CHEG325 Aspen Homework 4 Benzene-Toluene

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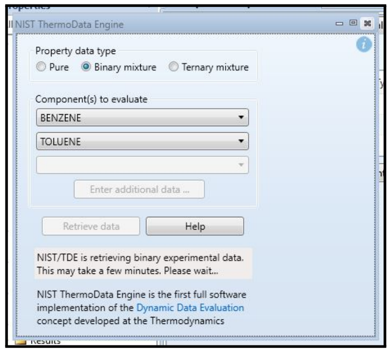
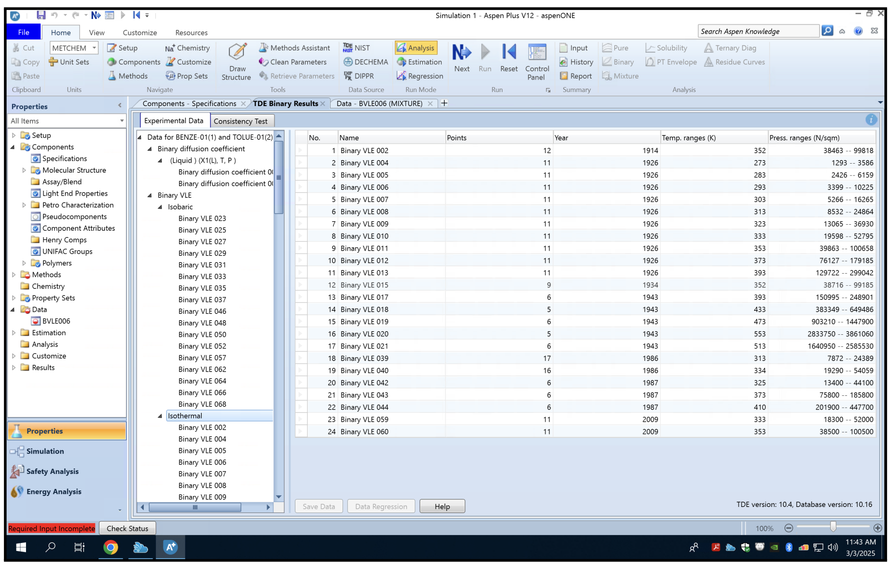
We obtained the data from Aspen's NIST TDE via adding Benzene and Toluene as components, selecting binary mixture in the TDE, and locating the isothermal VLE.





No.	Liquid mole fraction BENZE-01	Temperature (K)	Vapor mole fraction BENZE-01	Total pressure (N/sqm)
1	0	293.138	0	3399.7
2	0.1	293.138		4159.7
3	0.2	293.138		4932.9
4	0.3	293.138		5666.2
5	0.4	293.138		6466.1
6	0.5	293.138		7199.4
7	0.6	293.138		7879.4
8	0.7	293.138		8706
9	0.8	293.138		9265.9
10	0.9	293.138		9892.5
11	1	293.138	1	10225.8

The last piece of information we need is the pure component vapor pressures at this temperature. Luckily, our data set includes when the mole fraction is 0 and 1 so those points are the pure component vapor pressures. Now this data may be looked at inside a jupyter notebook on the next page.

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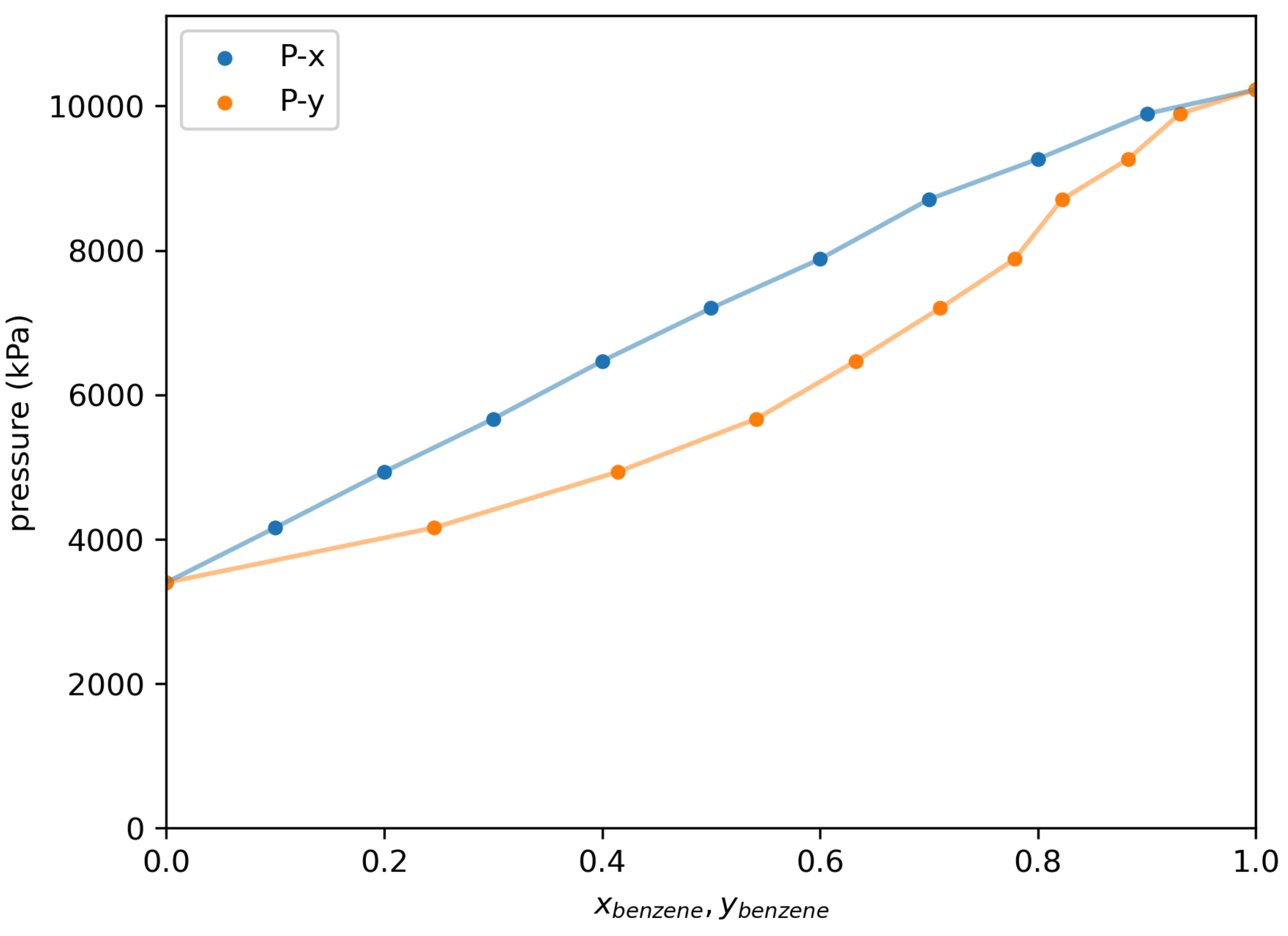
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt

df = pd.read_csv('data.txt', sep='\t')
pvap_benzene = float(df[df['benzene'] == 1.0]['pressure'].iloc[0])
pvap_toluene = float(df[df['toluene'] == 1.0]['pressure'].iloc[0])
df
```

	pressure	benzene	toluene
0	3399.7	0.0	1.0
1	4159.7	0.1	0.9
2	4932.9	0.2	0.8
3	5666.2	0.3	0.7
4	6466.1	0.4	0.6
5	7199.4	0.5	0.5
6	7879.4	0.6	0.4
7	8706.0	0.7	0.3
8	9265.9	0.8	0.2
9	9892.5	0.9	0.1
10	10225.8	1.0	0.0

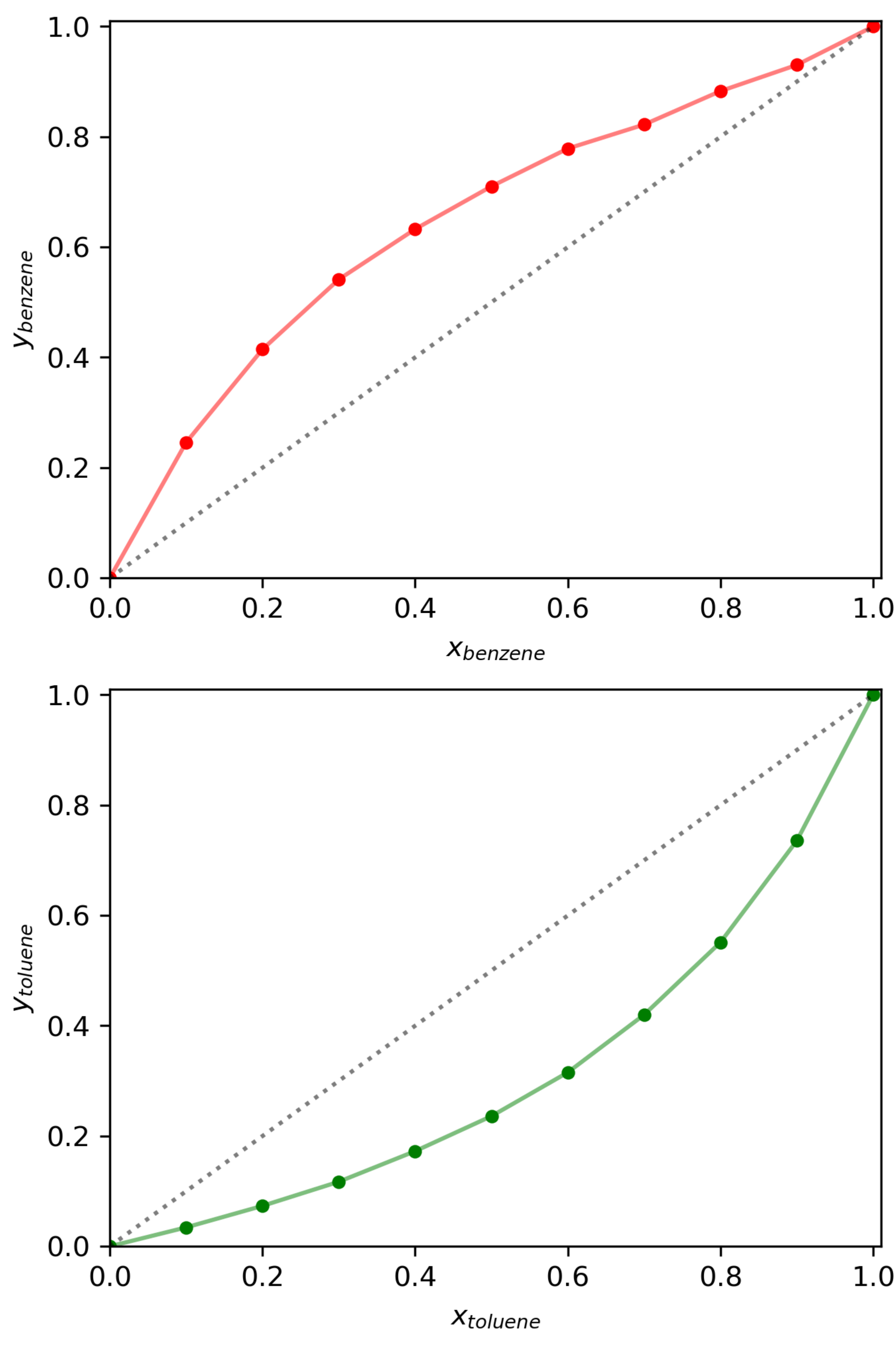
now calculate y_i using raults law

$$ x_i P^{}*i = y_i P*{}

```
fig, ax = plt.subplots(dpi=300,
                       subplot_kw={'xlim':(0,1),
                                   'ylim':(0, df['pressure'].max()*1.1),
                                   'ylabel':'pressure (kPa)',
                                   'xlabel':'$x_{benzene}, y_{benzene}$'})

P = df['pressure'] # kPa
xb = df['benzene']
xt = df['toluene']

yb = xb * pvap_benzene / P
yt = xt * pvap_toluene / P

ax.plot(xb, P, alpha=0.5, label='_nolegend_')
ax.scatter(xb, P, s=15, label='P-x')

ax.plot(yb, P, alpha=0.5, label='_nolegend_')
ax.scatter(yb, P, s=15, label='P-y')

ax.legend()
```




```
fig, (ax, ax2) = plt.subplots(2,dpi=300, figsize=(5,8),
                              subplot_kw={'xlim':(0,1.01),
                                          'ylim':(0, 1.01),
                                          'xlabel':'$x_{benzene}$',
                                          'ylabel':'$y_{benzene}$'})

ax.scatter(xb, yb, s=15, label='$y_{benzene}$', color='red')
ax.plot(xb, yb, alpha=0.5, color='red');
ax.plot(xb, xb, alpha=0.5, color='black', linestyle=':');

ax2.scatter(xt, yt, s=15, label='$y_{toluene}$', color='green')
ax2.plot(xt, yt, alpha=0.5, color='green');
ax2.plot(xb, xb, alpha=0.5, color='black', linestyle=':');
ax2.set(xlabel='$x_{toluene}$', ylabel='$y_{toluene}$')
```




```
# filler
```