Use the Peng-Robinson Equation of State and data in the back of S&VN 7th ed. (reproduced below) to determine:

1. 10 points
The vapor pressure of pure benzene and toluene at 250ºC in bar.

2. 30 points
The fugacity (in bar) of pure benzene and pure toluene at 250ºC and 15 bar total pressure.

3. 30 points
The fugacity (in bar) of pure liquid benzene and pure liquid toluene at 250ºC and 30 bar total pressure.

4. 30 points
The fugacities (in bar) of benzene and toluene in a 40/60 mole % mixture when T = 250ºC and P=15 bar.

Instructions for submitting the project: Use Excel to solve the problem. Each student should start with a blank worksheet in preparing their solution. Turn in a paper solution similar to an exam format. Show intermediate work and results as the problem parts are solved, and organize your solution logically. Your Excel sheet should parallel your hardcopy solution. Be sure to include comments on the sheet and include references to the parts of the problem you are working. Save the Excel sheet as “Project1-FirstName-LastName.xlsx” and email it to me before class the date it is due with the subject line: “ChE3063 Project 1 Solution”. Submit your paper solution at the beginning of class the date it is due.

The Peng-Robinson Equation of State:

\[ P = \frac{RT}{v - b} - \frac{a}{v(v + b) + b(v - b)} \]

\[ \alpha^{0.5} = 1 + \kappa(1 - T_r^{0.5}) \]
\[ \kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2 \]

\[ a = \frac{0.45724 R^2 T_c^2 \alpha}{P_c} \]

\[ b = \frac{0.07780 RT_c}{P_c} \]
also, for shorthand for the P-R equation, use:

\[
A = \frac{aP}{R^2T^2} \\
B = \frac{bP}{RT}
\]

Mixing rules:

\[
a = \sum_i \sum_j y_i y_j a_{ij}
\]

\[
b = \sum_i y_i b_i
\]

\[
a_{ij} = (1 - \delta_{ij})a_i^{0.5}a_j^{0.5}
\]

where \(\delta_{ij}\) is an empirical constant for the benzene/toluene mixture:

\[
\delta_{ii} = 0 \\
\delta_{ij} = 0.01
\]

Polynomial form:

\[
z^3 - (1 - B)z^2 + (A - 3B^2 - 2B)z - (AB - B^2 - B^3) = 0
\]

Fugacity coefficient for the mixture:

\[
\ln\left(\frac{f_i}{y_i P}\right) = \ln(\phi_i) = \\
\frac{b_1}{b} (z - 1) - \ln(z - B) - \frac{A}{2\sqrt{2}B} \left(\frac{2\sum_j y_j a_{1j}}{a} - \frac{b_1}{b}\right) \ln\left(\frac{z + 2.414B}{z - 0.414B}\right)
\]

Fugacity coefficient for the pure component:

\[
\ln(f / P) = \ln(\phi) = (z - 1) - \ln(z - B) - \left(\frac{A}{2\sqrt{2}B}\right) \ln\left(\frac{z + 2.414B}{z - 0.414B}\right)
\]

Data:

<table>
<thead>
<tr>
<th></th>
<th>Benzene</th>
<th>Toluene</th>
</tr>
</thead>
<tbody>
<tr>
<td>MW (g/mole)</td>
<td>78.114</td>
<td>92.141</td>
</tr>
<tr>
<td>(T_c), K</td>
<td>562.1</td>
<td>591.8</td>
</tr>
<tr>
<td>(P_c), bar</td>
<td>48.98</td>
<td>41.06</td>
</tr>
<tr>
<td>(z_c)</td>
<td>0.271</td>
<td>0.264</td>
</tr>
<tr>
<td>(\omega)</td>
<td>0.210</td>
<td>0.262</td>
</tr>
</tbody>
</table>
### Constants for Antoine vapor pressure equation

<table>
<thead>
<tr>
<th></th>
<th>Value 1</th>
<th>Value 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>13.7819</td>
<td>13.9320</td>
</tr>
<tr>
<td>B</td>
<td>2726.81</td>
<td>3056.96</td>
</tr>
<tr>
<td>C</td>
<td>217.572</td>
<td>217.625</td>
</tr>
</tbody>
</table>

\[
\ln(P_{Sat}) = A - \frac{B}{t + C}
\]

where:

- \( P \) is in kPa
- \( t \) is in °C