cheg325 homework 5 SIS 9.9

AUTHOR
k. wodehouse

PUBLISHED
March 28, 2025

using the data we need to relate the regular solution theory parameters to our van laar parameters (alpha and beta) usig this equation

$$\alpha = A_{12} = \frac{V_1}{RT}(\delta_1 - \delta_2)^2$$

$$\beta = A_{21} = \frac{V_2}{RT}(\delta_1 - \delta_2)^2$$

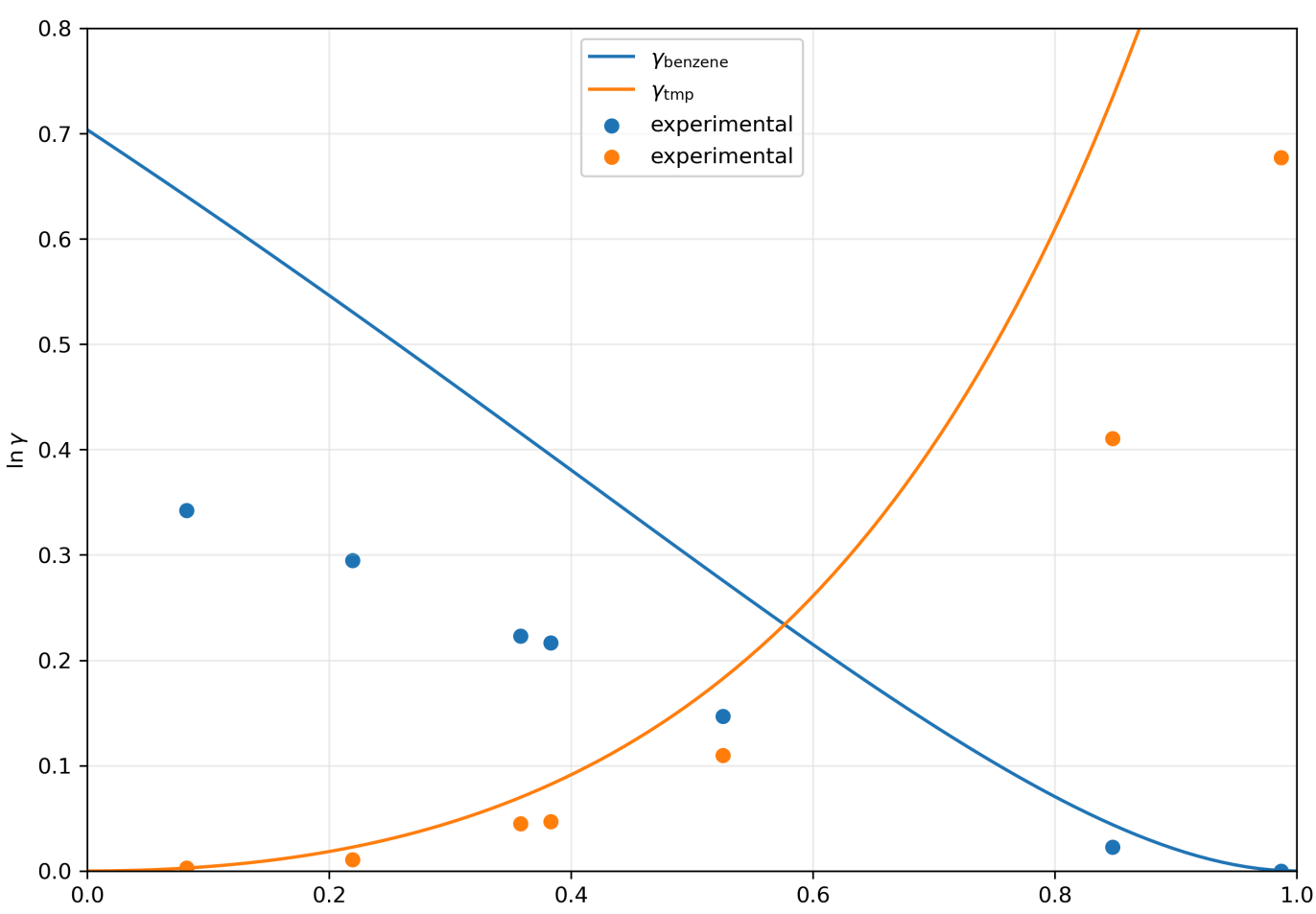
now calculating them up with the data in the table and the illustration where they calculate it for the trimethyl. also, arbitrarily let benzene be component 1

```
from scipy.constants import R
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

T = 273 + 55.0
R *= 0.239006 # convert to calories
V1 = 89.0
V2 = 165.0
delta1 = 9.2
delta2 = 6.93

alpha = (V1/(R*T))*(delta1 - delta2)**2
beta = (V2/(R*T))*(delta1 - delta2)**2

print(f"alpha: {alpha:.4f}")
print(f"beta: {beta:.4f}")

def van_laar1(x1, alpha, beta):
    return alpha / (1 + (alpha/beta) * (x1/(1-x1)))**2

def van_laar2(x1, alpha, beta):
    return beta / (1 + (beta/alpha) * ((1-x1)/(x1)))**2
```

```
alpha: 0.7036
beta: 1.3044
```

not looking too hot but let's plot with the experimental data and see

```
df = pd.read_csv('data.txt', sep=' ')
fig, ax = plt.subplots(figsize=(10,7), dpi=300, subplot_kw={'xlim':(0,1), 'ylim':(0,0.8),

x1 = np.linspace(0.001,0.999,100)
y1 = van_laar1(x1, alpha, beta)
y2 = van_laar2(x1, alpha, beta)

plt.plot(x1, y1)
plt.plot(x1, y2)


plt.scatter(df['xb'], np.log(df['gb']))
plt.scatter(df['xb'], np.log(df['gtmp']))



ax.legend([r'$\gamma_{\text{benzene}}$', r'$\gamma_{\text{tmp}}$', 'experimental', 'exper
ax.grid(alpha=0.2)
```



regular solution theory seems pretty far from experiment.

(B)

α and β correspond to our infinite dilution $\ln \gamma$ values. could be just visually guessed but i did it by measuring pixels in the graph. then beta can come from the data given in the textbook

```
alpha = (0.4/294)*304
beta = 0.6870
print(f'alpha: {alpha:.4f}\nbeta: {beta:.4f}')
```

```
alpha: 0.4136
beta: 0.6870
```

comparing to our experimental data now

```
df = pd.read_csv('data.txt', sep=' ')
fig, ax = plt.subplots(figsize=(10,7), dpi=300, subplot_kw={'xlim':(0,1), 'ylim':(0,0.8),

x1 = np.linspace(0.001,0.999,100)
y1 = van_laar1(x1, alpha, beta)
y2 = van_laar2(x1, alpha, beta)

plt.plot(x1, y1)
plt.plot(x1, y2)


plt.scatter(df['xb'], np.log(df['gb']))
plt.scatter(df['xb'], np.log(df['gtmp']))

ax.legend([r'$\gamma_{\text{benzene}}$', r'$\gamma_{\text{tmp}}$', 'experimental', 'exper
ax.grid(alpha=0.2)
```

a much better fit

```
# filler
```