Preliminary selection for VLE (without azeotrope)

methanol + water

Model:
NRTL with the following parameters:
Non-randomness parameter: 0.1
Dimensionless interaction parameters (form: $A + B/T$):

\[
\begin{array}{ll}
A & B \\
1 & 9.23811 \quad -2432.61 \\
2 & -5.70743 \quad 1538.74 \\
\end{array}
\]

0.1 MPa pressure as an example
butane + propane

Model:
Peng-Robinson equation with the following parameters:
Parameters:
\[ k_{12} = k_{21} = -0.00291821 \]

A few literature examples:


Phase boundary pressure [L, G] - Original Peng-Robinson (Non-translated)
butane + propane


General statistics:

Pressure deviations: 2% on average above T=320K; 4% on average at 240 K (the points with larger deviations are from two unreliable sources)
Gas mole fraction deviations: ±0.01 on average above T=320 K; 0.04 on average at T=240 K.
Isobars at 353-383 K
Model: NRTL with the following parameters:
Non-randomness parameter: 0.1
Dimensionless interaction parameters (form: A + B/T):

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.031069</td>
<td>453.935</td>
</tr>
<tr>
<td>2</td>
<td>0.280097</td>
<td>-428.145</td>
</tr>
</tbody>
</table>

0.1 MPa pressure as an example
Isotherms at 293-383 K

Model: NRTL with the following parameters:
Non-randomness parameter: 0.1

Dimensionless interaction parameters (form: A + B/T):

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-0.0885548</td>
<td>181.52</td>
</tr>
<tr>
<td>2</td>
<td>-0.527958</td>
<td>144.496</td>
</tr>
</tbody>
</table>

Phase boundary pressure [L, G] - NRTL/HOC: Percent deviation from equation
toluene + cyclohexane

Gas mole fraction of toluene - NRTL/HOC: Absolute deviation from equation
toluene + cyclohexane