Modelling Unit Operations II. ENSGTI/3A/CAPD

Modeling of a two phases distillation column with multiple trays in steady state operation

The goal is to build a mathematical model of a two phases distillation column with multiple trays, partial condenser and operating in steady state operation. The mathematical model will be solved using Newton Raphson's method, with coding in Fortran 90 Language. The resulting software will be used to analyze the working of the unit as a function of its working parameters.

- Heat provided to the boiler (Q_b)
- Heat withdrawn from the condenser (Q_c)
- Number of trays
- Operating Pressure
- Feeding tray
- Number of feedings.
- Nature of the feedings (vapor, liquid…)
- ….

The Jacobian matrix of the system will be estimated using numerical perturbations. The ordering of the set of equations as well as of the solution vector will be handled to render the structure of the Jacobian matrix tridiagonal by blocks. The linear system resolution, involved in NR's method, will be solved using appropriate Fortran Subroutine MRSL21. Its calling syntax and arguments are provided in Appendix.

-I- As a test case, the software will be used to simulate the following system:

Operating Pressure: 1atm

Components: ACETONE
BENZENE
CHLOROFORM

$V_j = D - L_1$

AV Alim : $L_j = L_1$

FP Alim : $L_j = \sum_{NP} F_j + L_1$

Feeding:

Temperature: Bubble point
Pressure: 1 atm
Partial molar flowrates [mol/s] :

ACETONE:	0.6
BENZENE:	0.3
CHLOROFORME:	0.1

Column:

Number of trays (ideal): 30
Feeding tray: 14
Heat to boiler: 19 10^3 cal/s
Heat from condenser: 15. 10^3 cal/s

Activity coefficients involved in the equilibrium equations will be computed according to NRTL Thermodynamical model. The binary interactions parameters will be recovered from the ProSim Plus database. NRTL thermodynamical model will also be used to evaluate the enthalpy in excess involved in the model for enthalpy of the liquid phase.

The mathematical derivation of NRTL model is the following:

$$Ln(\gamma_i) = \frac{\sum_{l=1}^{nc} \tau_{li} G_{li} x_l}{\sum_{l=1}^{nc} G_{li} x_l} + \sum_{j=1}^{nc} \frac{x_j G_{ij}}{\sum_{l=1}^{nc} G_{lj} x_l} \cdot \left(\tau_{ij} - \frac{\sum_{l=1}^{nc} \tau_{lj} G_{lj} x_l}{\sum_{l=1}^{nc} G_{lj} x_l} \right)$$

$$[\tau] = \begin{bmatrix} 0 & 569,931 & 228,454 \\ -193,340 & 0 & 0 \\ -643,277 & 0 & 0 \end{bmatrix} \begin{matrix} \text{Ac} \\ \text{Benz} \\ \text{Chlor} \end{matrix}$$

where

nc stands for the total number of chemical species involved in the model

$$\tau_{ij} = \frac{(g_{ij} - g_{jj})}{R.T}$$

$$\tau_{ii} = 0$$

$$G_{ij} = \exp(-\alpha_{ij} . \tau_{ij})$$

$$G_{ii} = 1$$

$$[\alpha] = \begin{bmatrix} 0 & & \\ 0,3007 & 0 & 0 \\ 0,3043 & 0 & 0 \end{bmatrix}$$

The binary interaction parameters of the model are (for a binary system i,j): ($g_{ij} - g_{jj}$), ($g_{ji} - g_{ii}$) and α_{ij} (equal to α_{ji}). The first two ones are expressed in cal/mol while the third is dimensionless.

$T_{ref} = 288,15$ K

$T_{bulle} = 334,7176$ Compo Liq (0,6 ; 0,3 ; 0,1)

$H_L = -26990,79$ J.mol^{-1} → y = 0,7323 ; 0,2052 ; $6,25 . 10^{-2}$

$H_V = 3083,55$ J.mol^{-1}

Auxiliary data

		Acetone	Benzene	Chloroform
T_{eb} at 1 atm	[K]	329.44	353.24	334.33
H_{vap} at Teb, 1 atm	[J/kmol]	2.96 E+07	3.08 E+07	2.95 E+07
Cp^{vap}	[J/kmol/K]	8.05 E+04	9.60 E+04	6.89 E+04
Cp^{liq}	[J/kmol/K]	1.34 E+05	1.47 E+5	1.17 E+05
P^{sat}	[Pa]			
	A	69.006	83.107	146.43
	B	-5599.6	-6486.2	-7792.3
	C	-7.0985	-9.2194	-20.614
	D	6.2237 E-06	6.9844 E-06	0.024578
	E	2	2	1

$P^{sat}(T) = \exp[A + \frac{B}{T} + C.Ln(T) + D.T^E]$. In this expression, unit for T is K.

-II- Application to the study of the ternary system Acetone-Benzene-Chloroform
Singular points of the ternary mixture are depicted on the following figure:

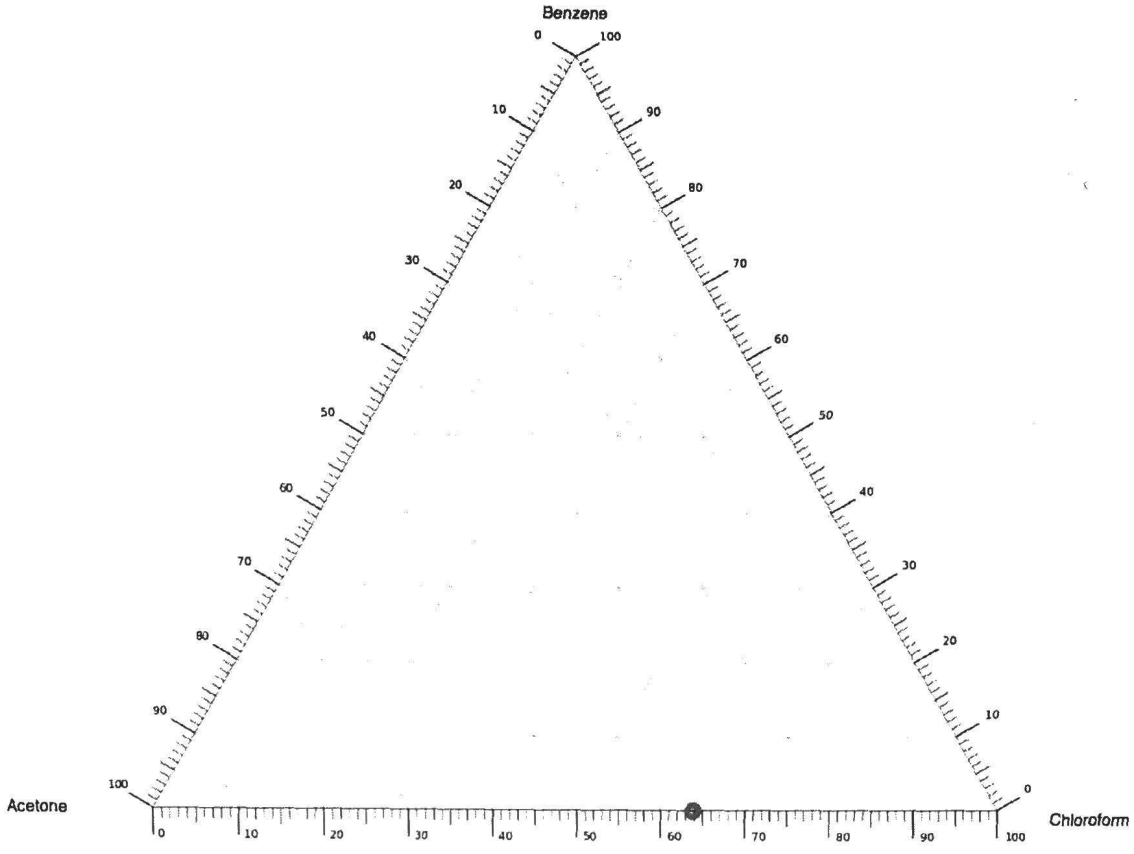
- Pure components
- Azeotrope for the binary mixture Acetone-Chloroform.

The goal is to determine the distillation domains of the ternary mixture. To do so, the software will be used to study the separation of the two following feeds:

- $Alim_1$: 0.6 0.3 0.1
- $Alim_2$: 0.1 0.2 0.7

For each feeding, heat withdrawn from the condenser will be varied from 11. 10^3 cal/s to 19. 10^3 cal/s.
Then, determine:

- The nature of the singular points of the ternary mixture: stable node, unstable node, saddle point,
- The distillation domain.



Binary mixture Acetone-Chloroform: Azeotrope characteristics:

- Molar composition
  - Acetone: 0.66 (-)
  - Chloroform: 0.34 (-)
- Temperature: 337.5 K

0,6	0,3	0,1	X	L1
0,1	0,2	0,7	X	L2
0,5	3	2		L3
6	2	2		L4
5	4	1		L5
1	3	6		L6
4	1	5		L7
3	1	6		L8
6	3	1		L9
1	8	1		L10
0,2	0,4	0,4		L11

Azeotrope problème

Acétone	Benzène	Chloroforme	
T=338,197 0,3535	0	0,6465	Ternaire Bi
1	0	0	selle stable
0	1	0	instable
0	0	1	stable
			instable

02 / 08 / 05

0,107 / 0,519 / 0,374

ANNEXE : Sous programme MRSL01

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      SUBROUTINE MRSL01(A,B,N,NL,IER,INDIC)
        IMPLICIT REAL*8 (A-H,O-Z)
C
C     SOUS PROGRAMME DE RESOLUTION DE SYSTEMES LINEAIRES
C
C     A   MATRICE PREMIER MEMBRE
C     B   EN ENTREE VECTEUR SECOND MEMBRE
C         EN SORTIE VECTEUR SOLUTION
C     N   NOMBRE D'EQUATIONS
C     NL  NOMBRE DE LIGNES REEL DE LA MATRICE A (DIMENSION)
C     IER INDICATEUR D'ERREUR
C         0 AUCUNE ERREUR DETECTEE
C         1 PIVOT TROP PETIT EN COURS D'ELIMINATION
C     INDIC  NON UTILISE DANS CETTE VERSION
C
C     ATTENTION  LA MATRICE A EST DETRUITE PAR LE SOUS PROGRAMME
C
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ANNEXE : Sous programme MRSL21

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      SUBROUTINE MRSL21(A,B,C,F,N,M,N1A,NLA,NC,IER,IRAZ,IMET)
      IMPLICIT REAL*8 (A-H,O-Z)
C*
C*   RESOLUTION D'UN SYSTEME LINEAIRE DONT LA MATRICE
C*   PREMIER MEMBRE EST TRIDIAGONALE PAR BLOCS
C*
C    LA MATRICE PREMIER MEMBRE SE PRESENTE SOUS LA FORME:
C     B1 C1
C     A2 B2 C2
C       A3 B3 C3
C
C           .........
C
C              AM BM
C
C    CETTE VERSION PERMET DANS CERTAINS CAS REELS D'ECONOMISER
C    PLUS D'UN TIERS DE LA PLACE MEMOIRE UTILISE AVEC L'ALGORITHME
C    TRADITIONNEL EN UTILISANT COMME DIMENSIONS :
C     A(NLA,N1A:N,M) PARTIE NON NULLE DE A COLLEE A B
C     B(N,N,M)
C     C(N,NC,M) PARTIE NON NULLE DE C COLLEE A B
C
C    ON PEUT AVOIR N1A=1 , NLA=N , NC=N
C
C    PARAMETRES DU S.P.
C    ----------------
C    A,B,C     DESCRIPTION MATRICE PREMIER MEMBRE VOIR CI DESSUS
C    F         VECTEUR 2EME MEMBRE EN ENTREE
C              VECTEUR SOLUTION EN SORTIE
C
C          ATTENTION: A,B,C ET F DETRUITS PAR LE S.P.
C
C    N         NOMBRE D'EQUATIONS PAR BLOC
C              SERT AU DIMENSIONNEMENT POUR A B C ET F
C    N1A       1ER INDICE COLONNE DE A UTILISE (1 A N) ATTENTION
C    NLA       NOMBRE DE LIGNES UTILES DE A (1 A N) ATTENTION
C    NC        NOMBRES DE COLONNES UTILES DE C (1 A N) ATTENTION
C
C    IER       INDICATEUR D'ERREUR  DOIT ETRE TESTE EN SORTIE
C              0  VALEUR NORMALE
C              >0 NOMBRE DE PIVOTS < EPS
C              <0 PIVOT NUL RENCONTRE  CALCUL ARRETE NE PAS UTILISER
C              LE RESULTAT
C
C    IRAZ      PARAMETRE D'ENTREE
C              0 LES TABLEAUX A B C DOIVENT ETRE ENTIEREMENT
REINITIALISES
C              PAR L'UTILISATEUR (MEME LES ELEMENTS NULS)
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```
C               1 EN SORTIE DU S.P. LES TABLEAUX A B C SONT REMIS A ZERO
C
C   IMET        PARAMETRE D'ENTREE
C               O PAS DE RECHERCHE DE PIVOT MAXIMUM
C               1 RECHERCHE DE PIVOT MAXIMUM POUR CHAQUE BLOC B
C
C
      DIMENSION A(NLA,N1A:N,M),B(N,N,M),C(N,NC,M),F(N,M)
C
C   EPS VALEUR EN DESSOUS DE LAQUELLE UN PIVOT EST CONSIDERE
C   COMME TROP PETIT  (IER INCREMENTE  CALCUL POURSUIVI)
C   SI UN PIVOT NUL EST RENCONTRE IER RECOIT UNE VALEUR NEGATIVE
C   ET LE CALCUL EST ARRETE (VERIFIER IER EN SORTIE)
C
      EPS=1.E-12
```