cheg325 homework 6 SIS 11.2-39

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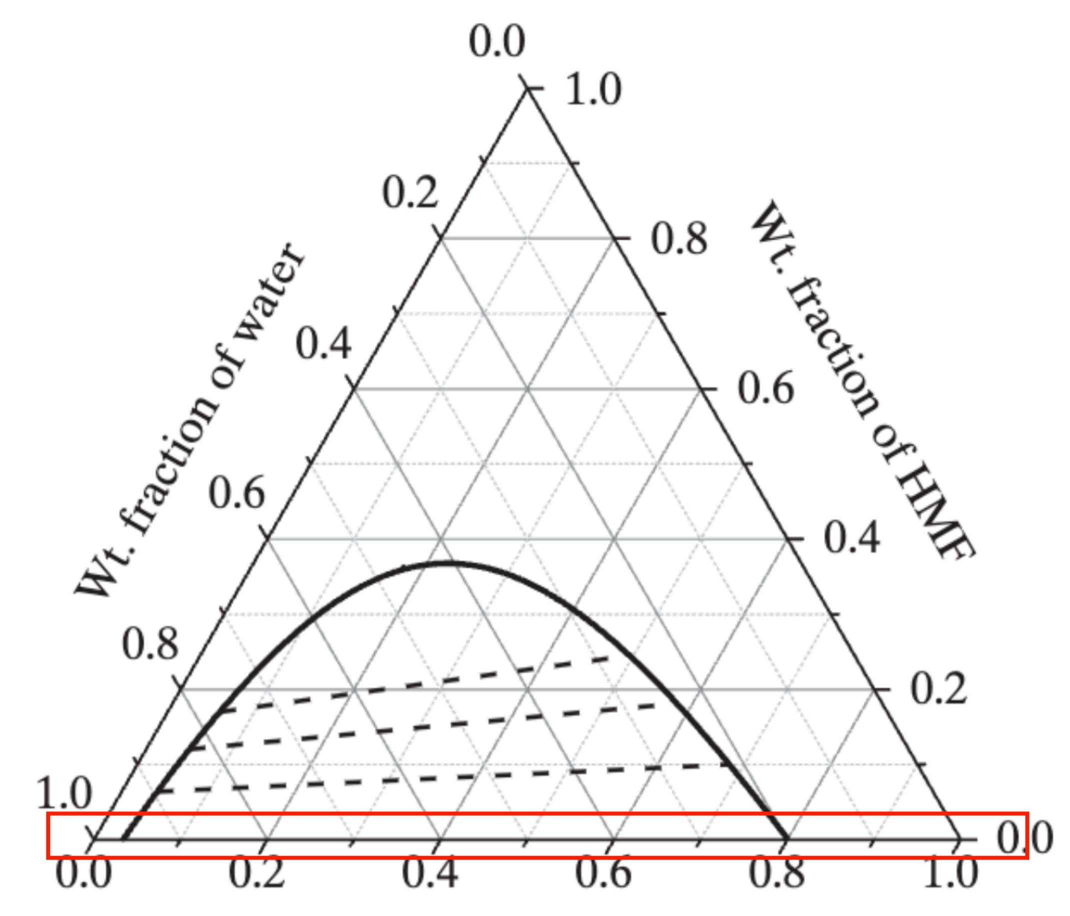
a

if any of the mole fractions are zero (if we have a binary mixture), we will be confined to sides of the triangle. now the question becomes on which sides of the triangle will there be a region with two phases.

we very quickly see only the bottom side (for when there is no HMF) will have a possible 2 phases, and the others will always be miscible.



the two phase region exist on this side of the triangle

miscible

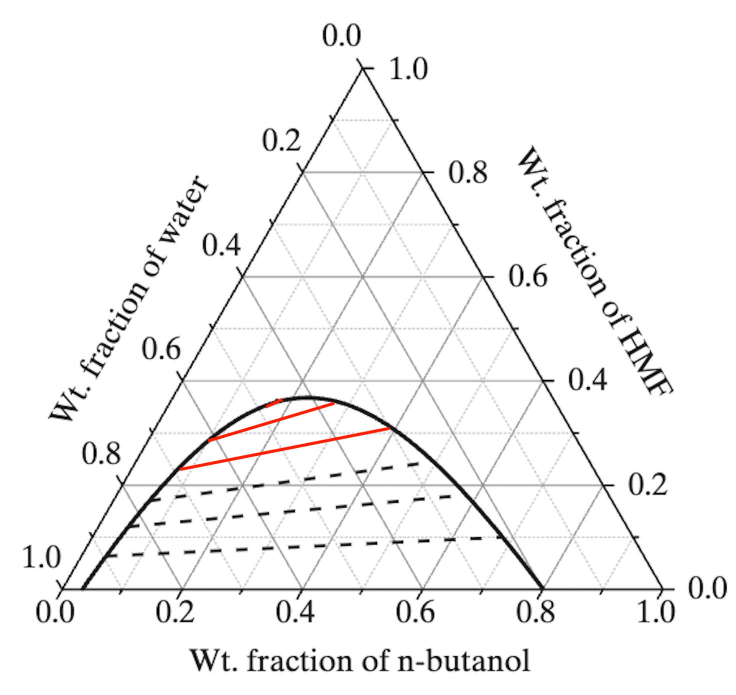
- HMF + Water
- HMF + n-butanol

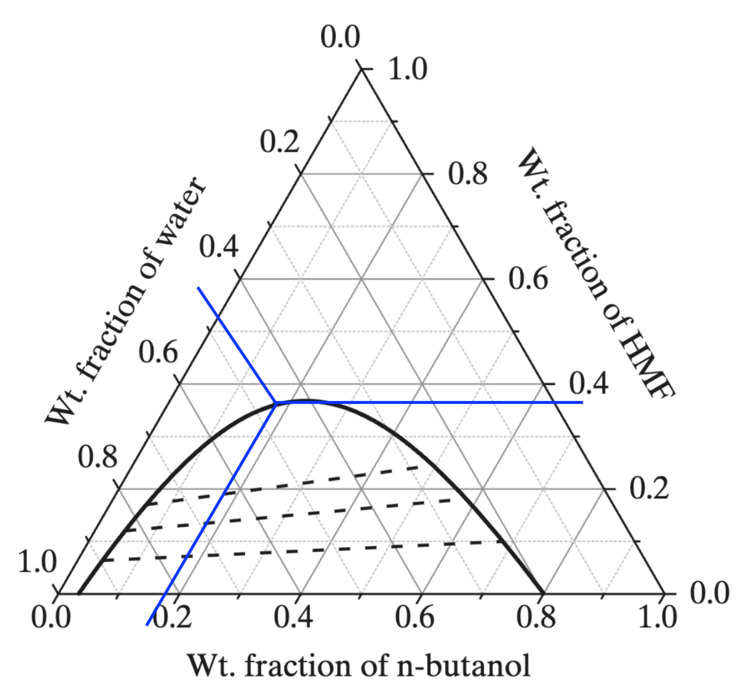
will form 2 phases at some concentration

- water + n-butanol

b

the plait point is where the tie lines end up intersecting the 2 phase region edge at the same point. this can be estimated by estimating some more tie lines going up.





i did this by measuring pixels to try and get some half accurate answers, so

```
import numpy as np

x_butanol = 129/720
x_hmf = np.hypot(129,227) / np.hypot(359, 623)
x_water =  np.hypot(361 - 192,623 - 329) / np.hypot(361, 623)

print(f'x_water: {x_water:.3f}')
print(f'x_hmf: {x_hmf:.3f}')
print(f'x_butanol: {x_butanol:.3f}\n')
print(f'sum: {x_water + x_butanol + x_hmf:.3f}')
```

```
x_water: 0.471
x_hmf: 0.363
x_butanol: 0.179

sum: 1.013
```

comparing these numbers from measuring pixels (because i think this is the most reasonable way to try and get decent numbers from a graph on a computer) to my eyes they all make sense from where the coordinates look to be on the graph.

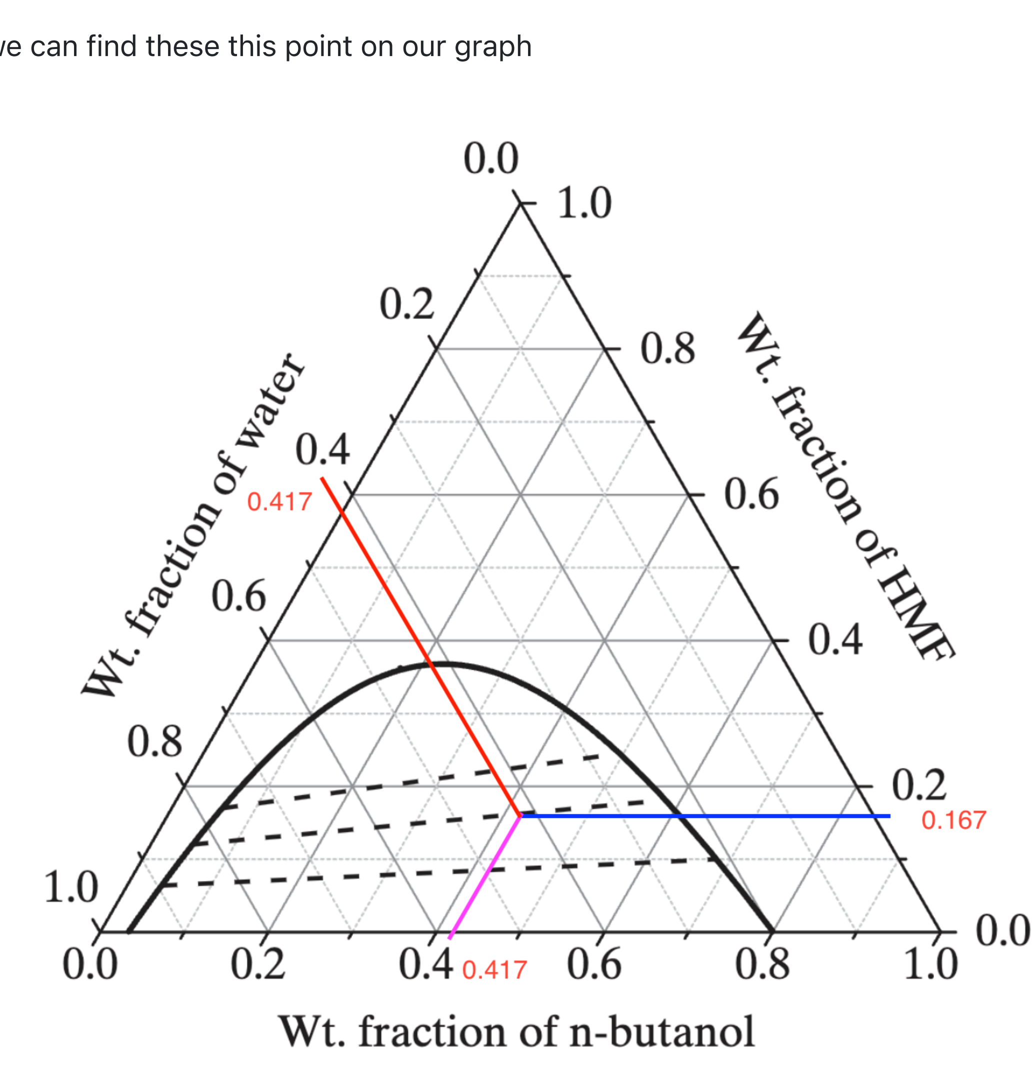
c

luckily the axes are in wt. fractions already, so we can easily calculate all the weight fractions…

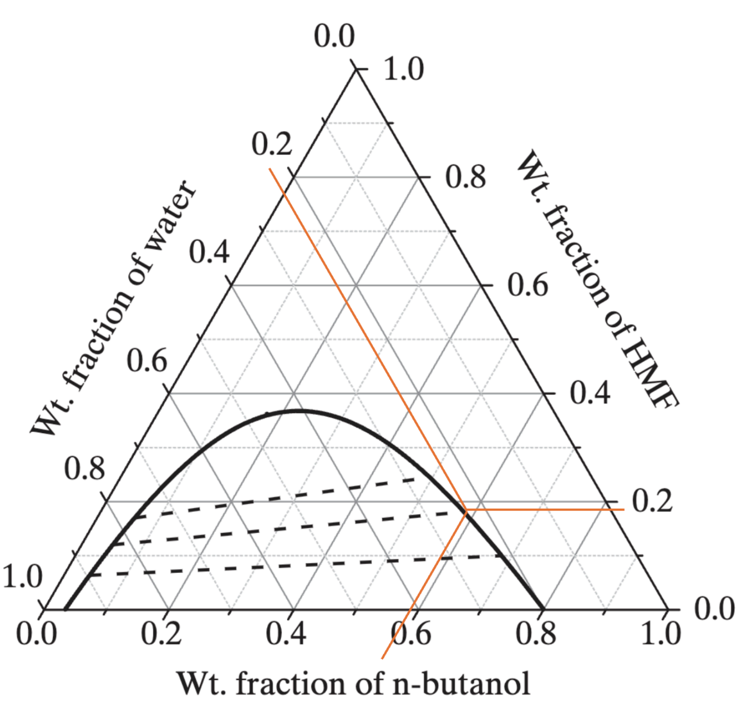
```
x_water = 5/12
x_butanol = 5/12
x_hmf = 2/12
print(f'x_water = x_butanol: {x_water:.3f}')
print(f'x_hmf: {x_hmf:.3f}')
```

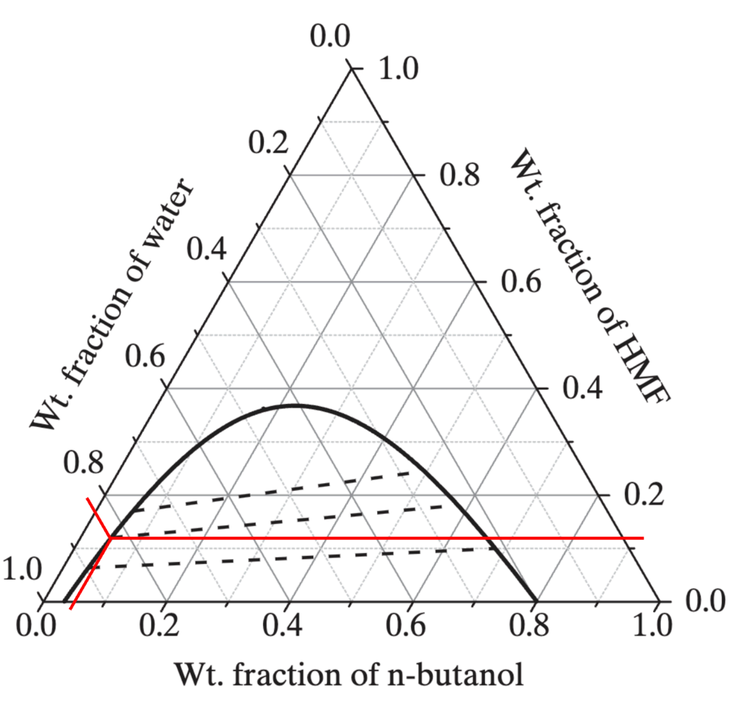
```
x_water = x_butanol: 0.417
x_hmf: 0.167
```

now we can find these this point on our graph



so we see that **there will be 2 phases**, and now we can figure out their compositions by following the tie line that this composition nicely falls on.





and again i did this by measuring pixels

```
x_butanol_r = 331/564
x_water_r =  np.hypot(67,114) / np.hypot(282,488)
x_hmf_r = np.hypot(53,91) / np.hypot(281,488)

print(f'----- butanol rich phase -----')
print(f'x_water: {x_water_r:.3f}')
print(f'x_hmf: {x_hmf_r:.3f}')
print(f'x_butanol: {x_butanol_r:.3f}')
print(f'sum: {x_water_r + x_butanol_r + x_hmf_r:.3f}\n')

x_butanol_l = 44/860
x_hmf_l = np.hypot(42,74) / np.hypot(349,605)
x_water_l =  np.hypot(292,503) / np.hypot(350,606)

print(f'----- water rich phase -----')
print(f'x_water: {x_water_l:.3f}')
print(f'x_hmf: {x_hmf_l:.3f}')
print(f'x_butanol: {x_butanol_l:.3f}')
print(f'sum: {x_water_l + x_butanol_l + x_hmf_l:.3f}\n')
```

```
----- butanol rich phase -----
x_water: 0.235
x_hmf: 0.187
x_butanol: 0.587
sum: 1.008

----- water rich phase -----
x_water: 0.831
x_hmf: 0.122
x_butanol: 0.051
sum: 1.004
```

to answer how many kg are in each phase, we need to use a mass balance. we know that if we put 5kg of water into our mixture, there will be 5kg split across both phases. let m_w be the mass of the water rich phase and m_b be the mass of the n-butanol rich phase. then, let x_w^b be the

$$m_w + m_b = 12 \qquad \text{(first equation)}$$

$$x_w^w m_w + x_w^b m_b = 5$$

now we have 2 equations and 2 unknows! this is easily done by substituting either m_w or m_b using the (first equation)

$$x_w^w m_w + x_w^b(12 - m_w) = 5$$

$$x_w^w m_w + 12x_w^b - x_w^b m_w = 5$$

$$m_w(x_w^w - x_w^b) + 12x_w^b = 5$$

$$m_w = \frac{5 - 12x_w^b}{x_w^w - x_w^b}$$

and then of course if we know m_w we can use (first equation). calculating, (also noting that the “left” is the water rich and “right” is the butanol rich)

```
m_w = (5 - 12 * x_water_r)/(x_water_l - x_water_r)
m_b = 12 - m_w

print(f'mass of water rich: {m_w:.2f} kg')
print(f'mass of n-butanol rich: {m_b:.2f} kg')
```

```
mass of water rich: 3.66 kg
mass of n-butanol rich: 8.34 kg
```

another way to do this would be to let X be the proportion of the mixture in the water rich phase. then,

$$x_w^w X + x_w^b(1 - X) = x_w$$

which using similar algebra as before gives

$$X = \frac{x_w - x_w^b}{x_w^w - x_w^b} \qquad \text{(lever ruleee)}$$

now plugging in

```
X = (x_water - x_water_r)/(x_water_l - x_water_r)
print(f'mass of water rich: {X*12:.2f}')
print(f'mass of water rich: {12 - X*12:.2f}')
```

```
mass of water rich: 3.66
mass of water rich: 8.34
```

and thankfully these agree.

```
# filler
```