cheg325 homework 5 SIS 11.2-3

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(a)

regular solutions should have $\underline{S}^{\text{ex}} = 0$, but we can clearly see that $\underline{G}^{\text{ex}} \neq \underline{H}^{\text{ex}}$ for the benzene-CCl4 system and that $\underline{G}^{\text{ex}} \approx \underline{H}^{\text{ex}}$ for our benzene-CS2 system.

since $\underline{S}^{\text{ex}} \neq 0$ for the benzene-CCl4 system, it is not a regular solution. and since excess entropy is visually 0 for the benzene-CS2 system, the regular solution model applies

(b)

we can see that the excess gibbs energy looks like a symmetric parabola, and will probably be fit well by a one-constant margules. we only need one point to fit the equation to since there is... one constant. i'll pick the middle point to fit to and read off the y value and then solve for the value of A

$$\underline{G}^{\text{ex}} = Ax_1x_2 \qquad \text{(one constant margules)}$$

visually, the maximum value looks to be about 107 J/mol, so

$$107 = A\left(\frac{1}{2}\right)^2$$

$$A = 427$$

now using this equation we may relate our A to the upper consulate temperature

$$T_{\text{uc}} = \frac{A}{2R} \qquad (11.2\text{-}14)$$

```
from scipy.constants import R
A = 427
Tuc = A / (2*R)
print(f'upper consulate temp: {Tuc:.2f} K')
```

```
upper consulate temp: 25.68 K
```

since melting temperatures are way way higher than the upper consulate temperature, there will not be a liquid liquid phase separation.

(c)

one fun way to do this question would be to literally just make any of our vle diagrams and see if we see an azeotrope.

note that the equation i built earlier isn't in the typical form, so

$$\frac{\underline{G}^{\text{ex}}}{RT} = \frac{A}{RT}x_1x_2$$

which makes our activity coefficients

$$\ln\gamma_1 = \frac{A}{RT}x_2^2$$

$$\ln\gamma_2 = \frac{A}{RT}x_1^2$$

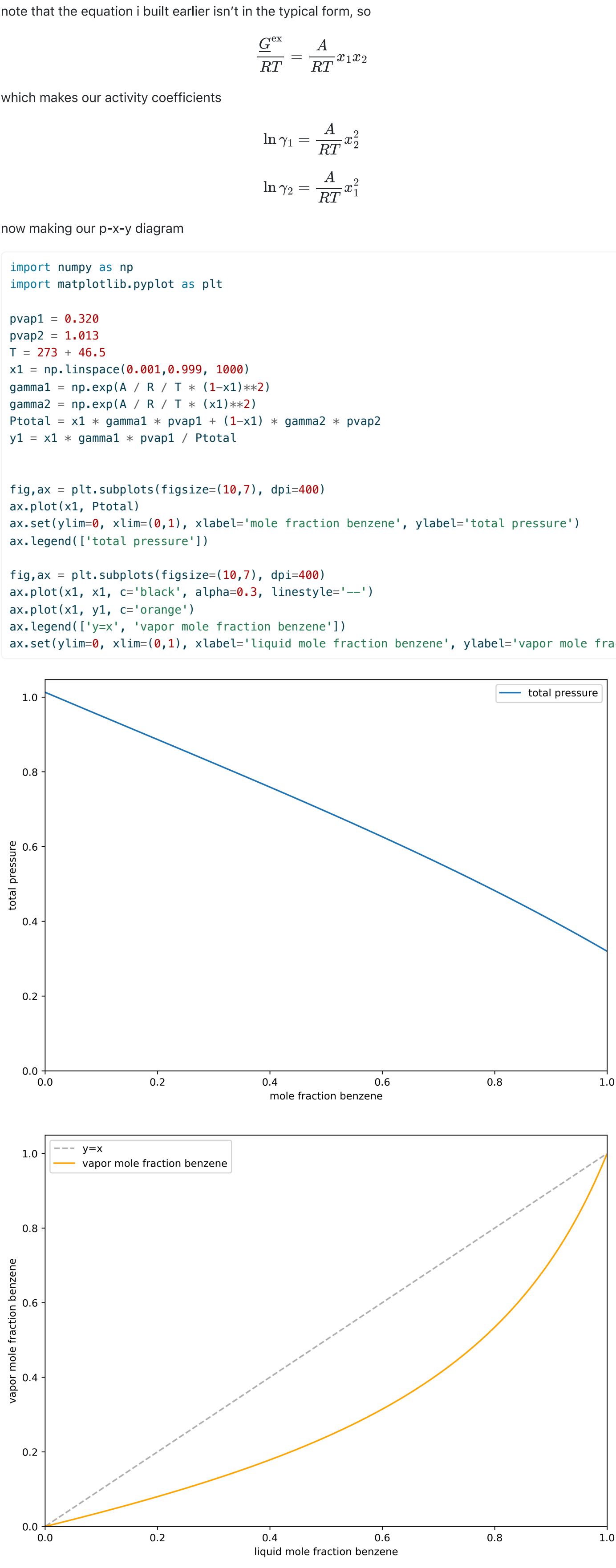
now making our p-x-y diagram

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

pvap1 = 0.320
pvap2 = 1.013
T = 273 + 46.5
x1 = np.linspace(0.001,0.999, 1000)
gamma1 = np.exp(A / R / T * (1-x1)**2)
gamma2 = np.exp(A / R / T * (x1)**2)
Ptotal = x1 * gamma1 * pvap1 + (1-x1) * gamma2 * pvap2
y1 = x1 * gamma1 * pvap1 / Ptotal


fig,ax = plt.subplots(figsize=(10,7), dpi=400)
ax.plot(x1, Ptotal)
ax.set(ylim=0, xlim=(0,1), xlabel='mole fraction benzene', ylabel='total pressure')
ax.legend(['total pressure'])

fig,ax = plt.subplots(figsize=(10,7), dpi=400)
ax.plot(x1, x1, c='black', alpha=0.3, linestyle='--')
ax.plot(x1, y1, c='orange')
ax.legend(['y=x', 'vapor mole fraction benzene'])
ax.set(ylim=0, xlim=(0,1), xlabel='liquid mole fraction benzene', ylabel='vapor mole frac
```



and we see that no azeotrope will occur

```
# filler text
```