657000	0.015963	0.0243
2) WATER		0.486000	0.486000	0.000000	0.0000	0.327037	0.343000	-0.015963	-0.0465
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000
Point 37									
* Temperature - Calc		78.900	CENT	- Exp	78.900	CENT	- dT	0.000	CENT
* Pressure - Calc		748.672	MMHG	- Exp	759.998	MMHG			
- dP		-11.326	MMHG	- dP/P	-0.01490				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.673000	0.673000	0.000000	0.0000	0.753831	0.737500	0.016331	0.0221
2) WATER		0.327000	0.327000	0.000000	0.0000	0.246169	0.262500	-0.016331	-0.0622
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000
Point 38									
* Temperature - Calc		78.260	CENT	- Exp	78.260	CENT	- dT	0.000	CENT
* Pressure - Calc		753.287	MMHG	- Exp	759.998	MMHG			
- dP		-6.711	MMHG	- dP/P	-0.00883				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.840000	0.840000	0.000000	0.0000	0.860273	0.850000	0.010273	0.0121
2) WATER		0.160000	0.160000	0.000000	0.0000	0.139727	0.150000	-0.010273	-0.0685
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000

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* XPSIM, Vers. 1.07 *                               * Page 0024 *
* Cust/User "STAFF"                               " *
* Proj/Problem "REGRESSION TEST"                   " *
* Date MAR 05, 2009 *

II) * REGRESSION DEVIATIONS & STATISTICS *

No of experimental points 38
variable parameters 6

Estimated fit variance 1471.1

- Maximum deviations -

- Temperature 0.000 CENT at point 38
- Pressure (ABS) -87.9125 MMHG at points 27
- Pressure (REL) 0.2076 at point 8

Comp 1 - ETHANOL
Abs dX 0.000000 at point 38 - Rel dX 0.000 at point 38
Abs dY -.092801 at point 7 - Rel dY -0.229 at point 28

Comp 2 - WATER
Abs dX 0.000000 at point 38 - Rel dX 0.000 at point 38
Abs dY 0.042501 at point 29 - Rel dY -0.120 at point 23

Comp 3 - METHYL ACETATE
Abs dX 0.000000 at point 27 - Rel dX 0.000 at point 27
Abs dY 0.086490 at point 7 - Rel dY 4.346 at point 7

- STANDARD DEVIATIONS -
- Temperature 0.000 CENT
- Pressure 43.7778 MMHG

Comp 1 - ETHANOL
X fractions 0.000000 - Y fractions 0.022633

Comp 2 - WATER
X fractions 0.000000 - Y fractions 0.018245

Comp 3 - METHYL ACETATE
X fractions 0.000000 - Y fractions 0.018928

- AVERAGE DEVIATIONS -
- Temperature 0.000 CENT
- Pressure (ABS) 36.6204 MMHG - Pressure (REL) 0.0566

Comp 1 - ETHANOL
X fractions 0.000000 - Y fractions 0.015886

Comp 2 - WATER
X fractions 0.000000 - Y fractions 0.015269

Comp 3 - METHYL ACETATE
X fractions 0.000000 - Y fractions 0.009608

* At iter 1 - Weighted error sum 29912.4
X err sum 2770.52 Y err sum 24878.9
T err sum 711.861 P err sum 1551.11
Maximum uncorrected changes
Para 1.47898 - X comp 0.79643 - Temp 2.55999
Minimum Adj factors
Para 0.06761 - X comp 0.12556 - Temp 1.00000
Improuv Ratio -0.364588

* At iter 2 - Weighted error sum 24916.8
X err sum 3432.86 Y err sum 18083.3
T err sum 1676.95 P err sum 1723.63
Maximum uncorrected changes
Para 1.26926 - X comp 0.77935 - Temp 1.89066
Minimum Adj factors
Para 0.07879 - X comp 0.12831 - Temp 1.00000
Improuv Ratio -0.167007

* At iter 3 - Weighted error sum 22136.8
X err sum 3202.83 Y err sum 14692.5
T err sum 2377.32 P err sum 1864.11
Maximum uncorrected changes
Para 1.11243 - X comp 0.76475 - Temp 1.34348
Minimum Adj factors
Para 0.08989 - X comp 0.13076 - Temp 1.00000
Improuv Ratio -0.111572

* At iter 4 - Weighted error sum 19955.2
X err sum 2914.21 Y err sum 12193.5
T err sum 2868.18 P err sum 1979.31
Maximum uncorrected changes
Para 0.98860 - X comp 0.75213 - Temp 0.90314
Minimum Adj factors
Para 0.10115 - X comp 0.13296 - Temp 1.00000
Improuv Ratio -0.985499E-01

* At iter 5 - Weighted error sum 18226.0
X err sum 2688.26 Y err sum 10239.7
T err sum 3232.53 P err sum 2065.46
Maximum uncorrected changes
Para 1.02432 - X comp 0.73860 - Temp 0.56777
Minimum Adj factors
Para 0.09763 - X comp 0.13539 - Temp 1.00000
Improuv Ratio -0.866558E-01

* At iter 6 - Weighted error sum 16779.9
X err sum 2516.91 Y err sum 8678.88
T err sum 3460.49 P err sum 2123.61
Maximum uncorrected changes
Para 1.05090 - X comp 0.72331 - Temp 0.29700
Minimum Adj factors
Para 0.09516 - X comp 0.13825 - Temp 1.00000
Improuv Ratio -0.793422E-01

* At iter 7 - Weighted error sum 15447.1
X err sum 2360.37 Y err sum 7367.46
T err sum 3563.16 P err sum 2156.15
Maximum uncorrected changes
Para 1.02041 - X comp 0.70517 - Temp 0.02817
```


*** VAPOR-LIQUID EQUILIBRIUM DATA REGRESSION ANALYSIS ***

I) * FINAL VAPOUR-LIQUID EQUILIBRIUM DATA *

Point 1									
* Temperature - Calc		70.007 CENT	- Exp	70.000 CENT	- dT	0.007 CENT			
* Pressure - Calc		412.242 MMHG	- Exp	380.999 MMHG					
		- dP	31.243 MMHG	- dP/P	0.08200				
		*---	Liquid fraction		----	*---	Vapor	fraction	----
Component		Calc	Exp	dX	dX/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.078404	0.085700	-0.007296	-0.0851	0.377178	0.374500	0.002678	0.0071
2) WATER		0.919642	0.911400	0.008242	0.0090	0.535446	0.538200	-0.002754	-0.0051
3) METHYL ACETATE		0.001954	0.002900	-0.000946	-0.3263	0.087377	0.087300	0.000077	0.0009
Point 2									
* Temperature - Calc		69.838 CENT	- Exp	70.000 CENT	- dT	-0.162 CENT			
* Pressure - Calc		454.163 MMHG	- Exp	414.999 MMHG					
		- dP	39.164 MMHG	- dP/P	0.09437				
		*---	Liquid fraction		----	*---	Vapor	fraction	----
Component		Calc	Exp	dX	dX/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.182176	0.185100	-0.002924	-0.0158	0.493635	0.490500	0.003135	0.0064
2) WATER		0.814986	0.812000	0.002986	0.0037	0.458985	0.462400	-0.003415	-0.0074
3) METHYL ACETATE		0.002838	0.002900	-0.000062	-0.0214	0.047380	0.047100	0.000280	0.0059
Point 3									
* Temperature - Calc		69.524 CENT	- Exp	70.000 CENT	- dT	-0.476 CENT			
* Pressure - Calc		491.843 MMHG	- Exp	454.999 MMHG					
		- dP	36.845 MMHG	- dP/P	0.08098				
		*---	Liquid fraction		----	*---	Vapor	fraction	----
Component		Calc	Exp	dX	dX/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.386344	0.388900	-0.002556	-0.0066	0.592830	0.588800	0.004030	0.0068
2) WATER		0.609409	0.608300	0.001109	0.0018	0.376493	0.380900	-0.004407	-0.0116
3) METHYL ACETATE		0.004247	0.002800	0.001447	0.5168	0.030677	0.030300	0.000377	0.0125
Point 4									
* Temperature - Calc		69.285 CENT	- Exp	70.000 CENT	- dT	-0.715 CENT			
* Pressure - Calc		516.133 MMHG	- Exp	506.999 MMHG					
		- dP	9.135 MMHG	- dP/P	0.01802				
		*---	Liquid fraction		----	*---	Vapor	fraction	----
Component		Calc	Exp	dX	dX/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.592515	0.595400	-0.002885	-0.0048	0.685819	0.681700	0.004119	0.0060
2) WATER		0.402525	0.400300	0.002225	0.0056	0.290942	0.295800	-0.004858	-0.0164
3) METHYL ACETATE		0.004960	0.004300	0.000660	0.1534	0.023239	0.022500	0.000739	0.0328
Point 5									
* Temperature - Calc		69.247 CENT	- Exp	70.000 CENT	- dT	-0.753 CENT			
* Pressure - Calc		533.594 MMHG	- Exp	550.999 MMHG					
		- dP	-17.404 MMHG	- dP/P	-0.03159				
		*---	Liquid fraction		----	*---	Vapor	fraction	----
Component		Calc	Exp	dX	dX/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.796763	0.800500	-0.003737	-0.0047	0.805919	0.803100	0.002819	0.0035
2) WATER		0.197634	0.194500	0.003134	0.0161	0.173860	0.177400	-0.003540	-0.0200
3) METHYL ACETATE		0.005602	0.005000	0.000602	0.1204	0.020221	0.019500	0.000721	0.0370

Point 6									
* Temperature - Calc		69.905	CENT	-	Exp	70.000	CENT	-	dT -0.095
* Pressure - Calc		439.710	MMHG	-	Exp	401.999	MMHG		
- dP		37.711	MMHG	-	dP/P	0.09381			
*---		Liquid fraction			---	*---		Vapor	fraction
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.082110	0.087100	-0.004990	-0.0573	0.353182	0.351100	0.002082	0.0059
2) WATER		0.914043	0.907300	0.006743	0.0074	0.498786	0.500800	-0.002014	-0.0040
3) METHYL ACETATE		0.003847	0.005600	-0.001753	-0.3130	0.148032	0.148100	-0.000068	-0.0005
Point 7									
* Temperature - Calc		69.851	CENT	-	Exp	70.000	CENT	-	dT -0.149
* Pressure - Calc		449.826	MMHG	-	Exp	409.999	MMHG		
- dP		39.827	MMHG	-	dP/P	0.09714			
*---		Liquid fraction			---	*---		Vapor	fraction
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.204181	0.187000	0.017181	0.0919	0.524420	0.544400	-0.019980	-0.0367
2) WATER		0.794744	0.805400	-0.010656	-0.0132	0.459227	0.435700	0.023527	0.0540
3) METHYL ACETATE		0.001075	0.007600	-0.006525	-0.8585	0.016354	0.019900	-0.003546	-0.1782
Point 8									
* Temperature - Calc		69.251	CENT	-	Exp	70.000	CENT	-	dT -0.749
* Pressure - Calc		499.453	MMHG	-	Exp	415.999	MMHG		
- dP		83.454	MMHG	-	dP/P	0.20061			
*---		Liquid fraction			---	*---		Vapor	fraction
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.386513	0.389700	-0.003187	-0.0082	0.571968	0.565800	0.006168	0.0109
2) WATER		0.604517	0.601900	0.002617	0.0043	0.365865	0.372600	-0.006735	-0.0181
3) METHYL ACETATE		0.008970	0.008400	0.000570	0.0679	0.062167	0.061600	0.000567	0.0092
Point 9									
* Temperature - Calc		69.058	CENT	-	Exp	70.000	CENT	-	dT -0.942
* Pressure - Calc		520.704	MMHG	-	Exp	532.999	MMHG		
- dP		-12.294	MMHG	-	dP/P	-0.02307			
*---		Liquid fraction			---	*---		Vapor	fraction
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.590973	0.595900	-0.004927	-0.0083	0.669100	0.662600	0.006500	0.0098
2) WATER		0.398936	0.395900	0.003036	0.0077	0.284792	0.292400	-0.007608	-0.0260
3) METHYL ACETATE		0.010091	0.008200	0.001891	0.2306	0.046108	0.045000	0.001108	0.0246
Point 10									
* Temperature - Calc		69.191	CENT	-	Exp	70.000	CENT	-	dT -0.809
* Pressure - Calc		538.050	MMHG	-	Exp	555.999	MMHG		
- dP		-17.949	MMHG	-	dP/P	-0.03228			
*---		Liquid fraction			---	*---		Vapor	fraction
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.796453	0.800700	-0.004247	-0.0053	0.795859	0.792700	0.003159	0.0040
2) WATER		0.193891	0.190500	0.003391	0.0178	0.169833	0.173700	-0.003867	-0.0223
3) METHYL ACETATE		0.009657	0.008800	0.000857	0.0973	0.034308	0.033600	0.000708	0.0211
Point 11									
* Temperature - Calc		69.580	CENT	-	Exp	70.000	CENT	-	dT -0.420
* Pressure - Calc		564.088	MMHG	-	Exp	496.999	MMHG		
- dP		67.089	MMHG	-	dP/P	0.13499			
*---		Liquid fraction			---	*---		Vapor	fraction
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.093358	0.092900	0.000458	0.0049	0.258692	0.259100	-0.000408	-0.0016
2) WATER		0.889941	0.888200	0.001741	0.0020	0.381176	0.380000	0.001176	0.0031
3) METHYL ACETATE		0.016702	0.018900	-0.002198	-0.1163	0.360132	0.360900	-0.000768	-0.0021

Point 18									
* Temperature - Calc		69.303	CENT	- Exp	70.000	CENT	- dT	-0.697	CENT
* Pressure - Calc		582.619	MMHG	- Exp	542.999	MMHG			
- dP		39.620	MMHG	- dP/P	0.07297				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.599177	0.601400	-0.002223	-0.0037	0.592217	0.588800	0.003417	0.0058
2) WATER		0.357941	0.356100	0.001841	0.0052	0.244670	0.248400	-0.003730	-0.0150
3) METHYL ACETATE		0.042882	0.042500	0.000382	0.0090	0.163112	0.162800	0.000312	0.0019
Point 19									
* Temperature - Calc		69.508	CENT	- Exp	70.000	CENT	- dT	-0.492	CENT
* Pressure - Calc		590.991	MMHG	- Exp	549.999	MMHG			
- dP		40.992	MMHG	- dP/P	0.07453				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.803246	0.804400	-0.001154	-0.0014	0.731414	0.730400	0.001014	0.0014
2) WATER		0.152525	0.151400	0.001125	0.0074	0.131648	0.132600	-0.000952	-0.0072
3) METHYL ACETATE		0.044229	0.044200	0.000029	0.0007	0.136938	0.137000	-0.000062	-0.0005
Point 20									
* Temperature - Calc		70.194	CENT	- Exp	70.000	CENT	- dT	0.194	CENT
* Pressure - Calc		745.785	MMHG	- Exp	777.998	MMHG			
- dP		-32.213	MMHG	- dP/P	-0.04141				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.197241	0.198100	-0.000859	-0.0043	0.236454	0.233300	0.003154	0.0135
2) WATER		0.719447	0.717900	0.001547	0.0022	0.280284	0.284600	-0.004316	-0.0152
3) METHYL ACETATE		0.083312	0.084000	-0.000688	-0.0082	0.483262	0.482100	0.001162	0.0024
Point 21									
* Temperature - Calc		70.130	CENT	- Exp	70.000	CENT	- dT	0.130	CENT
* Pressure - Calc		679.173	MMHG	- Exp	715.998	MMHG			
- dP		-36.825	MMHG	- dP/P	-0.05143				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.401431	0.399500	0.001931	0.0048	0.394074	0.393100	0.000974	0.0025
2) WATER		0.514414	0.511800	0.002614	0.0051	0.267822	0.270900	-0.003078	-0.0114
3) METHYL ACETATE		0.084154	0.088700	-0.004546	-0.0512	0.338104	0.336000	0.002104	0.0063
Point 22									
* Temperature - Calc		69.752	CENT	- Exp	70.000	CENT	- dT	-0.248	CENT
* Pressure - Calc		655.091	MMHG	- Exp	609.998	MMHG			
- dP		45.093	MMHG	- dP/P	0.07392				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.608037	0.605700	0.002337	0.0039	0.527034	0.527000	0.000034	0.0001
2) WATER		0.306656	0.305100	0.001556	0.0051	0.205101	0.206300	-0.001199	-0.0058
3) METHYL ACETATE		0.085307	0.089200	-0.003893	-0.0436	0.267865	0.266700	0.001165	0.0044
Point 23									
* Temperature - Calc		71.109	CENT	- Exp	70.000	CENT	- dT	1.109	CENT
* Pressure - Calc		989.354	MMHG	- Exp	1077.997	MMHG			
- dP		-88.643	MMHG	- dP/P	-0.08223				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.198138	0.204500	-0.006362	-0.0311	0.138650	0.132900	0.005750	0.0433
2) WATER		0.516640	0.515300	0.001340	0.0026	0.209365	0.211400	-0.002035	-0.0096
3) METHYL ACETATE		0.285222	0.280200	0.005022	0.0179	0.651985	0.655700	-0.003715	-0.0057

Point 30									
* Temperature - Calc		85.173	CENT	- Exp	85.400	CENT	- dT	-0.227	CENT
* Pressure - Calc		750.843	MMHG	- Exp	759.998	MMHG			
- dP		-9.155	MMHG	- dP/P	-0.01205				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.129200	0.124000	0.005200	0.0419	0.466213	0.470000	-0.003787	-0.0081
2) WATER		0.870800	0.876000	-0.005200	-0.0059	0.533787	0.530000	0.003787	0.0071
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000
Point 31									
* Temperature - Calc		83.610	CENT	- Exp	83.700	CENT	- dT	-0.090	CENT
* Pressure - Calc		747.531	MMHG	- Exp	759.998	MMHG			
- dP		-12.467	MMHG	- dP/P	-0.01640				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.181389	0.176000	0.005389	0.0306	0.508030	0.514000	-0.005970	-0.0116
2) WATER		0.818611	0.824000	-0.005389	-0.0065	0.491970	0.486000	0.005970	0.0123
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000
Point 32									
* Temperature - Calc		82.780	CENT	- Exp	82.750	CENT	- dT	0.030	CENT
* Pressure - Calc		751.895	MMHG	- Exp	759.998	MMHG			
- dP		-8.103	MMHG	- dP/P	-0.01066				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.232809	0.230000	0.002809	0.0122	0.537851	0.542000	-0.004149	-0.0077
2) WATER		0.767191	0.770000	-0.002809	-0.0036	0.462149	0.458000	0.004149	0.0091
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000
Point 33									
* Temperature - Calc		82.114	CENT	- Exp	82.000	CENT	- dT	0.114	CENT
* Pressure - Calc		757.096	MMHG	- Exp	759.998	MMHG			
- dP		-2.902	MMHG	- dP/P	-0.00382				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.290427	0.288000	0.002427	0.0084	0.565604	0.570000	-0.004396	-0.0077
2) WATER		0.709573	0.712000	-0.002427	-0.0034	0.434396	0.430000	0.004396	0.0102
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000
Point 34									
* Temperature - Calc		81.233	CENT	- Exp	81.000	CENT	- dT	0.233	CENT
* Pressure - Calc		763.871	MMHG	- Exp	759.998	MMHG			
- dP		3.873	MMHG	- dP/P	0.00510				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.387111	0.385000	0.002111	0.0055	0.607525	0.612000	-0.004475	-0.0073
2) WATER		0.612889	0.615000	-0.002111	-0.0034	0.392475	0.388000	0.004475	0.0115
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000
Point 35									
* Temperature - Calc		80.629	CENT	- Exp	80.500	CENT	- dT	0.129	CENT
* Pressure - Calc		761.413	MMHG	- Exp	759.998	MMHG			
- dP		1.415	MMHG	- dP/P	0.00186				
--- Liquid fraction --- *--- Vapor fraction ---*									
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.441047	0.440000	0.001047	0.0024	0.630697	0.633000	-0.002303	-0.0036
2) WATER		0.558953	0.560000	-0.001047	-0.0019	0.369303	0.367000	0.002303	0.0063
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000

Point 36									
* Temperature - Calc		79.215	CENT	- Exp	79.800	CENT	- dT	-0.585	
* Pressure - Calc		737.798	MMHG	- Exp	759.998	MMHG			
- dP		-22.200	MMHG	- dP/P	-0.02921				
		--- Liquid fraction ---							
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.511398	0.514000	-0.002602	-0.0051	0.662156	0.657000	0.005156	0.0078
2) WATER		0.488602	0.486000	0.002602	0.0054	0.337844	0.343000	-0.005156	-0.0150
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000
Point 37									
* Temperature - Calc		78.095	CENT	- Exp	78.900	CENT	- dT	-0.805	
* Pressure - Calc		735.937	MMHG	- Exp	759.998	MMHG			
- dP		-24.061	MMHG	- dP/P	-0.03166				
		--- Liquid fraction ---							
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.669988	0.673000	-0.003012	-0.0045	0.741832	0.737500	0.004332	0.0059
2) WATER		0.330012	0.327000	0.003012	0.0092	0.258168	0.262500	-0.004332	-0.0165
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000
Point 38									
* Temperature - Calc		77.798	CENT	- Exp	78.260	CENT	- dT	-0.462	
* Pressure - Calc		745.925	MMHG	- Exp	759.998	MMHG			
- dP		-14.073	MMHG	- dP/P	-0.01852				
		--- Liquid fraction ---							
Component		Calc	Exp	dx	dx/X	Calc	Exp	dY	dY/Y
1) ETHANOL		0.838097	0.840000	-0.001903	-0.0023	0.851520	0.850000	0.001520	0.0018
2) WATER		0.161903	0.160000	0.001903	0.0119	0.148480	0.150000	-0.001520	-0.0101
3) METHYL ACETATE		0.000000	0.000000	0.000000	0.0000	0.000000	0.000000	0.000000	0.0000

II) * REGRESSION DEVIATIONS & STATISTICS *

No of experimental points 38
variable parameters 6

Estimated fit variance 197.89

- Maximum deviations -

- Temperature 1.109 CENT at point 23
- Pressure (ABS) -136.9688 MMHG at points 27
- Pressure (REL) 0.2006 at point 8

Comp 1 - ETHANOL
Abs dX 0.017181 at point 7 - Rel dX 0.092 at point 7
Abs dY -.019980 at point 7 - Rel dY 0.043 at point 23

Comp 2 - WATER
Abs dX -.010656 at point 7 - Rel dX 0.018 at point 10
Abs dY 0.023527 at point 7 - Rel dY 0.054 at point 7

Comp 3 - METHYL ACETATE
Abs dX -.006525 at point 7 - Rel dX -0.858 at point 7
Abs dY 0.008065 at point 27 - Rel dY -0.178 at point 7

- STANDARD DEVIATIONS -
- Temperature 0.499 CENT
- Pressure 49.9789 MMHG

Comp 1 - ETHANOL
X fractions 0.004400 - Y fractions 0.005079

Comp 2 - WATER
X fractions 0.003338 - Y fractions 0.005382

Comp 3 - METHYL ACETATE
X fractions 0.002377 - Y fractions 0.002157

- AVERAGE DEVIATIONS -
- Temperature 0.409 CENT
- Pressure (ABS) 37.8715 MMHG - Pressure (REL) 0.0592

Comp 1 - ETHANOL
X fractions 0.003359 - Y fractions 0.003769

Comp 2 - WATER
X fractions 0.002559 - Y fractions 0.003853

Comp 3 - METHYL ACETATE
X fractions 0.001481 - Y fractions 0.001092

III) * FINAL VALUES OF VARIABLE PARAMETERS *

1) * INTERACTION PARAMETERS *					
	*----	Binary	----	* * Para no	* * Optimum value * * Initial value *
1)	1	ETHANOL		1	456.94 185.78
	2	WATER			
2)	1	ETHANOL		2	883.74 895.59
	2	WATER			
3)	1	ETHANOL		1	815.86 1265.7
	3	METHYL ACETATE			
4)	1	ETHANOL		2	-352.89 -460.82
	3	METHYL ACETATE			
5)	2	WATER		1	1589.9 1832.3
	3	METHYL ACETATE			
6)	2	WATER		2	5655.2 753.46
	3	METHYL ACETATE			

```
* XPSIM, Vers. 1.07 *
* Cust/User "STAFF" " *
* Proj/Problem "REGRESSION TEST" " *
*** SIMULATION TRACE FOLLOWS ***
... New/output binary file 'VLE-DEMO' initialized ...

. Stream 'S1' flashed .
. Feed/Recycle streams processed .
Unit op 1 - 'F1' calculated

*** SOLUTION OBTAINED ***
... Base case results loaded on binary file 'VLE-DEMO' ...
```

*** UNIT 1 - 'F1' - 'FLASH' ***

--- Feed Streams ---

'S1'

- Product Streams -

'S2'

1) * OPERATING CONDITIONS *

Outlet temperature	150.00 °C
Outlet pressure	5000.0000 mmHg

2) * FEEDS *

Stream	S1
Temperature, °C	150.00
Pressure, mmHg	5000.000
Total rate, kmol/h	0.70000
Vapor, kmol/h	0.70000
Liquid, kmol/h	0.0000

3) * PRODUCTS *

Stream	S2
Temperature, °C	150.00
Pressure, mmHg	5000.000
Total rate, kmol/h	0.70000
Vapor, kmol/h	0.70000
Liquid, kmol/h	0.0000

* STREAM 'S1', feed of unit(s) 1 'F1'

- Temperature 150.00 °C - Pressure 5000.0000 mmHg

Phase VAPOR

Molar Flow Rate kmol/h 0.700

Weight Flow Rate kg/h 21.029

Molar Fraction 1.000000

Weight Fraction 1.000000

Molecular Weight 30.0410

Std Vap Vol Rate N-m3/h 16.5514

Enthalpy Mcal/h 1.0744

Spec. Enthalpy kcal/kg 51.090

kcal/kmol 1534.806

Reference Gas Status - Temperature 15°C - Pressure 1 atm

No Components		-----	TOTAL	PHASE		-----
		Mol.	Rate	Mol. Fr	Wt. Rate	Wt. Fr.
			kmol/h		kg /h	
1	ETHANOL		0.300	0.428571	13.821	0.657230
2	WATER		0.400	0.571429	7.208	0.342770
***	TOTAL	***	0.700	1.000000	21.029	1.000000

* STREAM 'S2', product of unit 1 'F1'

- Temperature 150.00 °C - Pressure 5000.0000 mmHg

Phase VAPOR

Molar Flow Rate kmol/h 0.700

Weight Flow Rate kg/h 21.029

Molar Fraction 1.000000

Weight Fraction 1.000000

Molecular Weight 30.0410

Std Vap Vol Rate N-m3/h 16.5514

Enthalpy Mcal/h 1.0744

Spec. Enthalpy kcal/kg 51.090

kcal/kmol 1534.806

Reference Gas Status - Temperature 15°C - Pressure 1 atm

No Components	-----		TOTAL		PHASE		-----	
	Mol. Rate		Mol. Fr		Wt. Rate		Wt. Fr.	
		kmol/h				kg /h		
1 ETHANOL	0.300		0.428571		13.821		0.657230	
2 WATER	0.400		0.571429		7.208		0.342770	
*** TOTAL ***	0.700		1.000000		21.029		1.000000	

- Calculation time 0.28 sec

- Simulation no. 6 - Ended at 15.37.47 on MAR 05, 2009 -