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Appendix A: An example calculation of parameters used for bubble point calculation

Acetic acid: $V_{c1} = 179.7 cm^3/mol; Z_{c1} = 0.211; T_{c1} = 592K$

Ethanol: $V_{c2} = 167.0 cm^3/mol; Z_{c1} = 0.240; T_{c1} = 513.9K$

Water: $V_{c1} = 55.9 cm^3/mol; Z_{c1} = 0.229; T_{c1} = 647.1K$

Ethyl acetate: $V_{c1} = 286.0 cm^3/mol; Z_{c1} = 0.255; T_{c1} = 523.3K$

(a) Calculating molar volumes

$$V^{sat} = V_c Z_c^{(1-T/T_c)^{0.2857}}$$

Assume Temperature (T) 370K

$$V_1^{sat} = 179.7 \, cm^3/mol \times 0.211^{(1-370/592)^{0.2857}} = 55.45817$$

$$V_2^{sat} = 167.0 \, cm^3/mol \times 0.24^{(1-370/513.9)^{0.2857}} = 61.92824$$

$$V_3^{sat} = 55.90 \, cm^3/mol \times 0.229^{(1-370/647.1)^{0.2857}} = 17.579306$$

$$V_4^{sat} = 286.0 \, cm^3/mol \times 0.255^{(1-370/523.3)^{0.2857}} = 109.2657$$

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(b) Determination of temperature dependent parameters

$$G_{ij} = \frac{V_j}{V_i} \exp\left(\frac{-a_{ij}}{RT}\right)$$

$$G_{1,1} = \frac{V_1}{V_1} \exp\left(\frac{-a_{1,1}}{RT}\right) = 1$$

$$G_{1,2} = \frac{V_2}{V_1} \exp\left(\frac{-a_{1,2}}{RT}\right) = \frac{61.928}{55.458} \exp(130.6527/370) = 1.589567311$$

$$G_{1,3} = \frac{V_3}{V_1} \exp\left(\frac{-a_{1,3}}{RT}\right) = \frac{17.579306}{55.458} \exp(-2.0311/370) = 0.3152488279$$

$$G_{1,4} = \frac{V_4}{V_1} \exp\left(\frac{-a_{1,4}}{RT}\right) = \frac{109.2657}{55.458} \exp(-1749.9343/370) = 0.0173980767$$

$$G_{2,1} = \frac{V_1}{V_2} \exp\left(\frac{-a_{2,1}}{RT}\right) = \frac{55.458}{61.928} \exp(-101.6588/370) = 0.6803826245$$

$$G_{2,2} = \frac{V_2}{V_2} \exp\left(\frac{-a_{2,2}}{RT}\right) = 1$$

$$G_{2,3} = \frac{V_3}{V_2} \exp\left(\frac{-a_{2,3}}{RT}\right) = \frac{17.579306}{61.928} \exp(-198.1757/370) = 0.166150711$$

$$G_{2,4} = \frac{V_4}{V_2} \exp\left(\frac{-a_{2,4}}{RT}\right) = \frac{109.2657}{61.928} \exp(-288.2011/370) = 0.8096835545$$

$$G_{3,1} = \frac{V_1}{V_3} \exp\left(\frac{-a_{3,1}}{RT}\right) = \frac{55.458}{17.579306} \exp(-403.1564/370) = 1.061084683$$

$$G_{3,2} = \frac{V_2}{V_3} \exp\left(\frac{-a_{3,2}}{RT}\right) = \frac{61.928}{17.579306} \exp(-466.1059/370) = 0.9995044523$$

$$G_{3,3} = \frac{V_3}{V_3} \exp(0) = 1$$

$$G_{3,4} = \frac{V_4}{V_3} \exp\left(\frac{-a_{3,4}}{RT}\right) = \frac{109.2657}{17.579306} \exp(-1195.67/370) = 0.2454945763$$

$$G_{4,1} = \frac{V_1}{V_4} \exp\left(\frac{-a_{4,1}}{RT}\right) = \frac{55.458}{109.2657} \exp(464.1529/370) = 1.779461417$$

$$G_{4,2} = \frac{V_2}{V_4} \exp\left(\frac{-a_{4,2}}{RT}\right) = \frac{61.928}{109.2657} \exp(-28.8790/370) = 0.5242107598$$

$$G_{4,3} = \frac{V_3}{V_4} \exp\left(\frac{-a_{4,3}}{RT}\right) = \frac{17.579306}{109.2657} \exp(-26981.1/370) = 3.4430 \times 10^{-33}$$

$$G_{4,4} = \frac{V_4}{V_4} \exp(0) = 1$$

(c) Determination of activity coefficient

$$\ln \gamma_i = 1 - \ln\left(\sum_j x_j G_{ij}\right) - \sum_k \left(\frac{x_k G_{ki}}{\sum_j x_j G_{kj}}\right)$$

$$\ln \gamma_1 = 1 - \ln\left(x_1 G_{1,1} + x_2 G_{1,2} + x_3 G_{1,3} + x_4 G_{1,4}\right) - \frac{x_1 G_{1,1}}{x_1 G_{1,1} + x_2 G_{1,2} + x_3 G_{1,3} + x_4 G_{1,4}} \cdots$$

$$\ln \gamma_1 = -0.0551539989$$

$$\gamma_1 = \underline{0.9463394014}$$

$$\ln \gamma_2 = 1 - \ln\left(x_1 G_{2,1} + x_2 G_{2,2} + x_3 G_{2,3} + x_4 G_{2,4}\right) - \frac{x_1 G_{1,2}}{x_1 G_{1,1} + x_2 G_{1,2} + x_3 G_{1,3} + x_4 G_{1,4}} \cdots$$

$$\ln \gamma_2 = 0.5781461348$$

$$\gamma_2 = \underline{1.782730423}$$

$$\ln \gamma_3 = 1 - \ln\left(x_1 G_{3,1} + x_2 G_{3,2} + x_3 G_{3,3} + x_4 G_{3,4}\right) - \frac{x_1 G_{1,3}}{x_1 G_{1,1} + x_2 G_{1,2} + x_3 G_{1,3} + x_4 G_{1,4}} \cdots$$

$$\ln \gamma_3 = 0.6604718476$$

$$\gamma_3 = \underline{\underline{1.935705477}}$$

$$\ln \gamma_4 = 1 - \ln\left(x_1 G_{4,1} + x_2 G_{4,2} + x_3 G_{4,3} + x_4 G_{4,4}\right) - \frac{x_1 G_{4,3}}{x_1 G_{1,1} + x_2 G_{1,2} + x_3 G_{1,3} + x_4 G_{1,4}} \cdots$$

$$\ln \gamma_4 = 0.4620788076$$

$$\gamma_4 = \underline{\underline{1.587370395}}$$

(d) Calculating vapor pressure

Anotoine equation for vapour pressure

$$\log P^{sat} = A - \frac{B}{T + C}$$

For Acetic acid

$$A = 7.5596, B = 1644.05, C = 233.524$$

$$P_1^{sat} = 383.063 mmHg$$

For Ethanol

$$A = 8.20417, B = 1642.89, C = 230.3$$

$$P_2^{sat} = 1519.83 mmHg$$

For Water

$$A = 8.07131, B = 1730.63, C = 233.426$$

$$P_3^{sat} = 678.202 mmHg$$

For Ethyl Acetate

$$A = 7.2597, B = 1369.41, C = 235.5$$

$$P_4^{sat} = 1378.21 mmHg$$

Appendix B: bubble point temperature determination example calculation

First Iteration of bubble point calculation

P=760mmHg

Let's assume

    (1) Acetic acid mole fraction=0.45

    (2) Ethanol mole fraction=0.45

    (3)Water mole fraction=0.1

    (4) Ethyl acetate mole fraction=0

$$T_i^{sat} = \frac{B_i}{A_i - \log P} - C_i$$

For Acetic acid $\quad A = 7.5596, B = 1644.05, C = 233.524$

$T_1^{sat} = 117.86$

For Ethanol $\quad A = 8.20417, B = 1642.89, C = 230.3$

$T_2^{sat} = 78.32$

For Water $\quad A = 8.07131, B = 1730.63, C = 233.426$

$T_3^{sat} = 100$

For Ethyl Acetate $\quad A = 7.2597, B = 1369.41, C = 235.5$

$T_4^{sat} = 77.23$

$$T = \sum_i x_i T_i^{sat} = x_1 T_1^{sat} + x_2 T_2^{sat} + x_3 T_3^{sat} + x_4 T_4^{sat}$$

$$T = 98.28^0 C$$

$$\log P_i^{sat} = A_i - \frac{B_i}{T + C_i}$$

$$P_1^{sat} = 14375.13 \quad P_2^{sat} = 114.038 \quad P_3^{sat} = 0.6776 \quad P_4^{sat} = 3.1569$$

$$\ln \gamma_i = 1 - \ln \sum_j x_j \Lambda_{i,j} - \sum_k \frac{x_k \Lambda_{ki}}{\sum x_j \Lambda_{kj}}$$

$$\Lambda_{ij} = \frac{V_j}{V_i} \exp \frac{-a_{ij}}{RT}$$

$$a_{1,2} = -130.6527 \quad a_{2,1} = 101.6588 \quad a_{3,1} = 403.1564 \quad a_{4,1} = -464.1529$$

$$a_{1,3} = 2.0311 \quad a_{2,3} = 198.1757 \quad a_{3,2} = 466.1059 \quad a_{4,2} = 28.8790$$

$$a_{1,4} = 1749.9343 \quad a_{2,4} = 198.1757 \quad a_{3,2} = 466.1059 \quad a_{4,2} = 28.879$$

$$a_{i,j} = 0 \ (for \ i = j)$$

(1) Acetic acid: $V_{c1} = 179.7 cm^3 / mol; Z_{c1} = 0.211; T_{c1} = 592K$

(2)Ethanol: $V_{c2} = 167.0 cm^3 / mol; Z_{c1} = 0.240; T_{c1} = 513.9K$

(3) Water: $V_{c1} = 55.9 cm^3 / mol; Z_{c1} = 0.229; T_{c1} = 647.1K$

(4) Ethyl acetate: $V_{c1} = 286.0 cm^3 / mol; Z_{c1} = 0.255; T_{c1} = 523.3K$

$$V^{sat} = V_c Z_c^{\left(1 - T/T_c\right)^{0.2857}}$$

$T = 98.28$

$V_1 = 1.550876 \quad V_2 = 1.423288 \quad V_3 = 1.409967 \quad V_4 = 1.52938$

$\Lambda_{1,1} = 1 \quad \Lambda_{1,2} = 1.344 \quad \Lambda_{1,3} = 0.903 \quad \Lambda_{1,4} = 0.005903543$

$\Lambda_{2,1} = 0.809382492 \quad \Lambda_{2,2} = 1.009447632 \quad \Lambda_{2,3} = 0.554864221 \quad \Lambda_{2,4} = 0.462530073$

$\Lambda_{3,1} = 0.338271289 \quad \Lambda_{3,2} = 0.258238087 \quad \Lambda_{3,3} = 1 \quad \Lambda_{3,4} = 0.024490565$

$\Lambda_{4,1} = 3.941342859 \quad \Lambda_{4,2} = 0.855252092 \quad \Lambda_{4,3} = 0 \quad \Lambda_{4,4} = 1$

$$\ln \gamma_i = 1 - \ln \sum_j x_j \Lambda_{i,j} - \sum_k \frac{x_k \Lambda_{ki}}{\sum_j x_j \Lambda_{kj}}$$

$\ln \gamma_1 = -0.03929 \quad \gamma_1 = 0.961471$

$\ln \gamma_2 = 0.037237 \quad \gamma_2 = 1.037939$

$\ln \gamma_3 = 1.010128 \quad \gamma_3 = 2.745953$

$\ln \gamma_4 = 0.03834 \quad \gamma_4 = 1.039085$

$$P_j^{sat} = \frac{P}{\sum_i (x_i \gamma_i / \Phi_i)(P_i^{sat} / P_j^{sat})}$$

Select Acetic acid as j component from the set (i)

$P_j^{sat} = 183.607$

Calculate Temperature

$$T = \frac{B_j}{A_j - \ln P_j^{sat}} - C_j \quad T = 76.92536$$

$$\log P_i^{sat} = A_i - \frac{B_i}{T + C_i}$$

$P_1^{sat} = 3536.322 \quad P_2^{sat} = 36190.02 \quad P_3^{sat} = 9345.951 \quad P_4^{sat} = 38788.75$

$$y_i = \frac{x_i \gamma_i P_i^{sat}}{P}$$

$y_1 = 2.013199 \quad y_2 = 22.24128 \quad y_3 = 3.376782 \quad y_4 = 0$

$T = 76.92536$

$\Lambda_{1,1} = 1 \quad \Lambda_{1,2} = 1.3296 \quad \Lambda_{1,3} = 0.9085 \quad \Lambda_{1,4} = 0.00662$

$\Lambda_{2,1} = 0.8170055 \quad \Lambda_{2,2} = 1.001833 \quad \Lambda_{2,3} = 0.56669 \quad \Lambda_{2,4} = 0.470607162$

$\Lambda_{3,1} = 0.34593 \quad \Lambda_{3,2} = 0.2645796 \quad \Lambda_{3,3} = 1 \quad \Lambda_{3,4} = 0.0265743$

$\Lambda_{4,1} = 3.83674 \quad \Lambda_{4,2} = 0.8589740 \quad \Lambda_{4,3} = 0 \quad \Lambda_{4,4} = 1$

$$\ln \gamma_i = 1 - \ln \sum_j x_j \Lambda_{i,j} - \sum_k \frac{x_k \Lambda_{ki}}{\sum x_j \Lambda_{kj}}$$

$\ln \gamma_1 = -0.03776 \quad \gamma_1 = 0.962942$

$\ln \gamma_2 = 0.02238 \quad \gamma_2 = 1.022632$

$\ln \gamma_3 = 1.06441 \quad \gamma_3 = 2.899127$

$\ln \gamma_4 = 0.000163 \quad \gamma_4 = 1.000163$

$$P_j^{sat} = \frac{P}{\sum_i \left(x_i \gamma_i / \Phi_i \right) \left(P_i^{sat} / P_j^{sat} \right)}$$

Select Acetic acid as j component from the set (i)

$P_j^{sat} = 147.7789$

Calculate Temperature

$$T = \frac{B_j}{A_j - \ln P_j^{sat}} - C_j \quad T = 71.49526$$

By Iterating

Table 3.2:Bubble point temperature and vapor composition

Temperature	Y_1	Y_2	Y_3	Y_4
98.28026	2.013199	22.24128	3.376782	0
76.92541	1.317713	15.55649	2.37511	0
71.49528	1.138841	13.78373	2.096188	0

Proceed the iteration till $\sum y_i = 1$.

Appendix C:Solving model equations

First Iteration of bubble point calculation

P=760mmHg

Let us assume

(1) Acetic acid mole fraction=0.45

(2) Ethanol mole fraction=0.45

(3)Water mole fraction=0.1

(4) Ethyl acetate mole fraction=0

$$T_i^{sat} = \frac{B_i}{A_i - \log P} - C_i$$

For Acetic acid $A = 7.5596, B = 1644.05, C = 233.524$

$T_1^{sat} = 117.86$

For Ethanol $A = 8.20417, B = 1642.89, C = 230.3$

$T_2^{sat} = 78.32$

For Water $A = 8.07131, B = 1730.63, C = 233.426$

$T_3^{sat} = 100$

For Ethyl Acetate $A = 7.2597, B = 1369.41, C = 235.5$

$T_4^{sat} = 77.23$

$$T = \sum_i x_i T_i^{sat} = x_1 T_1^{sat} + x_2 T_2^{sat} + x_3 T_3^{sat} + x_4 T_4^{sat}$$

$T = 98.28^0 C$

$$\log P_i^{sat} = A_i - \frac{B_i}{T + C_i}$$

$$P_1^{sat} = 402.4583 \quad P_2^{sat} = 1600.311 \quad P_3^{sat} = 714.4188 \quad P_4^{sat} = 1435.393$$

$$\ln \gamma_i = 1 - \ln \sum_j x_j \Lambda_{i,j} - \sum_k \frac{x_k \Lambda_{ki}}{\sum x_j \Lambda_{kj}}$$

$$\Lambda_{ij} = \frac{V_j}{V_i} \exp \frac{-a_{ij}}{RT}$$

$$a_{1,2} = -130.6527 \quad a_{2,1} = 101.6588 \quad a_{3,1} = 403.1564 \quad a_{4,1} = -464.1529$$

$$a_{1,3} = 2.0311 \quad a_{2,3} = 198.1757 \quad a_{3,2} = 466.1059 \quad a_{4,2} = 28.8790$$

$$a_{1,4} = 1749.9343 \quad a_{2,4} = 198.1757 \quad a_{3,2} = 466.1059 \quad a_{4,2} = 28.879$$

$$a_{i,j} = 0 \ (for\ i = j)$$

(1) Acetic acid: $V_{c1} = 179.7 cm^3/mol; Z_{c1} = 0.211; T_{c1} = 592K$

(2) Ethanol: $V_{c2} = 167.0 cm^3/mol; Z_{c1} = 0.240; T_{c1} = 513.9K$

(3) Water: $V_{c1} = 55.9 cm^3/mol; Z_{c1} = 0.229; T_{c1} = 647.1K$

(4) Ethyl acetate: $V_{c1} = 286.0 cm^3/mol; Z_{c1} = 0.255; T_{c1} = 523.3K$

$$V^{sat} = V_c Z_c^{\left(1 - T/T_c\right)^{0.2857}}$$

$T = 98.28$

$$V_1 = 55.5768 \quad V_2 = 62.1010 \quad V_3 = 17.6089 \quad V_4 = 109.5433$$

$$\Lambda_{1,1} = 1 \quad \Lambda_{1,2} = 1.1656 \quad \Lambda_{1,3} = 0.3166 \quad \Lambda_{1,4} = 1.1183$$

$$\Lambda_{2,1} = 0.8659 \quad \Lambda_{2,2} = 1.009447632 \quad \Lambda_{2,3} = 0.2659 \quad \Lambda_{2,4} = 1.606$$

$$\Lambda_{3,1} = 2.7698 \quad \Lambda_{3,2} = 3.0325 \quad \Lambda_{3,3} = 1 \quad \Lambda_{3,4} = 4.2236$$

$$\Lambda_{4,1} = 0.5896 \quad \Lambda_{4,2} = 0.5616 \quad \Lambda_{4,3} = 0 \quad \Lambda_{4,4} = 1$$

$$\ln \gamma_i = 1 - \ln \sum_j x_j \Lambda_{i,j} - \sum_k \frac{x_k \Lambda_{ki}}{\sum x_j \Lambda_{kj}}$$

$\ln \gamma_1 = -0.00542 \quad \gamma_1 = 0.9945$

$\ln \gamma_2 = -0.00908 \quad \gamma_2 = 0.990957$

$\ln \gamma_3 = -0.31399 \quad \gamma_3 = 0.730527$

$\ln \gamma_4 = 0.167025 \quad \gamma_4 = 0.167025$

$$P_j^{sat} = \frac{P}{\sum_i (x_i \gamma_i / \Phi_i)(P_i^{sat} / P_j^{sat})}$$

Select Acetic acid as j component from the set (i)

$P_j^{sat} = 323.347$

Calculate Temperature

$$T = \frac{B_j}{A_j - \ln P_j^{sat}} - C_j \quad T = 92.0349$$

$$\log P_i^{sat} = A_i - \frac{B_i}{T + C_i}$$

$P_1^{sat} = 323.347 \quad P_2^{sat} = 1280.348 \quad P_3^{sat} = 567.3297 \quad P_4^{sat} = 1198.784$

$$y_i = \frac{x_i \gamma_i P_i^{sat}}{P}$$

$y_1 = 0.19042 \quad y_2 = 0.751245 \quad y_3 = 0.054533 \quad y_4 = 0$

$T = 92.0349$

$$\Lambda_{1,1} = 1 \quad \Lambda_{1,2} = 1.1632 \quad \Lambda_{1,3} = 0.3172 \quad \Lambda_{1,4} = 1.1056$$

$$\Lambda_{2,1} = 0.86790 \quad \Lambda_{2,2} = 1 \quad \Lambda_{2,3} = 0.2669 \quad \Lambda_{2,4} = 1.6059$$

$$\Lambda_{3,1} = 2.7582 \quad \Lambda_{3,2} = 3.01034 \quad \Lambda_{3,3} = 1 \quad \Lambda_{3,4} = 4.1803$$

$$\Lambda_{4,1} = 0.5921 \quad \Lambda_{4,2} = 0.5609 \quad \Lambda_{4,3} = 0 \quad \Lambda_{4,4} = 1$$

$$\ln \gamma_i = 1 - \ln \sum_j x_j \Lambda_{i,j} - \sum_k \frac{x_k \Lambda_{ki}}{\sum x_j \Lambda_{kj}}$$

$$\ln \gamma_1 = -0.00551 \quad \gamma_1 = 0.9945$$

$$\ln \gamma_2 = -0.00888 \quad \gamma_2 = 0.9911$$

$$\ln \gamma_3 = -0.30934 \quad \gamma_3 = 0.7339$$

$$\ln \gamma_4 = 0.172688 \quad \gamma_4 = 1.1884$$

$$P_j^{sat} = \frac{P}{\sum_i \left(x_i \gamma_i / \Phi_i \right) \left(P_i^{sat} / P_j^{sat} \right)}$$

Select Acetic acid as j component from the set (i)

$$P_j^{sat} = 324.4535$$

Calculate Temperature

$$T = \frac{B_j}{A_j - \ln P_j^{sat}} - C_j \quad T = 92.13057$$

By Iterating

Calculated through trial and error

Table C.1:Bubble point temperature and vapor composition

Iteration number	Input temperature for Iteration	Y_1	Y_2	Y_3	Y_4	Output temperature of the Iteration
1	-	0.237007	0.938975	0.055173	0	98.28026
2	98.28026	0.19042	0.751245	0.054533	0	92.0349
3	92.0349	0.191055	0.75402	0.054985	0	92.13057
4	92.13057	0.191045	0.753976	0.054978	0	92.12905
5	92.12905	0.191045	0.753977	0.054978	0	92.12908
6	92.12908	0.191045	0.753977	0.054978	0	92.12908

Solving Algebraic equations

Assume

$$(A_1)_1 = 5000 \quad (A_0)_1 = 100 \quad \Delta t = 1\,\text{min}$$

Condenser holdup 100 moles assumed to be constant throughout the process.

Applying Euler method

$$(A_0)_{t+\Delta t} = \Delta t\,(V_1 - L_0 - D) + (A_0)_t$$

Let us say $V_1 = 90;$ $\quad L_0 / V_1 = 0.95;$

$$L_0 = 0.95 \times 90 = 85.5$$

$$D = V_1 - L_0$$

$$D = 90 - 85.5 = 4.5$$

$$(x_{0,i})_{t+\Delta t} = (x_{0,i})_t + \frac{\Delta t V_1}{A_0}(y_{1,i} - x_{0,i}) \quad + \quad \Delta t R_{0,i}$$

$$(x_{0,i})_2 = (x_{0,i})_1 + \frac{\Delta t V_1}{A_0}(y_{1,i} - x_{0,i}) \quad + \quad \Delta t R_{0,i}$$

$$R = \frac{\rho \sum x_i}{\left(\sum x_i M_i\right)}(K_f x_1 x_2 - K_r x_3 x_4)$$

Where $K_f = 4.76 \times 10^{-4} \, litre/gmol.\min$ (Mujtaba and Macchietto,1997).

$K_r = 1.63 \times 10^{-4} \, litre/gmol.\min$ (Mujtaba and Macchietto,1997).

$M_1 = 60.05 \quad M_2 = 46.068 \quad M_3 = 18.015 \quad M_4 = 88.105$

$$R = \frac{10^3 \times \left(4.76 \times 10^{-4} \times 0.45 \times 0.45 - 1.63 \times 10^{-4} \times 0.1 \times 0\right)}{(0.45 \times 60.05 + 0.45 \times 46.068 + 0.1 \times 18.01528 + 0 \times 88.105)} = 0.00195$$

$\Delta H_r = -14.5 kJ/mol$ (Glessler et al., 2001).

Calculation of Condenser composition at t=1minute

$$(x_{0,1})_2 = 0.45 + 0.9 \times (0.191045 - 0.45) \quad + \quad 0.0019 = \underline{0.2150}$$

$$(x_{0,2})_2 = (x_{0,2})_1 + \frac{\Delta t V_1}{A_0}(y_{1,2\backslash} - x_{0,2}) \quad + \quad \Delta t R_{0,2}$$

$$(x_{0,2})_2 = 0.45 + 0.9 \times \times (0.753977 - 0.45) \quad - 0.00195 = \underline{0.7216}$$

$$(x_{0,3})_2 = (x_{0,3})_1 + \frac{\Delta t V_1}{A_0}(y_{1,3} - x_{0,3}) \quad + \quad \Delta t R_{0,3}$$

$$(x_{0,3})_2 = 0.1 + 0.9 \times (0.054978 - 0.1) \quad + \quad 0.0019 = \underline{0.0614}$$

$$(x_{0,4})_2 = (x_{0,4})_1 + \frac{\Delta t V_1}{A_0}(y_{1,4} - x_{0,4}) \quad + \quad \Delta t R_{0,4}$$

$$(x_{0,4})_2 = 0.9 \times (0. - 0) \quad + \quad 0.0019 = \underline{0.0019}$$

Calculation of reactor composition at t=1minute

$$(x_{1,i})_{t+\Delta t} = (x_{1,i})_t + \frac{\Delta t\, L_0}{A_1}(x_{0,i} - x_{1,i}) \;+\; \frac{\Delta t\, V_1}{A_1}(x_{1,i} - y_{1,i}) + R_{1,i}\Delta t$$

$$(x_{1,i})_2 = (x_{1,i})_1 + \frac{\Delta t\, L_0}{A_1}(x_{0,i} - x_{1,i}) \;+\; \frac{\Delta t\, V_1}{A_1}(x_{1,i} - y_{1,i}) + R_{1,i}\Delta t$$

$$(x_{1,1})_2 = (x_{1,1})_1 + \frac{\Delta t\, L_0}{A_1}(x_{0,1} - x_{1,1}) \;+\; \frac{\Delta t\, V_1}{A_1}(x_{1,1} - y_{1,1}) + R_{1,1}\Delta t$$

$$(x_{1,1})_2 = 0.45 + 85.5\times10^{-3}(0.45 - 0.45) \;+ 90\times10^{-3}(0.45 - 0.191045) = \underline{\underline{0.4523}}$$

$$(x_{1,2})_2 = (x_{1,2})_1 + \frac{\Delta t\, L_0}{A_1}(x_{0,2} - x_{1,2}) \;+\; \frac{\Delta t\, V_1}{A_1}(x_{1,2} - y_{1,2}) + R_{1,2}\Delta t$$

$$(x_{1,2})_2 = 0.45 + 90\times10^{-3}(0.45 - 0.753977) = \underline{\underline{0.4473}}$$

$$(x_{1,3})_2 = (x_{1,2})_1 + \frac{\Delta t\, L_0}{A_1}(x_{0,3} - x_{1,3}) \;+\; \frac{\Delta t\, V_1}{A_1}(x_{1,3} - y_{1,3}) + R_{1,3}\Delta t$$

$$(x_{1,3})_2 = 0.1 + 85.5\times10^{-3}(0.1 - 0.1) \;+ 90\times10^{-3}(0.1 - 0.054978) = \underline{\underline{0.1004}}$$

$$(x_{1,4})_2 = (x_{1,4})_1 + \frac{\Delta t\, L_0}{A_1}(x_{0,3} - x_{1,3}) \;+\; \frac{\Delta t\, V_1}{A_1}(x_{1,3} - y_{1,3}) + R_{1,3}\Delta t$$

$$(x_{1,4})_2 = 0.9\times10^{-2}(0 - 0) = \underline{\underline{0}}$$

Calculation of condenser heat load

$$(H_{L,0})_{t+\Delta t} = (H_{L,0})_t + \frac{\Delta t\, V_1}{A_0}(H_{V,1} - H_{L,0}) + \Delta t R_0 \Delta H_r - \frac{\Delta t\, Q_0}{A_0}$$

$$(H_{L,0})_2 = (H_{L,0})_1 + \frac{\Delta t\, V_1}{A_0}(H_{V,1} - H_{L,0}) + \Delta t R_0 \Delta H_r - \frac{\Delta t\, Q_0}{A_0}$$

$$H_{L,0}(1) = T_0(1) \times \left(x_{0,1}(1) \times cp1 + x_{0,2}(1) \times cp2 + x_{0,3}(2) \times cp3 + x_{0,4}(2) \times cp4 \right)$$

$$H_{L,0}(1) = 92.129 \times \left(0.45 \times 123.1 + 0.45 \times 125.305 + 0.1 \times 75.3759 + 0 \times 170 \right)$$

$$H_{L,0}(1) = \underline{10993 J / mol}$$

$$H_{V,1}(t) = y_{1,1}(t) \times cp1 \times T_1(t) + hfg1 \times y_{1,1}(t) + y_{1,2}(t) \times cp2 \times T_1(t) + \dots$$
$$hfg2 \times y_{1,2}(t) + y_{1,3}(t) \times cp3 \times T_1(t) + hfg3 \times y_{1,3}(t) + y_{1,4}(t) \times cp4 \times T_1(t) + hfg4 \times y_{1,4}(t)$$

$$H_{V,1}(1) = 92.129 \times \left(0.1910 \times 123.1 + 0.7539 \times 125.305 + 0.054978 \times 75.3759 + 0 \times 170 \right) + \dots$$
$$\left(24140 \times .1910 + 39388 \times 0.7539 + 0.0549 \times 40715 + 31940 \times 0 \right)$$

$$H_{V,1}(1) = \underline{47805 J / mol}$$

$$T_0(2) = 84.1866 \quad x_{01}(2) = 0.215 \quad x_{02}(2) = 0.7217 \quad x_{03}(2) = 0.0614 \quad x_{04}(2) = 0.0019$$

$$H_{L,0}(2) = T_0(2) \times \left(x_{0,1}(2) \times cp1 + x_{02}(2) \times cp2 + x_{0,3}(2) \times cp3 + x_{0,4}(2) \times cp4 \right)$$

$$H_{L,0}(2) = \underline{10259 J / mol}$$

$$T_1(2) = 92.3066 \quad x_{11}(2) = 0.4527 \quad x_{12}(2) = 0.4426 \quad x_{13}(2) = 0.1028 \quad x_{14}(2) = 0.0019$$

$$Q_0(t) = \frac{A_0(t)\left(H_{L,0}(t) - H_{L,0}(t + \Delta t)\right)}{\Delta t} + V_1\left(\left(H_{V,1}(t) - H_{L,0}(t)\right)\right) + A_0(t) \times R_0(t) \times \Delta H_r$$

$$Q_0(1) = \frac{100 \times (10993 - 10259)}{1} + 90 \times \left(47805 - 10259 \right) + 100 \times 0.00195 \times 14500$$

$$Q_0(1) = \underline{3455367 J / \min}$$

Calculation of reactor heat load

$$(H_{L,1})_{t+\Delta t} = (H_{L,1})_t + \frac{\Delta t\, Q_1}{A_1} - \frac{\Delta t\, L_0}{A_1}(H_{L,1} - H_{L,0}) - \frac{\Delta t\, V_1}{A_1}(H_{V,1} - H_{L,1}) + \Delta t\, R_1 \Delta H_r$$
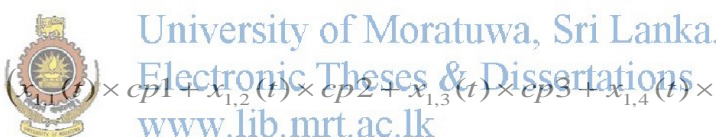
$$(H_{L,1})_2 = (H_{L,1})_1 + \frac{\Delta t\, Q_1}{A_1} - \frac{\Delta t\, L_0}{A_1}(H_{L,1} - H_{L,0}) - \frac{\Delta t\, V_1}{A_1}(H_{V,1} - H_{L,1}) + \Delta t\, R_1 \Delta H_r$$

$$H_{L,1}(t) = T_1(t) \times \left(x_{1,1}(t) \times cp1 + x_{1,2}(t) \times cp2 + x_{1,3}(t) \times cp3 + x_{1,4}(t) \times cp4\right)$$

$$H_{L,1}(1) = T_1(1) \times \left(x_{1,1}(1) \times cp1 + x_{1,2}(1) \times cp2 + x_{1,3}(1) \times cp3 + x_{1,4}(1) \times cp4\right)$$

$$H_{L,1}(1) = 92.129 \times \left(0.45 \times 123.1 + 0.45 \times 125.305 + 0.1 \times 75.3759 + 0 \times 170\right)$$

$$H_{L,1}(1) = \underline{10993 J/mol}$$

$$H_{L,1}(t) = T_1(t) \times \left(x_{1,1}(t) \times cp1 + x_{1,2}(t) \times cp2 + x_{1,3}(t) \times cp3 + x_{1,4}(t) \times cp4\right)$$

$$H_{L,1}(2) = T_1(2) \times \left(x_{1,1}(2) \times cp1 + x_{1,2}(2) \times cp2 + x_{1,3}(2) \times cp3 + x_{1,4}(2) \times cp4\right)$$

$$H_{L,1}(2) = 92.3066 \times \left(0.4527 \times 123.1 + 0.4426 \times 125.305 + 0.1028 \times 75.3759 + 0.0019 \times 170\right)$$

$$H_{L,1}(2) = \underline{\underline{11008\ J/mol}}$$

$$Q_1(t) = \frac{A_1(t)\left(H_{L,1}(t+\Delta t) - H_{L,1}(t)\right)}{\Delta t} + L_0\left(H_{L,1}(t) - H_{L,0}(t)\right) + V_1\left(H_{V,1}(t) - H_{L,1}(t)\right) + A_1(t) \times R_1(t) \times \Delta H_r$$

$$Q_1(1) = \frac{A_1(1)\left(H_{L,1}(2) - H_{L,1}(1)\right)}{\Delta t} + L_0\left(H_{L,1}(1) - H_{L,0}(1)\right) + V_1\left(H_{V,1}(1) - H_{L,1}(1)\right) + A_1(t) \times R_1(t) \times \Delta H_r$$

$$Q_1(1) = \frac{5000 \times (11008 - 10993)}{1} + 85.5 \times (10993 - 10993) + 90 \times (47805 - 10993) + 5000 \times 0.00195 \times 1450$$

Appendix D:

M file for solving algebraic equations in reactive distillation modeling

```matlab
% This M file simulates batch reactive distillation column for acetic acid
esterification
Reflux=19; %Reflux can be specified
R=Reflux;
V1=90;    %V1 can be specified
L0OverV1=0.95;
L0=V1*L0OverV1;
D=L0/R;
A1(1)=5000;  % initial molar holdup of reactor
A0(1)=100;    % A0 can be specified initial molar hold up of condenser
% 1-Acetic acid 2-Ethanol 3-Water 4-Ethyl Acetate
x01(1)=0.45;x02(1)=0.45;x03(1)=0.1;x04(1)=0;  % xoi can be specified,molar
fraction of condenser
x11(1)=0.45;x12(1)=0.45;x13(1)=0.1;x14(1)=0;  % molar fraction of reactor

i=1:4;
M(i)=[60.05 46.068 18.01528 88.105]; % Molecular mass of substances
kf=4.76*10^-4;
kr=1.63*10^-4;  % rate constants

cp1=123.1;cp2=125.3050;cp3=75.3759;cp4=170; %specific heat capacity J/mol.K
hfg1=24140;hfg2=39388;hfg3=40715;hfg4=31940; % latent heat of vaporization
J/mol
deltaH=14500; %heat of reaction,J/mol

delT=1;         % step size
totaltime=1050;

ap(1)=0;
qt=0;

for t=1:delT:totaltime % time interval,min

rho=1000;  % density




R0(t)=rho*(x01(t)+x02(t)+x03(t)+x04(t))*(kf*x01(t)*x02(t)-
kr*x03(t)*x04(t))/(x01(t)*M(1)+x02(t)*M(2)+x03(t)*M(3)+x04(t)*M(4));% rate
of reaction,condenser


R1(t)=rho*(x11(t)+x12(t)+x13(t)+x14(t))*(kf*x11(t)*x12(t)-
kr*x13(t)*x14(t))/(x11(t)*M(1)+x12(t)*M(2)+x13(t)*M(3)+x14(t)*M(4));%rate
of reaction boiler

a=[x11(t)  x12(t)  x13(t)  x14(t)];% molar fraction of components in reactor
[T1(t) y11(t) y12(t) y13(t) y14(t)]=bubble_point(760,a);

b=[x01(t)  x02(t)  x03(t)  x04(t)];% molar fraction of components in condenser
[T0(t) y01(t) y02(t) y03(t) y04(t)]=bubble_point(760,b);%calls bubble point
function
```

```matlab
A0(t+delT)=A0(t)+delT*(V1-L0-D);% molar holdup of condenser at time=t+delT
min

A1(t+delT)=A1(t)+delT*(L0-V1);% molar holdup of reboiler at time=t+delT min




x01(t+delT)=x01(t)+delT*V1*(y11(t)-x01(t))/A0(t)-delT*R0(t);
x02(t+delT)=x02(t)+delT*V1*(y12(t)-x02(t))/A0(t)-delT*R0(t);
x03(t+delT)=x03(t)+delT*V1*(y13(t)-x03(t))/A0(t)+delT*R0(t);
x04(t+delT)=x04(t)+delT*V1*(y14(t)-x04(t))/A0(t)+delT*R0(t);




x11(t+delT)=x11(t)+delT*L0*(x01(t)-x11(t))/A1(t)+delT*V1*(x11(t)-
y11(t))/A1(t)-delT*R1(t);
x12(t+delT)=x12(t)+delT*L0*(x02(t)-x12(t))/A1(t)+delT*V1*(x12(t)-
y12(t))/A1(t)-delT*R1(t);
x13(t+delT)=x13(t)+delT*L0*(x03(t)-x13(t))/A1(t)+delT*V1*(x13(t)-
y13(t))/A1(t)+delT*R1(t);
x14(t+delT)=x14(t)+delT*L0*(x04(t)-x14(t))/A1(t)+delT*V1*(x14(t)-
y14(t))/A1(t)+delT*R1(t);

ap(t+delT)=ap(t)+x04(t);% average product mole fraction
AP(t)=D*ap(t);%total product moles
totaldis(t)=5100-A1(t)-A0(t);%accumilated total distillate
EAcpercentage(t)=AP(t)*100./totaldis(t);%percentage of distillate in the
product

end
```
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```matlab
for t=1:totaltime-1
HL0(t)=T0(t)*(x01(t)*cp1+x02(t)*cp2+x03(t)*cp3+x04(t)*cp4);% molar enthalpy
of L0 flow, J/mole
HL0(t+delT)=T0(t+delT)*(x01(t+delT)*cp1+x02(t+delT)*cp2+x03(t+delT)*cp3+x04
(t+delT)*cp4);
HL1(t)=T1(t)*(x11(t)*cp1+x12(t)*cp2+x13(t)*cp3+x14(t)*cp4);% molar enthalpy
of reactor, J/mole
HL1(t+delT)=T1(t+delT)*(x11(t+delT)*cp1+x12(t+delT)*cp2+x13(t+delT)*cp3+x14
(t+delT)*cp4);

HV1(t)=y11(t)*cp1*T1(t)+hfg1*y11(t)+y12(t)*cp2*T1(t)+hfg2*y12(t)+y13(t)*cp3
*T1(t)+hfg3*y13(t)+y14(t)*cp4*T1(t)+hfg4*y14(t);% molar enthalpy of V1
flow,J/mole;
Q0(t)=A0(t)/delT*(HL0(t)-HL0(t+delT))+V1*(HV1(t)-
HL0(t))+A0(t)*R0(t)*deltaH; % condenser heat duty J/min
Q1(t)=A1(t)/delT*(HL1(t+delT)-HL1(t))+L0*(HL1(t)-HL0(t))+V1*(HV1(t)-
HL1(t))-A1(t)*R1(t)*deltaH; % Reboiler heat duty J/min

qt=qt+Q1(t);%total heat load of reactor J
end




Qt=qt/1000%total heat load reactor
Tb=(totaltime-1)/60%batch time
productionrate=AP(totaltime)/Tb%production rate moles/hr
```

Appendix E:

M file to calculate bubble point temperature

```matlab
function[T,y5,y6,y7,y8]=bubble_point(P,x)
%bubble point function calculates bubble point temperature
%and vapor phase composition , Input arguments
%(1)Acetic acid (2)Ethnol (3)Water (4)Ethyl acetate and PmmHg
%Output arguments bubble point temperature and vapor phase composition

i=1:4;
A(i)=[7.5596 8.20417 8.07131 7.2597];%Anotonie constants
B(i)=[1644.05 1642.89 1730.63 1369.41];
C(i)=[233.524 230.3 233.426 235.5];
y2(i)=[0 0 0 0];

Tsat(i)=B(i)./(A(i)-log10(P))-C(i); %Anotonie equation
Tapprox=sum(x(i).*Tsat(i));
Psat(i)=10.^(A(i)-(B(i)./(Tapprox+C(i))));

%Calculation of activity coefficient

% Calculating molar volumes
Vc(i)=[179.7 167 55.9 286];% Critical volume
Zc(i)=[0.211 0.24 0.229 0.255];%Critical Compressibility factor
Tc(i)=[592 513.9 647.1 523.3];%Critical temperature
Vsat(i)=Vc(i).*(Zc(i).^((1-(Tapprox+273.13)./Tc(i).^0.2857));
m=1:4;n=1:4;
a(m,n)=[1 -130.6527 2.0311749.2343.1901 6588.1981.1757 288.2011;403.1564
466.1059 1 1195.872 464.1529 28.8790 26981.1 1];
for m=1:4
for n=1:4
G(m,n)=(Vsat(n).*(exp(-a(m,n)./(8.314*(Tapprox+273.13))))))./Vsat(m);
end
end
for i=1:4
activity(i)=exp(1-log(x(1)*G(i,1)+x(2)*G(i,2)+x(3)*G(i,3)+x(4)*G(i,4))-
(x(1)*G(1,i)/(x(1)*G(1,1)+x(2)*G(1,2)+x(3)*G(1,3)+x(4)*G(1,4)))-
(x(2)*G(2,i)/(x(1)*G(2,1)+x(2)*G(2,2)+x(3)*G(2,3)+x(4)*G(2,4)))-
(x(3)*G(3,i)/(x(1)*G(3,1)+x(2)*G(3,2)+x(3)*G(3,3)+x(4)*G(3,4)))-
(x(4)*G(4,i)/(x(1)*G(4,1)+x(2)*G(4,2)+x(3)*G(4,3)+x(4)*G(4,4))));
end
i=1:4;
Pjsat=P*Psat(1)/sum(x(i).*activity(i).*Psat(i));
Temp1=B(1)./(A(1)-log10(Pjsat))-C(1);
P1sat(i)=10.^(A(i)-(B(i)./(Temp1+C(i))));
i=1:4;
y1(i)=x(i).*activity(i).*P1sat(i)./P;

Error_tolerance=0.0001;
old_guess=Tapprox;
new_guess=Temp1;

while abs(new_guess-old_guess)>Error_tolerance

old_guess=new_guess;
Temp1=old_guess;

Vsat2(i)=Vc(i).*(Zc(i).^((1-(Temp1+273.13)./Tc(i)).^0.2857));
```

```
for m=1:4
for n=1:4
G2(m,n)=(Vsat2(n).*(exp(-a(m,n)./(8.314*(Temp1+273.13))))))./Vsat2(m);
end
end
for i=1:4
activity2(i)=exp(1-
log(x(1)*G2(i,1)+x(2)*G2(i,2)+x(3)*G2(i,3)+x(4)*G2(i,4))-
(x(1)*G2(1,i)/(x(1)*G2(1,1)+x(2)*G2(1,2)+x(3)*G2(1,3)+x(4)*G2(1,4)))-
(x(2)*G2(2,i)/(x(1)*G2(2,1)+x(2)*G2(2,2)+x(3)*G2(2,3)+x(4)*G2(2,4)))-
(x(3)*G2(3,i)/(x(1)*G2(3,1)+x(2)*G2(3,2)+x(3)*G2(3,3)+x(4)*G2(3,4)))-
(x(4)*G2(4,i)/(x(1)*G2(4,1)+x(2)*G2(4,2)+x(3)*G2(4,3)+x(4)*G2(4,4))));
end
i=1:4;
P2jsat=P*P1sat(1)/sum(x(i).*activity2(i).*P1sat(i));
Temp2=B(1)./(A(1)-log10(P2jsat))-C(1);
P2sat(i)=10.^(A(i)-(B(i)./(Temp2+C(i))));
i=1:4;
y2(i)=x(i).*activity2(i).*P2sat(i)./P;

new_guess=Temp2;
end

T=new_guess;
y5=y2(1);
y6=y2(2);
y7=y2(3);
y8=y2(4);
```

Appendix F

M file for heterogeneous catalyst

```
% This M file simulates batch reactive distillation column for acetic acid
% esterification with heterogeneous catalyst
Reflux=19; %Reflux can be specified
R=Reflux;
V1=90;    %V1 can be specified
L0OverV1=0.95;
L0=V1*L0OverV1;
D=L0/R;
A1(1)=5000;  % initial molar holdup of reactor
A0(1)=100;   % A0 can be specified initial molar hold up of condenser
% 1-Acetic acid 2-Ethanol 3-Water 4-Ethyl Acetate
x01(1)=0.5;x02(1)=0.5;x03(1)=0;x04(1)=0;  % xoi can be specified,molar
fraction of condenser
x11(1)=0.45;x12(1)=0.45;x13(1)=0.1;x14(1)=0;  % molar fraction of reactor

i=1:4;
M(i)=[60.05 46.068 18.01528 88.105]; % Molecular mass of substances
k=5.0*10^-4;
kw=3.2*10^-2;
ke=1.3*10^-1;  % rate constants

cp1=123.1;cp2=125.3050;cp3=75.3759;cp4=170; %specific heat capacity J/mol.K
hfg1=24140;hfg2=39388;hfg3=40715;hfg4=31940; % latent heat of vaporization
J/mol
deltaH=14500; %heat of reaction, J/mol


delT=1;       % step size
totaltime=1050;   % minutes

ap(1)=0;
qt=0;

for t=1:delT:totaltime % time interval,min

rho=1000;  % density




R0(t)=rho^2*265.28*k*(x01(t)*x02(t)-
(x03(t)*x04(t)/1.907))/((x01(t)*M(1)+x02(t)*M(2)+x03(t)*M(3)+x04(t)*M(4))^2
+kw*x03(t)*rho+ke*x02(t)*rho)^2;% rate of reaction,condenser


R1(t)=rho^2*13264*k*(x11(t)*x12(t)-
(x13(t)*x14(t)/1.907))/((x11(t)*M(1)+x12(t)*M(2)+x13(t)*M(3)+x14(t)*M(4))^2
+kw*x13(t)*rho+ke*x12(t)*rho)^2;%rate of reaction boiler

a=[x11(t)  x12(t)  x13(t)  x14(t)];% molar fraction of components in reactor
[T1(t) y11(t) y12(t) y13(t) y14(t)]=bubble_point(760,a);

b=[x01(t)  x02(t)  x03(t)  x04(t)];% molar fraction of components in condenser
[T0(t) y01(t) y02(t) y03(t) y04(t)]=bubble_point(760,b);%calls bubble point
function

A0(t+delT)=A0(t)+delT*(V1-L0-D);% molar holdup of condenser at time=t+delT
min
```
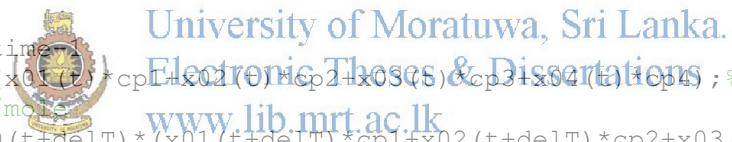
```matlab
A1(t+delT)=A1(t)+delT*(L0-V1);% molar holdup of reboiler at time=t+delT min




x01(t+delT)=x01(t)+delT*V1*(y11(t)-x01(t))/A0(t)-delT*R0(t)/A0(t);
x02(t+delT)=x02(t)+delT*V1*(y12(t)-x02(t))/A0(t)-delT*R0(t)/A0(t);
x03(t+delT)=x03(t)+delT*V1*(y13(t)-x03(t))/A0(t)+delT*R0(t)/A0(t);
x04(t+delT)=x04(t)+delT*V1*(y14(t)-x04(t))/A0(t)+delT*R0(t)/A0(t);




x11(t+delT)=x11(t)+delT*L0*(x01(t)-x11(t))/A1(t)+delT*V1*(x11(t)-
y11(t))/A1(t)-delT*R1(t)/A1(t);
x12(t+delT)=x12(t)+delT*L0*(x02(t)-x12(t))/A1(t)+delT*V1*(x12(t)-
y12(t))/A1(t)-delT*R1(t)/A1(t);
x13(t+delT)=x13(t)+delT*L0*(x03(t)-x13(t))/A1(t)+delT*V1*(x13(t)-
y13(t))/A1(t)+delT*R1(t)/A1(t);
x14(t+delT)=x14(t)+delT*L0*(x04(t)-x14(t))/A1(t)+delT*V1*(x14(t)-
y14(t))/A1(t)+delT*R1(t)/A1(t);

ap(t+delT)=ap(t)+x04(t);% average product mole fraction
AP(t)=D*ap(t);%total product moles
totaldis(t)=5100-A1(t)-A0(t);%accumilated total distillate
EAcpercentage(t)=AP(t)*100./totaldis(t);%percentage of distillate in the
product
Conversion(t)=(50-A0(t).*x01(t))/50;
end



for t=1:totaltime-1
HL0(t)=T0(t)*(x01(t)*cp1+x02(t)*cp2+x03(t)*cp3+x04(t)*cp4);% molar enthalpy
of L0 flow, J/mole
HL0(t+delT)=T0(t+delT)*(x01(t+delT)*cp1+x02(t+delT)*cp2+x03(t+delT)*cp3+x04
(t+delT)*cp4);
HL1(t)=T1(t)*(x11(t)*cp1+x12(t)*cp2+x13(t)*cp3+x14(t)*cp4);% molar enthalpy
of reactor, J/mole
HL1(t+delT)=T1(t+delT)*(x11(t+delT)*cp1+x12(t+delT)*cp2+x13(t+delT)*cp3+x14
(t+delT)*cp4);

HV1(t)=y11(t)*cp1*T1(t)+hfg1*y11(t)+y12(t)*cp2*T1(t)+hfg2*y12(t)+y13(t)*cp3
*T1(t)+hfg3*y13(t)+y14(t)*cp4*T1(t)+hfg4*y14(t);% molar enthalpy of V1
flow,J/mole;
Q0(t)=A0(t)/delT*(HL0(t)-HL0(t+delT))+V1*(HV1(t)-
HL0(t))+A0(t)*R0(t)*deltaH; % condenser heat duty J/min
Q1(t)=A1(t)/delT*(HL1(t+delT)-HL1(t))+L0*(HL1(t)-HL0(t))+V1*(HV1(t)-
HL1(t))-A1(t)*R1(t)*deltaH; % Reboiler heat duty J/min

qt=qt+Q1(t);%total heat load of reactor J
end




Qt=qt/1000 %total heat load reactor
Tb=(totaltime-1)/60 %batch time
productionrate=AP(totaltime)/Tb %production rate moles/hr
```