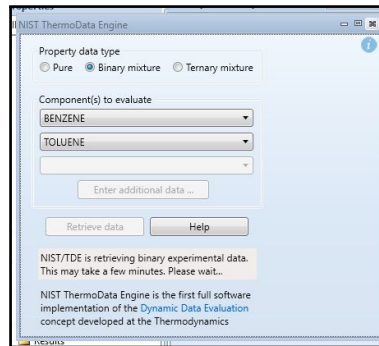


CHEG325 Aspen Homework 4 Benzene-Toluene

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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.	Name	Points	Year	Temp. ranges (K)	Press. ranges (N/sqm)
1	Binary VLE 002	12	1914	352	36483 - 99818
2	Binary VLE 004	11	1926	275	1293 - 3586
3	Binary VLE 005	11	1926	283	2426 - 6159
4	Binary VLE 006	11	1926	293	3399 - 10225
5	Binary VLE 007	11	1926	303	5266 - 16265
6	Binary VLE 008	11	1926	313	6532 - 24864
7	Binary VLE 009	11	1926	323	13065 - 36930
8	Binary VLE 010	11	1926	333	19598 - 52795
9	Binary VLE 011	11	1926	353	39863 - 100658
10	Binary VLE 012	11	1926	373	76127 - 179185
11	Binary VLE 013	11	1926	393	129732 - 299042
12	Binary VLE 015	9	1934	352	38716 - 99185
13	Binary VLE 017	6	1943	393	150095 - 248901
14	Binary VLE 018	5	1943	433	383149 - 649408
15	Binary VLE 019	6	1943	473	903210 - 1647900
16	Binary VLE 020	5	1943	553	2833750 - 3861060
17	Binary VLE 021	6	1943	513	1640950 - 2585350
18	Binary VLE 039	17	1986	313	7872 - 24389
19	Binary VLE 040	16	1986	334	10290 - 54059
20	Binary VLE 042	6	1987	325	13400 - 44100
21	Binary VLE 043	6	1987	373	75800 - 185800
22	Binary VLE 044	6	1987	410	201900 - 447700
23	Binary VLE 059	11	2009	353	18300 - 52000
24	Binary VLE 060	11	2009	353	38500 - 100500

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': '$x_{benzene}, y_{benzene}$'})

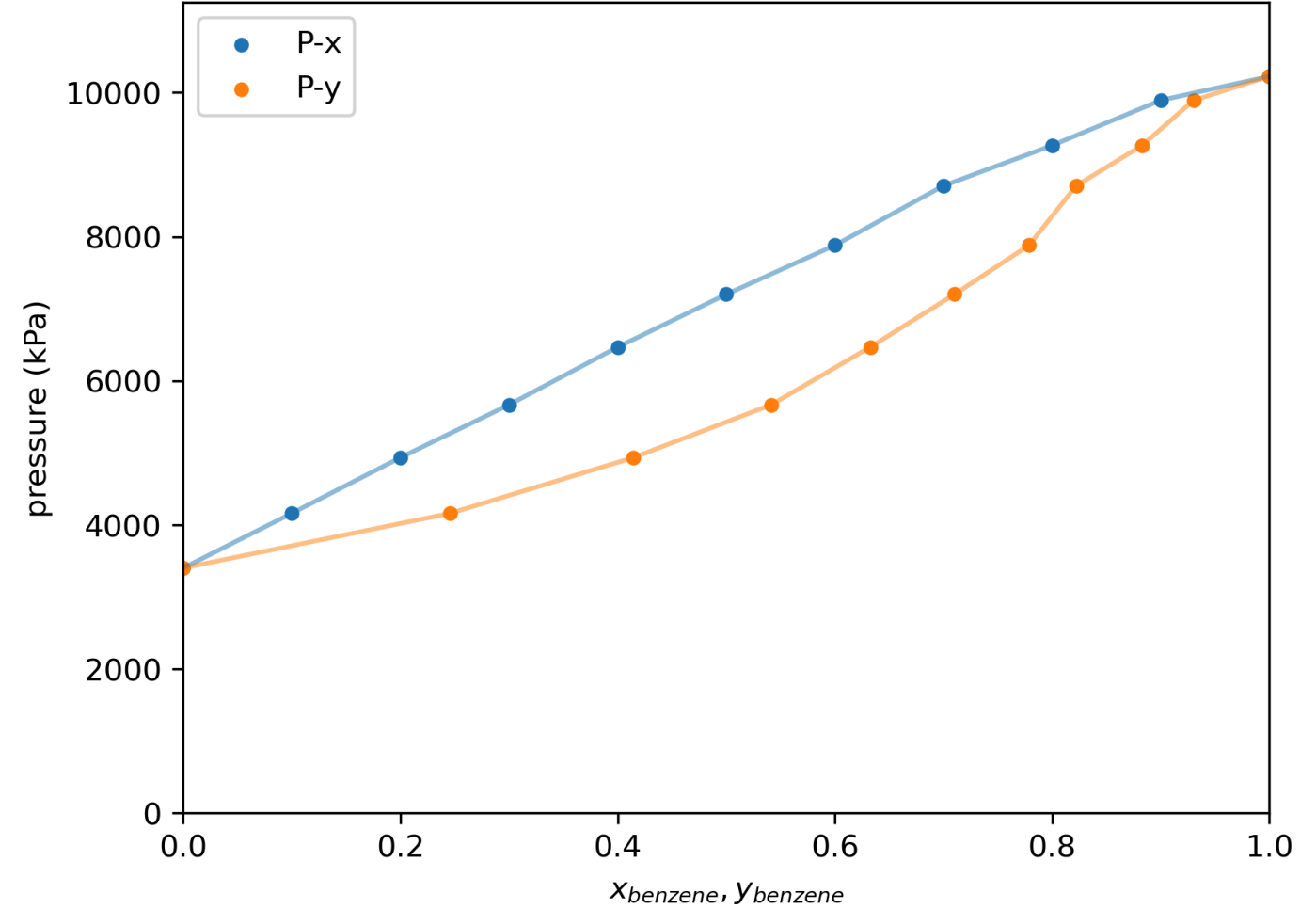
P = df['pressure'] # kPa
xb = df['benzene']
xt = df['toluene']

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')

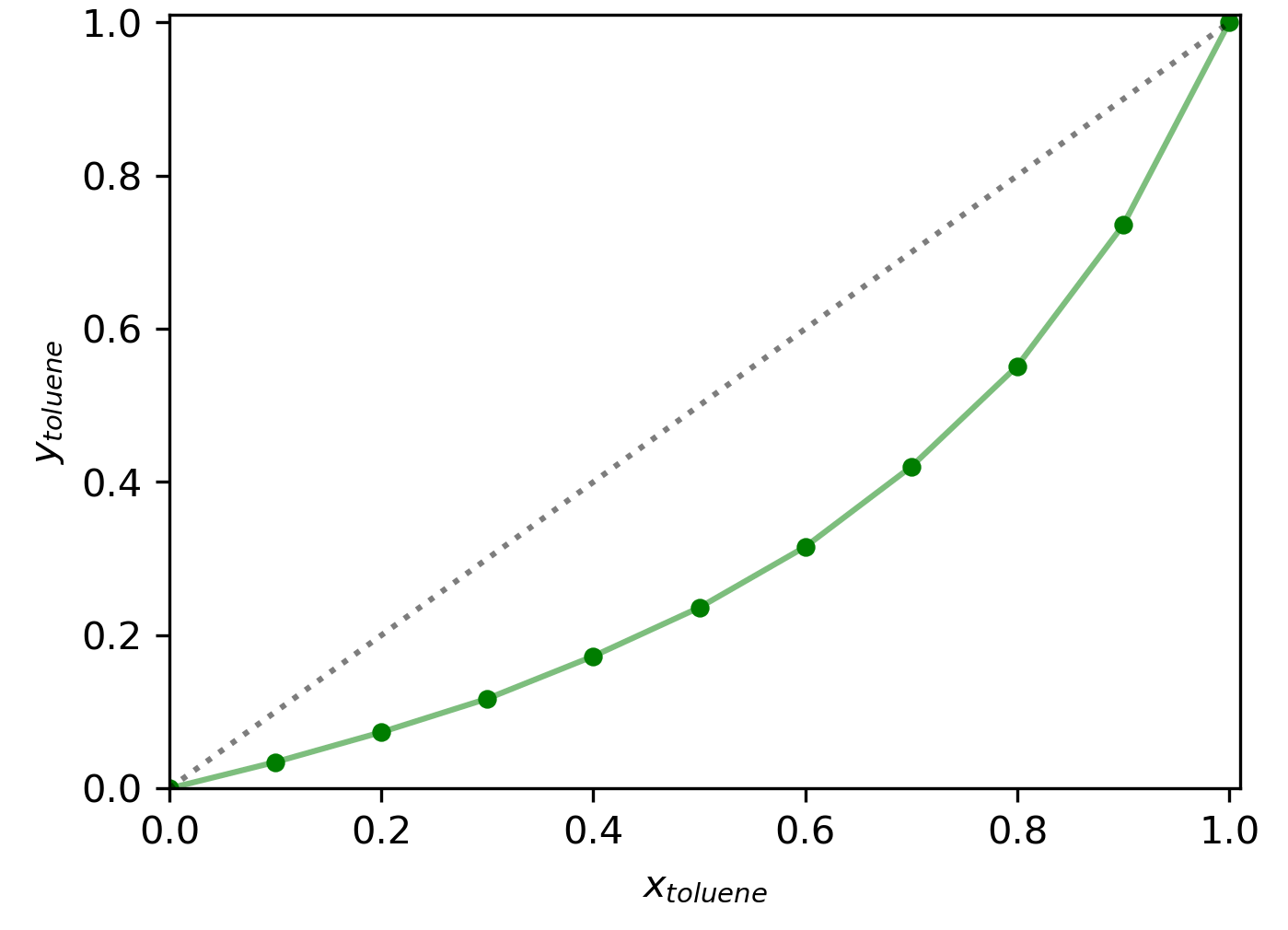
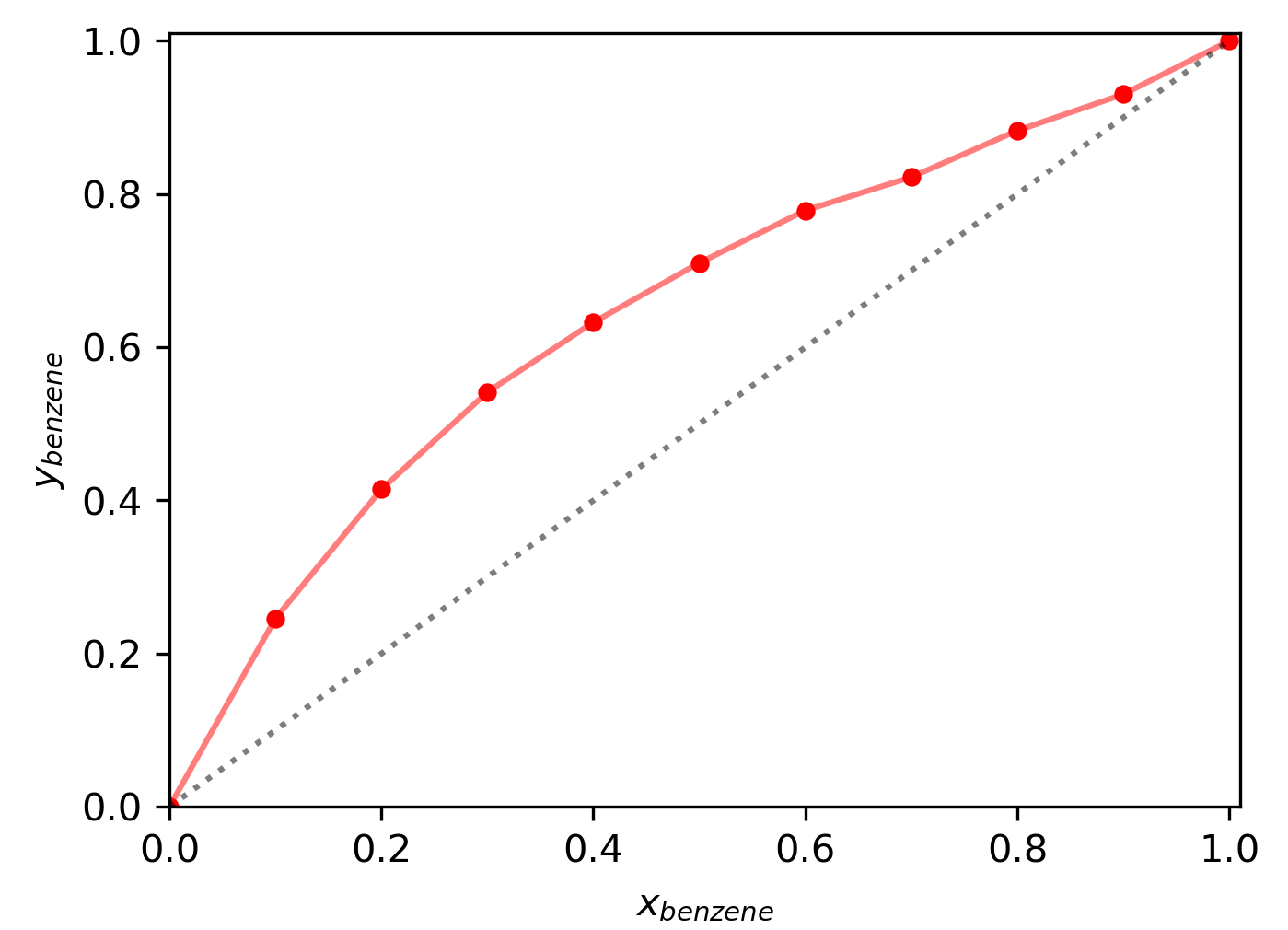
ax.legend()
```



```
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