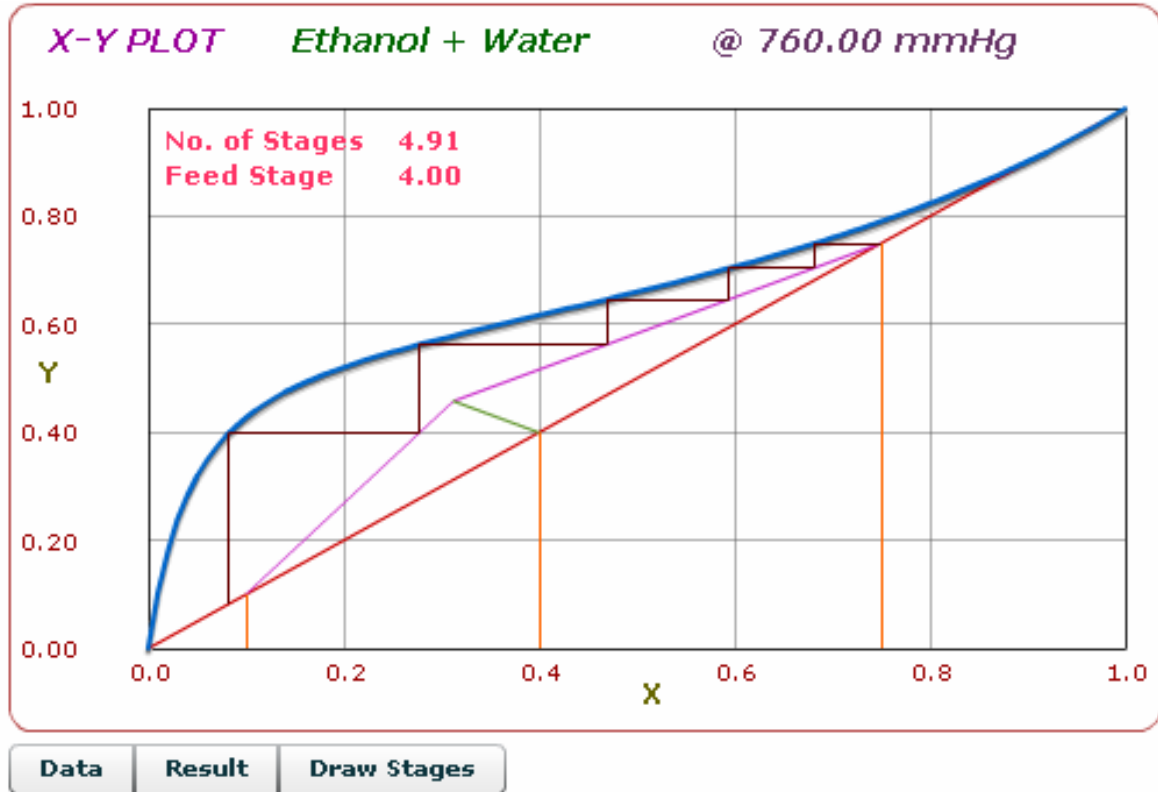


# BINARY VAPOR LIQUID EQUILIBRIUM (VLE) CALCULATOR



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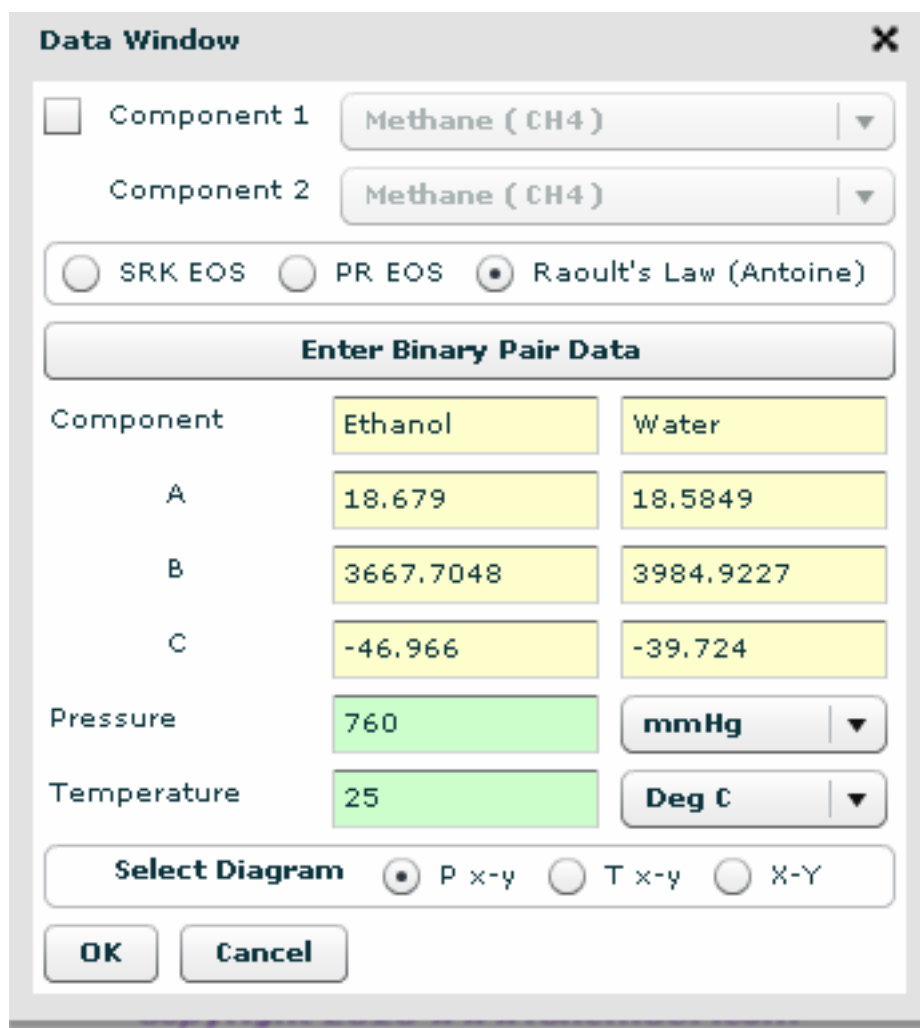
Binary Vapor Liquid Equilibrium (VLE) Calculator plots P x-y, T x-y, x-y diagrams for Binary Mixtures. It plots Mc-Cabe Thiele diagram and estimates number of stages required for Binary distillation.

It plots diagrams based on Soave Redlich Kwong (SRK) EOS, Peng Robinson (PR) EOS, Raoult's Law (Antoine Equation for Vapor Pressure) and Modified Raoult's Law with Wilson Interaction parameters.

To start the application Press Data Button



Following Data Window will appear



The Data Window dialog box contains the following fields and controls:

- Component 1: Methane (CH<sub>4</sub>)
- Component 2: Methane (CH<sub>4</sub>)
- EOS Selection:  SRK EOS,  PR EOS,  Raoult's Law (Antoine)
- Enter Binary Pair Data section:

Component	Ethanol	Water
A	18.679	18.5849
B	3667.7048	3984.9227
C	-46.966	-39.724
- Pressure: 760 mmHg
- Temperature: 25 Deg C
- Select Diagram:  P x-y,  T x-y,  X-Y
- Buttons: OK, Cancel

Select the appropriate EOS from SRK and PR or Raoult's Law.

For Raoult's law enter the Coefficients A, B, C for Antoine Vapor Pressure Equation in the following format –

$$\ln(P(\text{mmHg})) = A - \frac{B}{T(^{\circ}\text{K}) + C} \quad \text{----- (1)}$$

where Pressure P is in mmHg units and Temperature T is in  $^{\circ}\text{K}$  units. For SRK and PR EOS enter the Critical Temperature  $T_c$  ( $^{\circ}\text{K}$ ),  $P_c$  (Bar) and acentric factor  $\omega$ . Select the checkbox in front of Component 1 to select component properties from calculator's Databank.

Enter Pressure and Temperature at which plots are to be generated. Select the type of diagram to be made and press OK. A window will appear summarizing the data entered. Press OK to start plotting of the diagram.

Component	Ethanol	Water
<b>A</b>	<b>18.679</b>	<b>18.5849</b>
<b>B</b>	<b>3667.7048</b>	<b>3984.9227</b>
<b>C</b>	<b>-46.966</b>	<b>-39.724</b>

OK Cancel

To enter the binary interaction parameters Press the Button "Enter Binary Pair Data", Based on the type of model selected a window will appear for collection of data required for Binary Pair interaction.

For Raoult's Law following window will appear –

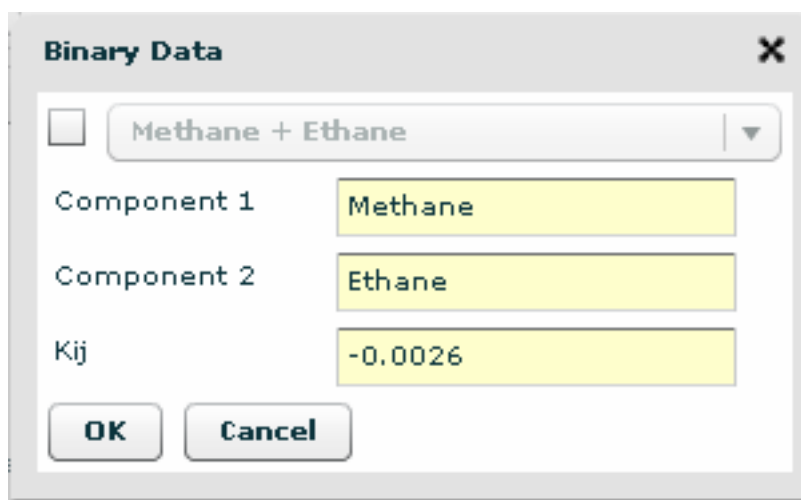
Component	Ethanol	Water
T <sub>c</sub> (K)	516.2	647.14
P <sub>c</sub> (Bar)	63.83	220.50042
ω	0.635	0.329
Z <sub>RA</sub>	0.2502	0.2338
A <sub>ij</sub>	325.0757	953.2792

Enter the Critical temperature  $T_c$  in °K,  $P_c$  in bar, acentric factor  $\omega$ ,  $Z_{RA}$  and Wilson interaction parameters  $A_{ij}$  in cal/mol.  $Z_{RA}$  is a pure component parameter for Rackett Liquid Volume correlation, it is used to estimate liquid molar volume of a pure component at different temperatures. Some binary pair information is provided in calculator's databank, Select the checkbox provided at top left corner and select the Binary Pair from the menu.

Press OK, so that calculator takes the new values provided. If a Binary Pair is selected from the Drop down menu at top, properties of the component in the main Data Window will also get updated to new binary pair selected.

After entering the remaining data press OK on main Data window it will show the summary of all data entered and will start plotting of the diagram.

For SRK and PR EOS following window will appear –



Binary Data

Methane + Ethane

Component 1: Methane

Component 2: Ethane

Kij: -0.0026

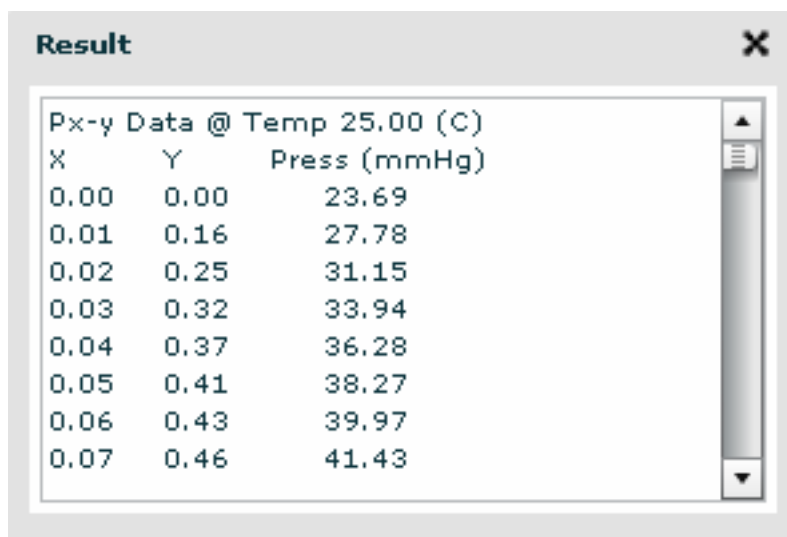
OK Cancel

Enter the interaction parameter  $K_{ij}$  for the binary components. To select the data from calculator's databank, select the checkbox at top left corner and select the pair from drop down menu.

After entering of data or selection of a pair Press OK so that calculator takes the values of binary interaction parameters.

*Note – If value for  $A_{ij}$  for any component or  $K_{ij}$  is left blank or provided 0, calculator will not consider interaction effects.*

For viewing results Press “Result” button. A Result window will appear showing data for 100 points.

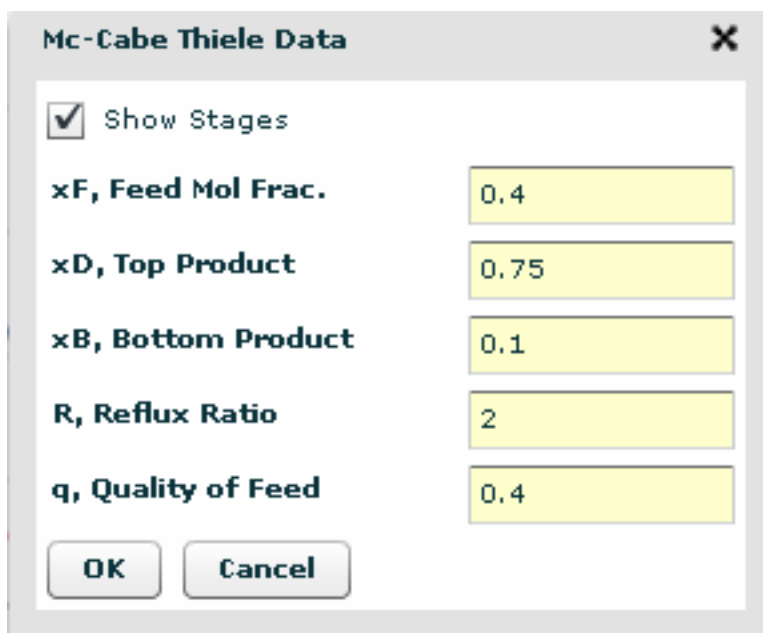


Result

Px-y Data @ Temp 25.00 (C)

X	Y	Press (mmHg)
0.00	0.00	23.69
0.01	0.16	27.78
0.02	0.25	31.15
0.03	0.32	33.94
0.04	0.37	36.28
0.05	0.41	38.27
0.06	0.43	39.97
0.07	0.46	41.43

For plotting of Mc-Cabe Thiele diagram press “Draw Stages” button, A Mc-Cabe Thiele Data window will appear.



The image shows a dialog box titled "Mc-Cabe Thiele Data" with a close button (X) in the top right corner. The dialog contains a checked checkbox labeled "Show Stages". Below this are five input fields with corresponding labels: "xF, Feed Mol Frac." with value 0.4, "xD, Top Product" with value 0.75, "xB, Bottom Product" with value 0.1, "R, Reflux Ratio" with value 2, and "q, Quality of Feed" with value 0.4. At the bottom of the dialog are two buttons: "OK" and "Cancel".

Parameter	Value
xF, Feed Mol Frac.	0.4
xD, Top Product	0.75
xB, Bottom Product	0.1
R, Reflux Ratio	2
q, Quality of Feed	0.4

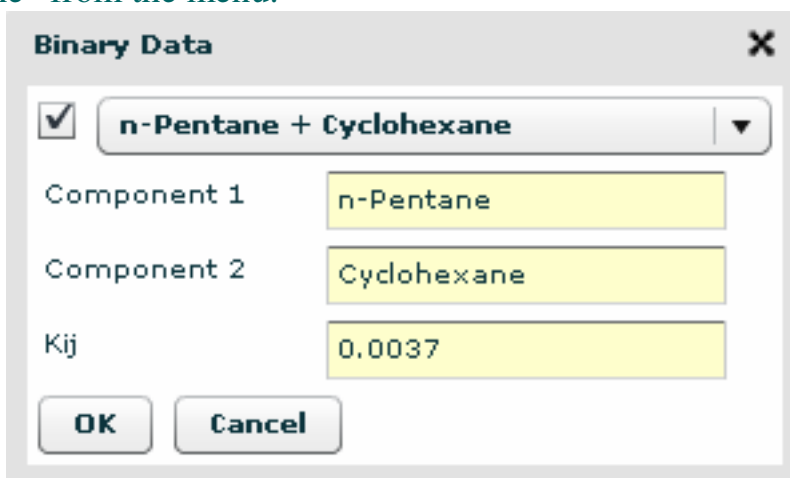
Enter the desired data and press OK to start plotting of Mc-Cabe Thiele Diagram.

### Example

A T<sub>x</sub>-y Plot is to be made for a binary mixture of n-Pentane and Cyclohexane using Peng Robinson EOS at 2 bar Pressure.

### Solution

Press “Data” Button to bring Data Window, Select “PR EOS” and Press “Enter Binary Pair Data” button to bring Binary Data Window. Select the checkbox at top corner and select the binary pair of “n-Pentane + Cyclohexane” from the menu.



**Binary Data**

n-Pentane + Cyclohexane

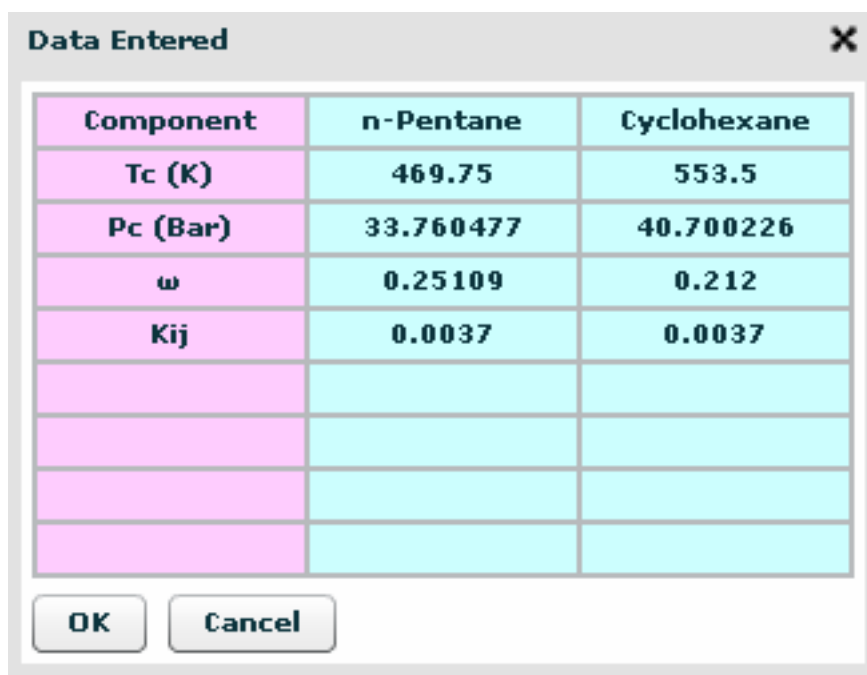
Component 1: n-Pentane

Component 2: Cyclohexane

Kij: 0.0037

OK Cancel

Press OK to return to Data Window. Enter the Pressure 2 and change the units to bar. Press OK and see the summary before starting plotting of the diagram.

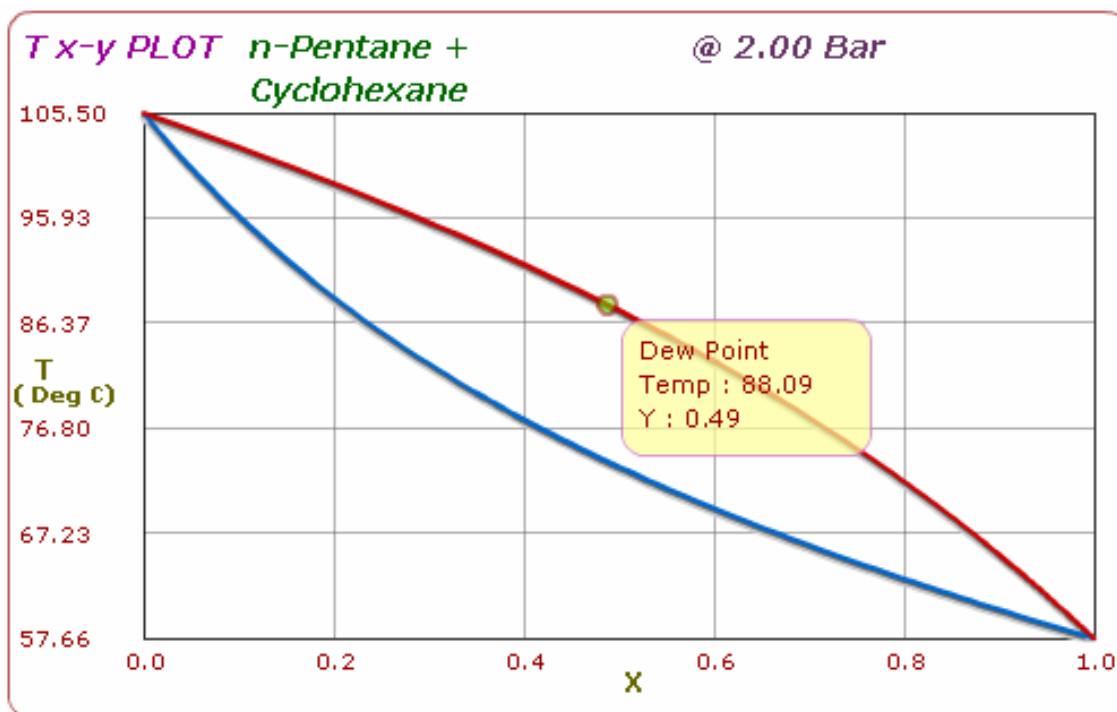


**Data Entered**

Component	n-Pentane	Cyclohexane
T <sub>c</sub> (K)	469.75	553.5
P <sub>c</sub> (Bar)	33.760477	40.700226
ω	0.25109	0.212
K <sub>ij</sub>	0.0037	0.0037

OK Cancel

Following window will appear with Tx-y plot for binary mixture of n-Pentane and Cyclohexane.



Press the Result button to get tabular data, to select data press “Ctrl+A”, then press “Ctrl+C” to copy data to clipboard, then open any text editor or spreadsheet and press “Ctrl+V” to paste data from clipboard.

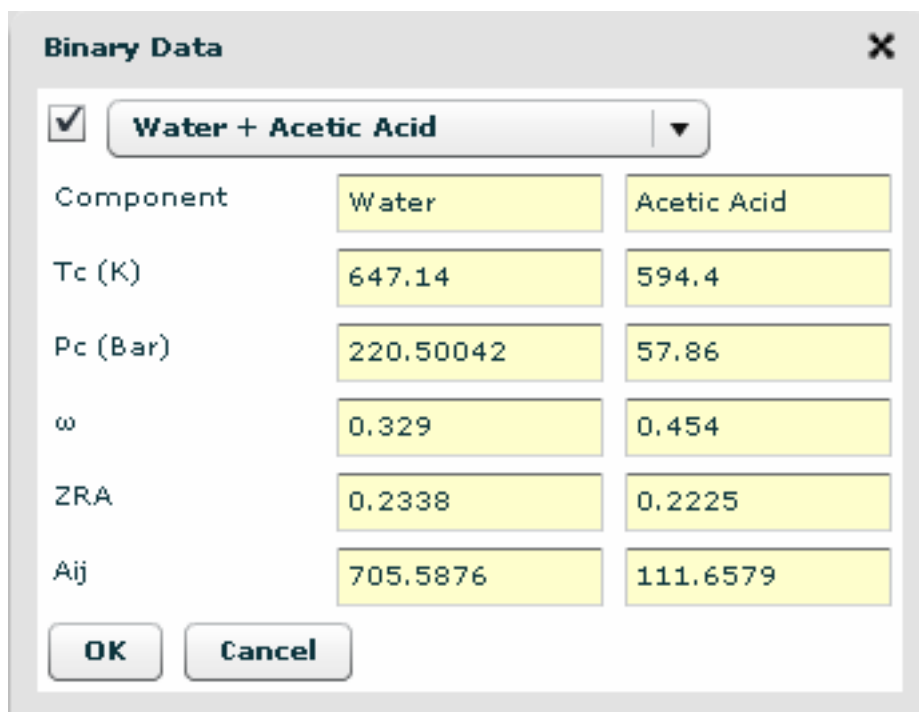
Tx-y Data @ Press 2.00 (Bar)		
X	Y	Temp (C)
0.00	0.00	105.50
0.01	0.03	104.46
0.02	0.07	103.45
0.03	0.10	102.47
0.04	0.13	101.50
0.05	0.16	100.56
0.06	0.18	99.64
0.07	0.21	98.75

**Example**

Plot x-y Diagram for a Binary mixture of Water and Acetic Acid at 2 bar pressure. Calculate the number of stages required for separation of a mixture containing 0.4 mol fraction of water with a top product containing 0.85 mol fraction of water and bottom product containing 0.1 mol fraction of water with Reflux ratio of 2 and quality of feed 0.4.

**Solution**

Press “Data” Button to bring Data Window, Select “Raoult’s Law” and Press “Enter Binary Pair Data” button to bring Binary Data Window. Select the checkbox at top corner and select the binary pair of “Water + Acetic Acid” from the menu.



The screenshot shows a dialog box titled "Binary Data" with a close button (X) in the top right corner. A checkbox is checked, and a dropdown menu is set to "Water + Acetic Acid". Below this, there are two columns of input fields for "Water" and "Acetic Acid". The fields contain the following values:

Component	Water	Acetic Acid
Tc (K)	647.14	594.4
Pc (Bar)	220.50042	57.86
$\omega$	0.329	0.454
ZRA	0.2338	0.2225
Aij	705.5876	111.6579

At the bottom of the dialog box, there are two buttons: "OK" and "Cancel".

Press OK Button and return to the Data window. Select x-y Diagram and change the pressure to 2 bar and press OK to see summary window.

**Data Entered** ✕

Component	Water	Acetic Acid
A	18.5849	18.469
B	3984.9227	4457.8276
C	-39.724	-14.609
Tc (K)	647.14	594.4
Pc (Bar)	220.50042	57.86
$\omega$	0.329	0.454
ZRA	0.2338	0.2225
Aij	705.5876	111.6579

OK Cancel

Press OK to start plotting of x-y Diagram. To calculate Mc-Cabe Thiele stages press “Draw Stages” button and enter the data as following

**Mc-Cabe Thiele Data** ✕

Show Stages

**x<sub>F</sub>, Feed Mol Frac.**

**x<sub>D</sub>, Top Product**

**x<sub>B</sub>, Bottom Product**

**R, Reflux Ratio**

**q, Quality of Feed**

OK Cancel

Press OK to start plotting of number of stages required for separation and feed stage.

