E.1 Data from Aspen Engineering Suite 2006

E.1.1 methanol/ethanol (20:80 wt %)

Component I = ethanol
Component J = methanol

VALUE I-J			VALUE J-I		
A_{ij}	=	-2.3127	A_{ji}	=	4.71190
B_{ij}	=	483.844	B_{ji}	=	-1162.29
C_{ij}	=	0.30000	C_{ji}	=	0.30000
D_{ij}	=	0.00000	D_{ji}	=	0.00000
E_{ij}	=	0.00000	E_{ji}	=	0.00000
F_{ij}	=	0.00000	F_{ji}	=	0.00000

E.1.2 acetone/methanol (80:20 wt %)

Component I = acetone
Component J = methanol

VALUE I-J			VALUE J-I		
A_{ij}	=	0.00000	A_{ji}	=	0.00000
B_{ij}	=	101.886	B_{ji}	=	114.135
C_{ij}	=	0.30000	C_{ji}	=	0.30000
D_{ij}	=	0.00000	D_{ji}	=	0.00000
E_{ij}	=	0.00000	E_{ji}	=	0.00000

E.1.3 isopropanol / acetone (80: 20 wt %)

Component I = isopropanol
Component J = acetone

VALUE I-J			VALUE J-I		
A_{ij}	=	2.44940	A_{ji}	=	-2.4106
B_{ij}	=	-583.345	B_{ji}	=	822.489
C_{ij}	=	0.30000	C_{ji}	=	0.30000
D_{ij}	=	0.00000	D_{ji}	=	0.00000
E_{ij}	=	0.00000	E_{ji}	=	0.00000
F_{ij}	=	0.00000	F_{ji}	=	0.00000

E.1.4 ethanol / acetone (50:50 wt %)

Component I = ethanol
Component J = acetone

VALUE I-J			VALUE J-I		
A_{ij}	=	-0.2589	A_{ji}	=	-1.0295
B_{ij}	=	228.279	B_{ji}	=	416.749
C_{ij}	=	0.30000	C_{ji}	=	0.30000
D_{ij}	=	0.00000	D_{ji}	=	0.00000
E_{ij}	=	0.00000	E_{ji}	=	0.00000
F_{ij}	=	0.00000	F_{ji}	=	0.00000

E.2 Calculations of activity coefficients (γ_i) of each compound in the mixture

The activity coefficients (γ_i) of each compound in the mixture are determined with the Non-Random Two Liquid model (NRTL) whereas, the variables in this model gets from program Aspen Engineering Suite 2006.

Non-Random Two Liquid models (NRTL):

$$\ln\gamma_I = X_J^2\left[\tau_{UA}\left(\frac{G_{JI}}{X_I+X_JG_{JI}}\right)^2+\left(\frac{\tau_{AU}G_{IJ}}{(X_J+X_IG_{IJ})^2}\right)\right]$$

$$\ln\gamma_J = X_I^2\left[\tau_{AU}\left(\frac{G_{IJ}}{X_J+X_IG_{IJ}}\right)^2+\left(\frac{\tau_{UA}G_{JI}}{(X_I+X_JG_{JI})^2}\right)\right]$$

Where

$$G_{IJ}=\exp\left(-\alpha\tau_{AU}\right)_{IJ}$$

$$\tau_{UA}=\frac{A_{IJ}+B_{IJ}}{T}+E_{IJ}\ln(T)+F_{IJ}T$$

$$\alpha = C_{IJ}+D_{IJ}\,(T-273.15\ K)$$

UNITS: K

E.2.1 methanol/ethanol (20:80 wt %)

From data E.1.1

$$\tau_{AU}=\frac{-2.31270+483.844}{273.15+55}+0+0=-0.86037$$

$$\alpha= 0.30+0\ (T-273.15\ K)= 0.30$$

$$G_{IJ}= \exp\ (-0.30\times -0.86037)_{IJ}=1.29448$$

$$\tau_{UA}=\frac{4.71190+(-1162.29)}{273.15+55}+0+0=1.2231$$

$$\alpha= 0.30+0\ (T-273.15\ K)= 0.30$$

$$G_{JI}=\exp\ (-0.30\times 1.2231)_{JI}=0.69285$$

$$\ln\gamma_I = 0.26^2\left[1.2231\left(\frac{0.69285}{0.74+(0.26\times 0.69285)}\right)^2+\left(\frac{-0.86037\times 1.29448}{(0.26+0.74\times 1.29448)^2}\right)\right]$$

$$\ln\gamma_I = -0.00388$$

$$\gamma_{EtOH} = 0.99613$$

$$\ln\gamma_J = 0.74^2\left[-0.86037\left(\frac{1.29448}{0.26+0.74\times 1.29448}\right)^2+\left(\frac{1.2231\times 0.69285}{(0.74+0.26\times 0.69285)^2}\right)\right]$$

$$\ln\gamma_J = 0.01586$$

$$\gamma_{MeOH} = 1.01599$$

E.2.2 acetone/methanol (80:20 wt %)

From data E.1.2

$$\tau_{AU}=\frac{0+101.886}{273.15+55}+0+0=0.3058$$

$$\alpha=0.30+0\ (T-273.15\ K)=0.30$$

$$G_{IJ}=\exp\ (-0.30\times0.3058)_{IJ}=0.91233$$

$$\tau_{UA}=\frac{0+114.135}{273.15+55}+0+0=0.34259$$

$$\alpha=0.30+0\ (T-273.15\ K)=0.30$$

$$G_{JI}=\exp\ (-0.30\times0.34259)_{JI}=0.902327$$

$$\ln\gamma_I = 0.31^2\left[0.34259\left(\frac{0.902327}{0.69+(0.31\times0.902327)}\right)^2+\left(\frac{0.3058\times 0.91233}{(0.31+0.69\times0.91233)^2}\right)\right]$$

$$\ln\gamma_I = 0.05888$$

$$\gamma_{Acetone} = 1.06065$$

$$\ln\gamma_J = 0.69^2\left[0.3058\left(\frac{0.91233}{0.31+0.69\times0.91233}\right)^2+\left(\frac{0.34259\times0.902327}{(0.69+0.31\times0.902327)^2}\right)\right]$$

$$\ln\gamma_J = 0.29381$$

$$\gamma_{MeOH} = 1.34153$$

E.2.3 isopropanol / acetone (80:20 wt %)

From data E.1.3

$$\tau_{AU}=\frac{2.44940+(-583.345)}{273.15+55}+0+0=0.6717$$

$\alpha = 0.30+0\ (T-273.15\ K) = 0.30$

$G_{IJ}= \exp\ (-0.30\times0.6717)_{IJ}= 0.8175$

$$\tau_{UA}= \frac{-2.41060+822.489}{273.15+55}+0+0=0.0958$$

$\alpha= 0.30+0\ (T-273.15\ K) = 0.30$

$G_{JI}= \exp\ (-0.30\times0.0958)_{JI}= 0.9717$

$$\ln\gamma_I=0.24^2\left[0.0958\left(\frac{0.9717}{0.76+(0.24\times0.9717)}\right)^2+\left(\frac{0.6717\times 0.8175}{(0.24+0.76\times0.8175)^2}\right)\right]$$

$\ln\gamma_I = 0.0490$

$\gamma_{isopropanol} = 1.0503$

$$\ln\gamma_J = 0.76^2\left[0.6717\left(\frac{0.8175}{0.24+0.76\times0.8175}\right)^2+\left(\frac{0.0958\times0.9717}{(0.76+0.24\times0.9717)^2}\right)\right]$$

$\ln\gamma_J = 0.4041$

$\gamma_{Acetone} = 1.4979$

E.2.4 ethanol / acetone (50:50 wt %)

From data E.1.4

$$\tau_{AU}=\frac{-0.258900+(228.279)}{273.15+55}+0+0=0.43675$$

$$\alpha=0.30+0\ (T-273.15\ K)=0.30$$

$$G_{IJ}=\exp\ (-0.30\times0.6717)_{IJ}=0.87719$$

$$\tau_{UA}=\frac{-1.02950_{+}416.749}{273.15+55}+0+0=0.24049$$

$$\alpha=0.30+0\ (T-273.15\ K)=0.30$$

$$G_{JI}=\exp\ (-0.30\times0.0958)_{JI}=0.93039$$

$$\ln\gamma_{I}=0.44^{2}\left[0.24049\left(\frac{0.9303}{0.56+(0.44\times0.9303)}\right)^{2}+\left(\frac{0.43675\times\ 0.87719}{(0.44+0.56\times0.87719)^{2}}\right)\right]$$

$$\ln\gamma_{I}=0.12842$$

$$\gamma_{EtOH}=1.13703$$

$$\ln\gamma_{J}=0.56^{2}\left[0.43675\left(\frac{0.87719}{0.44+0.56\times0.87719}\right)^{2}+\left(\frac{0.24049\times0.93039}{(0.56+0.44\times0.93039)^{2}}\right)\right]$$

$$\ln\gamma_{J}=0.19620$$

$$\gamma_{Acetone}=\ 1.21677$$