

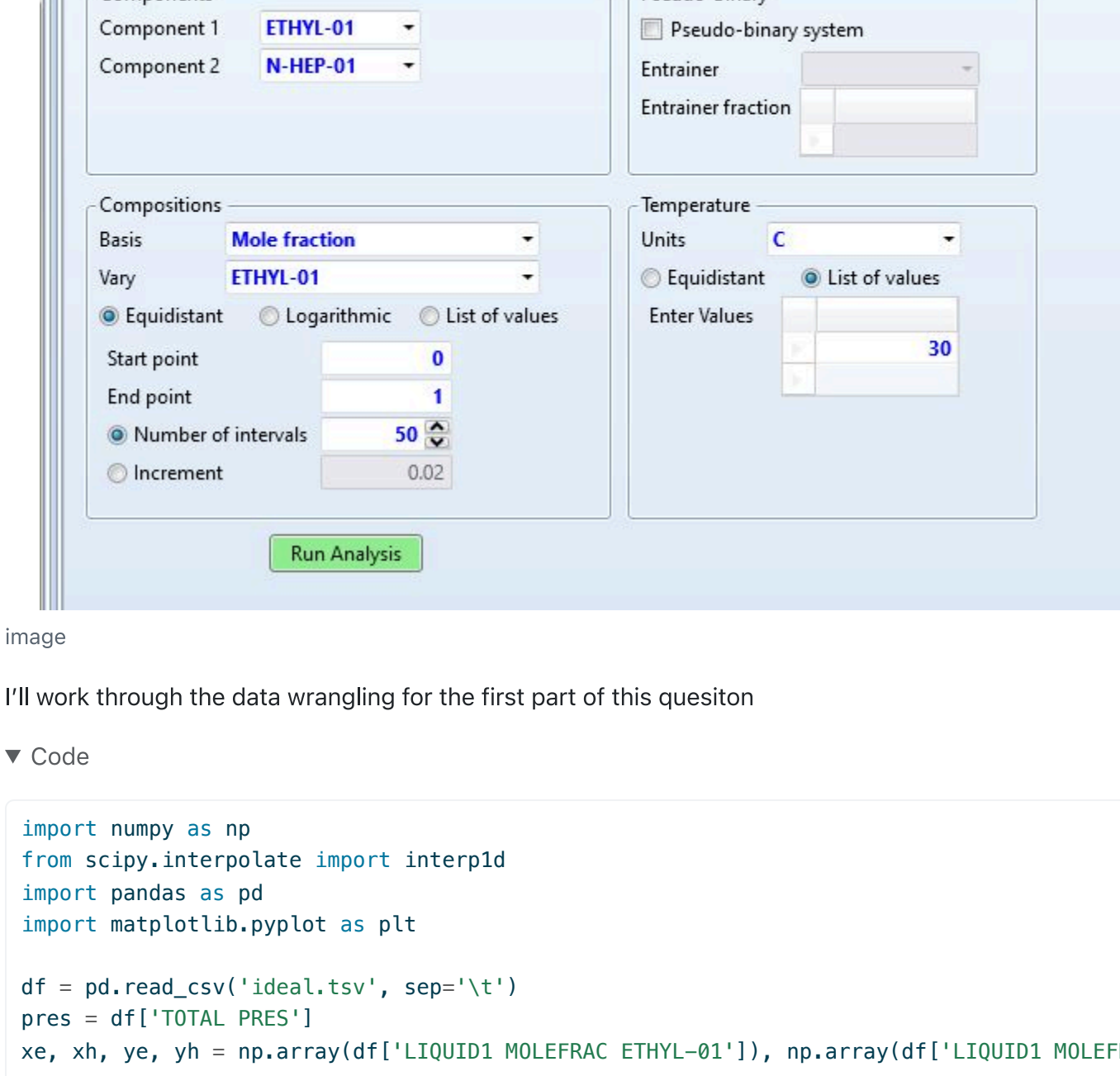
# SIS 10.2-1

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## part a

using **IDEAL** model in aspen and going to binary analysis

here's what my analysis page looked like when running these different models



image

I'll work through the data wrangling for the first part of this question

▼ Code

```
import numpy as np
from scipy.interpolate import interp1d
import pandas as pd
import matplotlib.pyplot as plt

df = pd.read_csv('ideal.tsv', sep='\t')
pres = df['TOTAL PRES']
xe, xh, ye, yh = np.array(df['LIQUID1 MOLEFRAC ETHYL-01']), np.array(df['LIQUID1 MOLEFRAC N-HEP-01']), np.array(df['VAPOR1 MOLEFRAC ETHYL-01']), np.array(df['VAPOR1 MOLEFRAC N-HEP-01'])

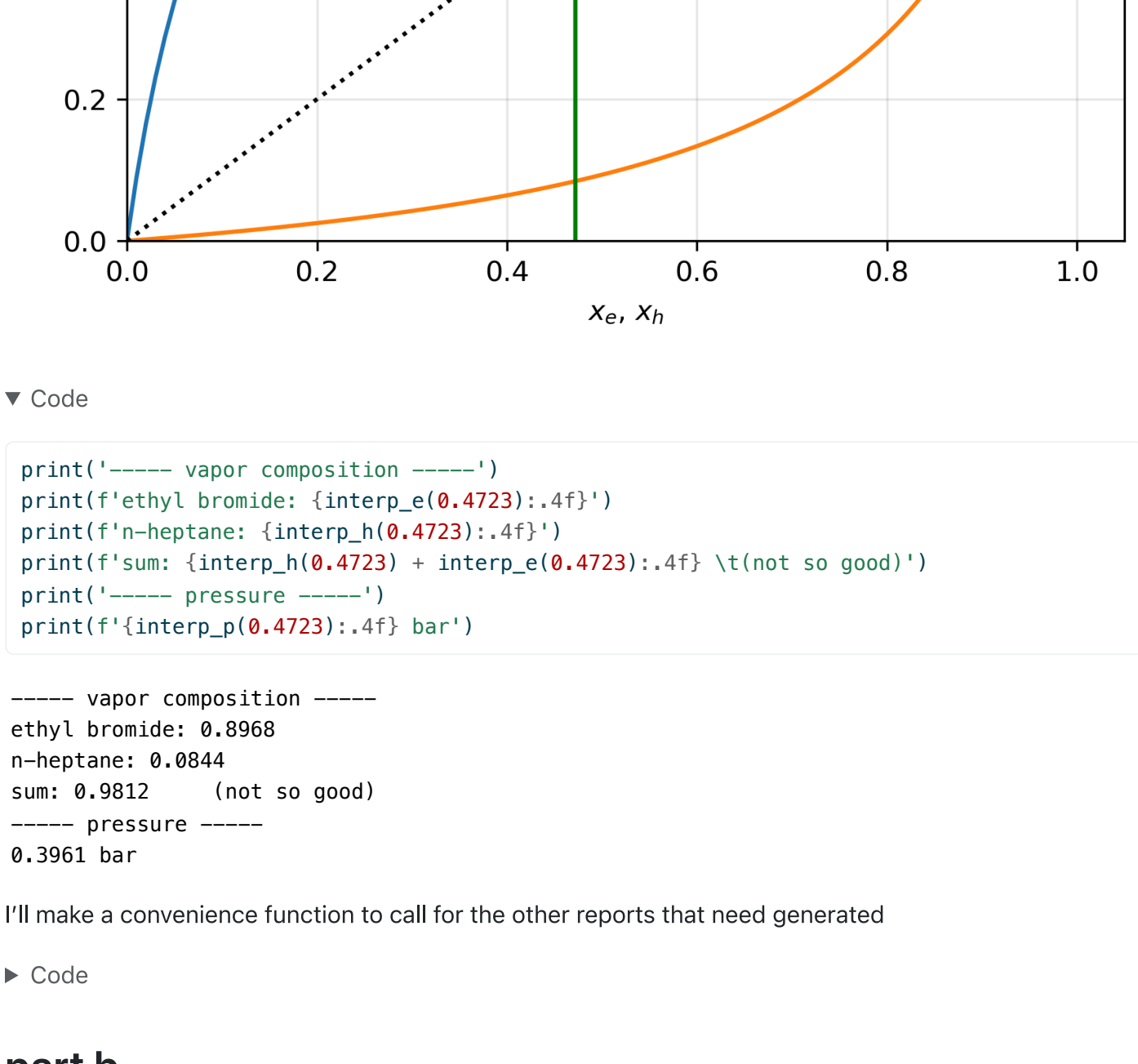
interp_p = interp1d(xe, pres, kind='linear', fill_value="extrapolate")
interp_e = interp1d(xe, ye, kind='linear', fill_value="extrapolate")
interp_h = interp1d(xh, yh, kind='linear', fill_value="extrapolate")

df.head(3)
```

TEMP	MOLEFRAC ETHYL-01	TOTAL PRES	TOTAL KVL ETHYL-01	TOTAL KVL N-HEP-01	LIQUID1 GAMMA ETHYL-01	LIQUID1 GAMMA N-HEP-01	LIQUID2 GAMMA ETHYL-01	LIQUID2 GAMMA N-HEP-01	TOTAL KVL2 ETHYL-01	TOTAL KVL2 N-HEP-01	TOTAL BE
0 30	0.00	0.077455	9.709034	1.000000	1	1	NaN	NaN	NaN	NaN	1
1 30	0.01	0.084201	8.931212	0.919887	1	1	NaN	NaN	NaN	NaN	1
2 30	0.02	0.090947	8.268773	0.851658	1	1	NaN	NaN	NaN	NaN	1

▼ Code

```
fig, ax = plt.subplots(dpi=300)
ax.grid(alpha=0.3)
ax.plot(xe, ye, label='ethyl')
ax.plot(xh, yh, label='n-heptane')
ax.plot(xe, ye, ':', c='black')
ax.set(xlim=0, ylim=0, xlabel='$x_e, x_h$', ylabel='$y_e, y_h$')
ax.vlines(0.4723, 0, 1, color='green', label='mixture comp')
ax.legend();
```



▼ Code

```
print('----- vapor composition -----')
print(f'ethyl bromide: {interp_e(0.4723):.4f}')
print(f'n-heptane: {interp_h(0.4723):.4f}')
print(f'sum: {interp_h(0.4723) + interp_e(0.4723):.4f} \t(not so good)')
print('----- pressure -----')
print(f'{interp_p(0.4723):.4f} bar')
```

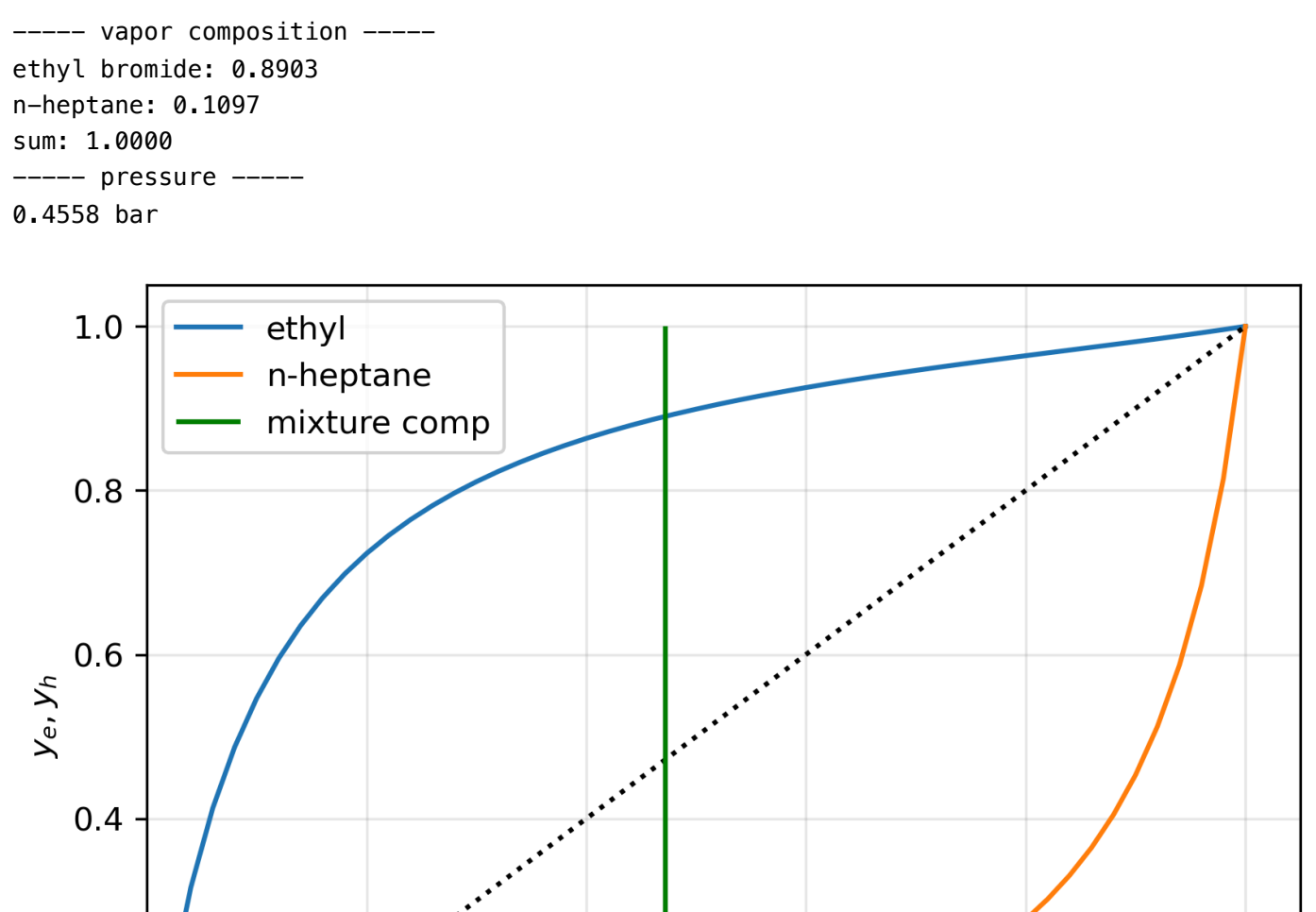
```
----- vapor composition -----
ethyl bromide: 0.8968
n-heptane: 0.0844
sum: 0.9812 (not so good)
----- pressure -----
0.3961 bar
```

I'll make a convenience function to call for the other reports that need generated

► Code

## part b

here's what the p-x-y plot looked like for the **GRAYSON** model

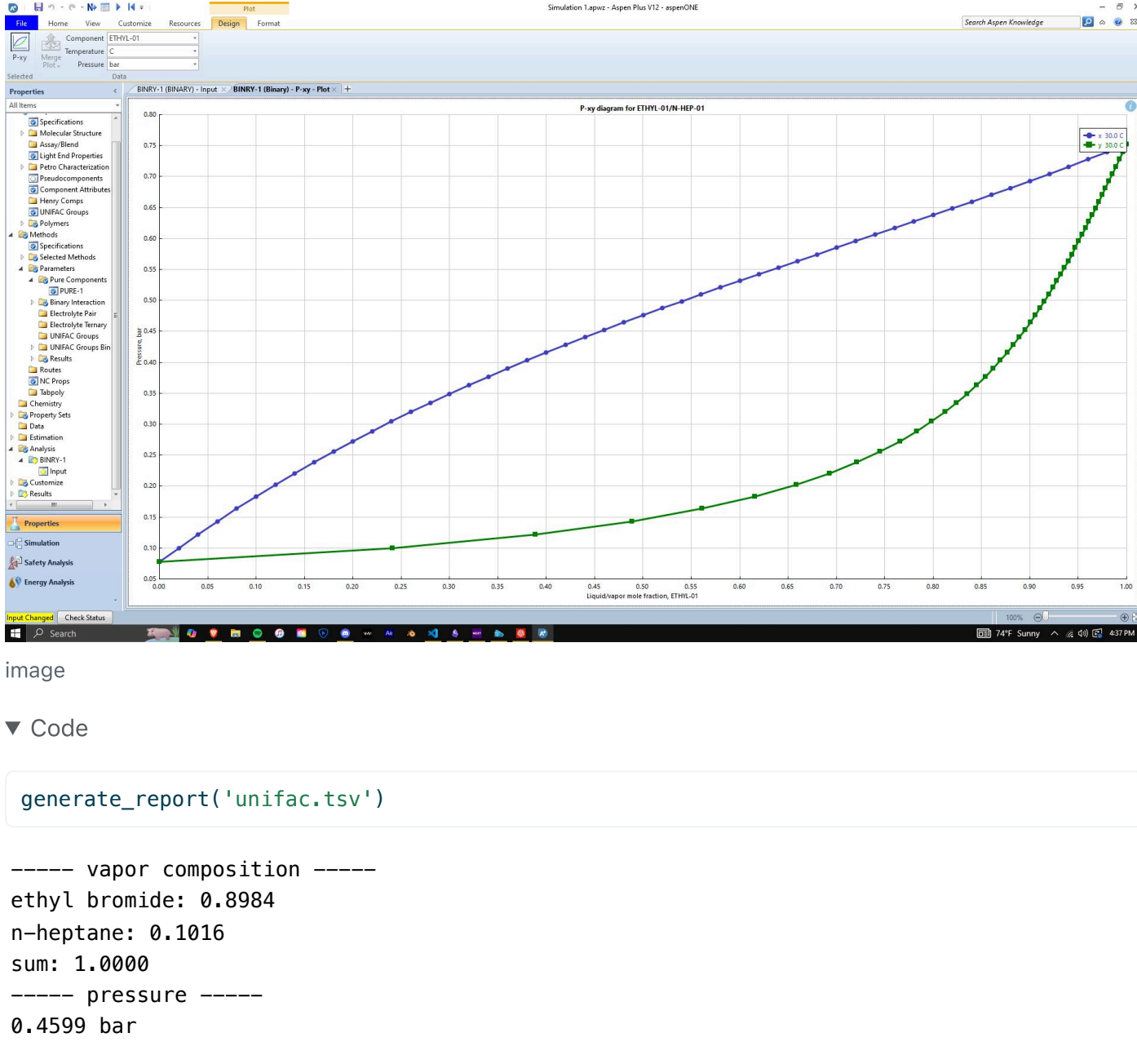


image

▼ Code

```
generate_report('ptb.tsv')
```

```
----- vapor composition -----
ethyl bromide: 0.8903
n-heptane: 0.1097
sum: 1.0000
----- pressure -----
0.4558 bar
```

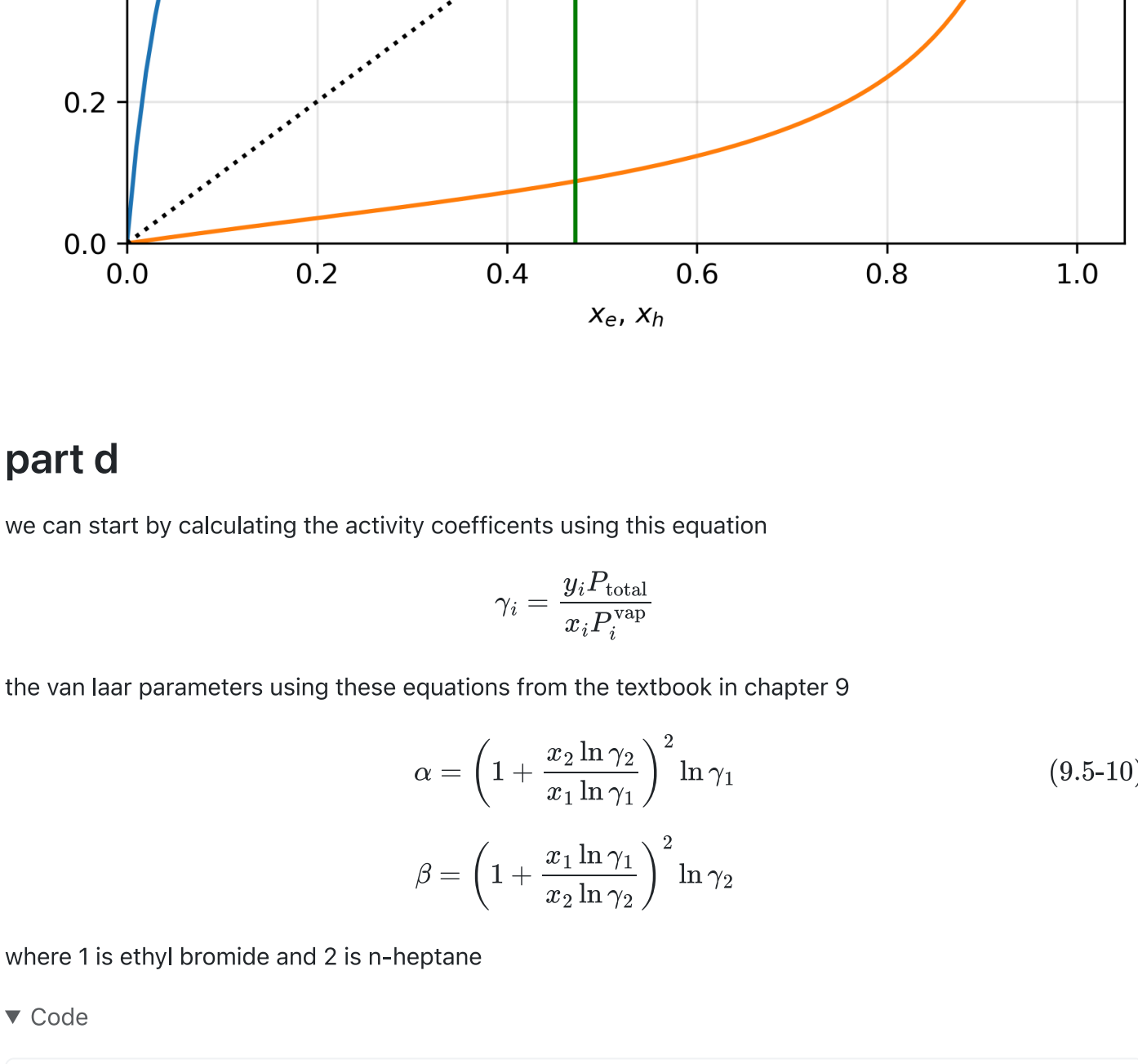


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▼ Code

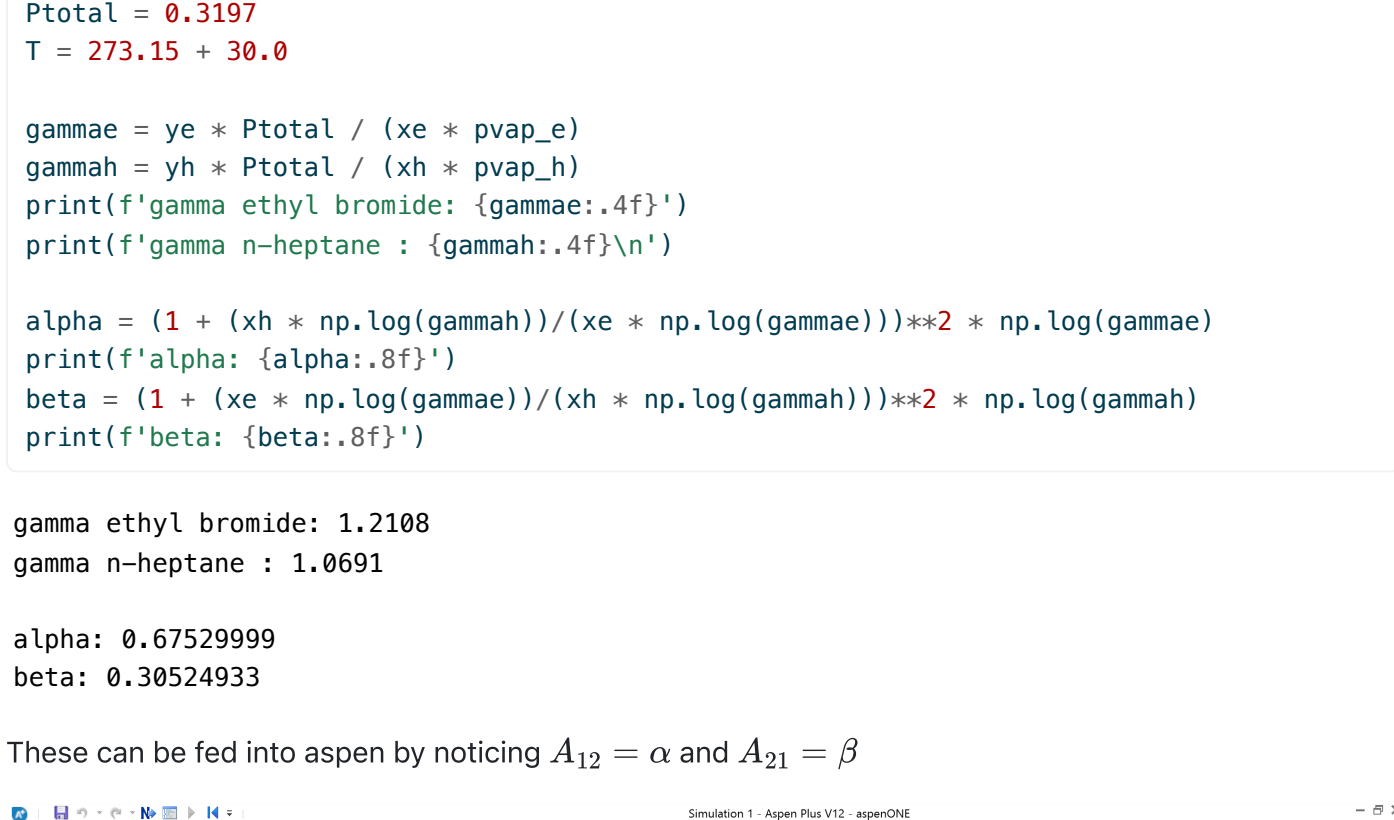
```
generate_report('unifac.tsv')
```

```
----- vapor composition -----
ethyl bromide: 0.8984
n-heptane: 0.1016
sum: 1.0000
----- pressure -----
0.4599 bar
```



## part c

here's what the p-x-y plot looked like for the **UNIFAC** model



image

▼ Code

```
ye = 0.815
yh = 1 - ye
xe = 0.2843
xh = 1 - xe

pvap_e = 0.7569
pvap_h = 0.0773

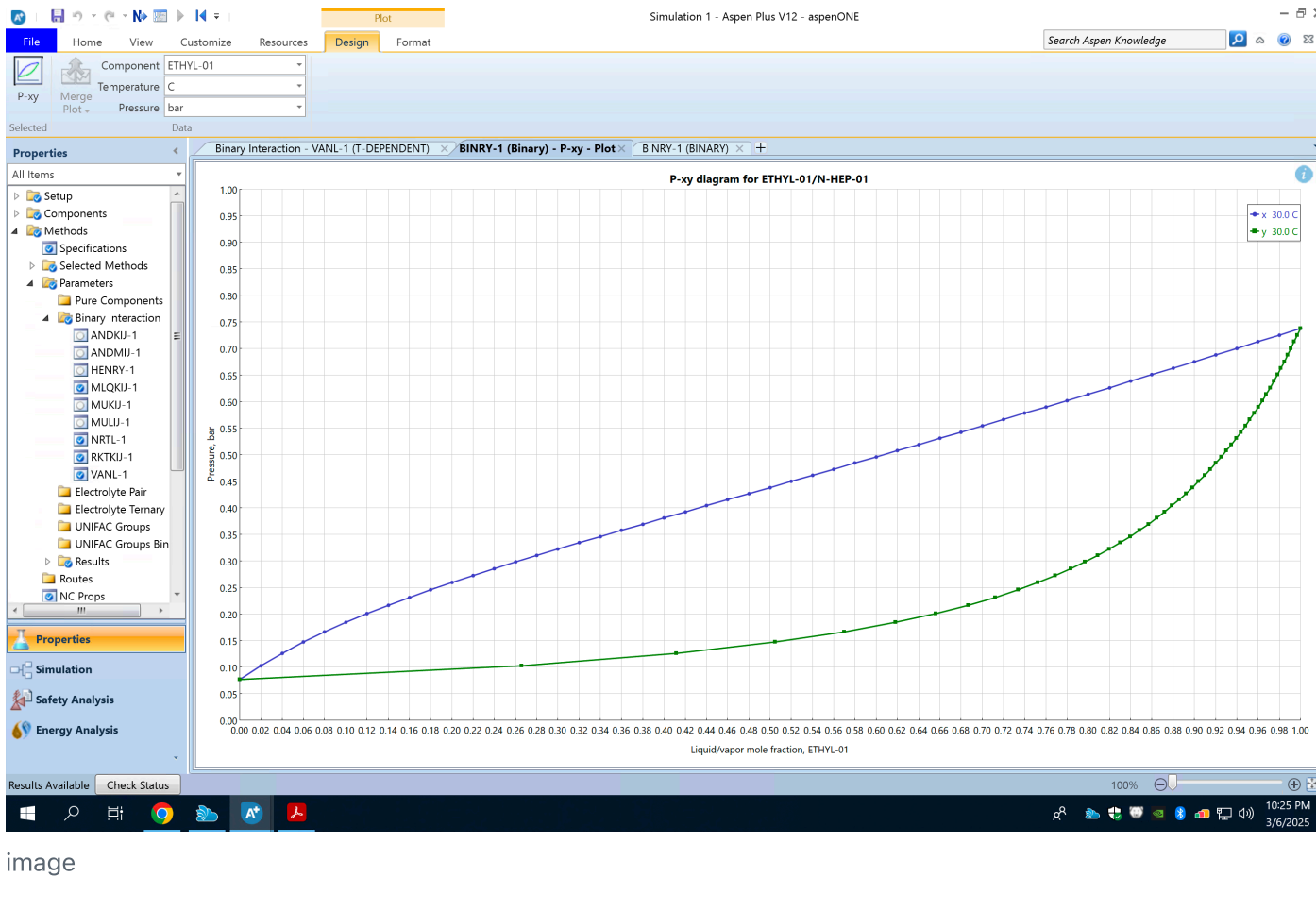
Ptotal = 0.3197
T = 273.15 + 30.0

gammae = ye * Ptotal / (xe * pvap_e)
gammah = yh * Ptotal / (xh * pvap_h)
print(f'gamma ethyl bromide: {gammae:.8f}')
print(f'gamma n-heptane : {gammah:.4f}\n')
```

```
gamma ethyl bromide: 1.2108
gamma n-heptane : 1.0691
```

```
alpha: 0.67529999
beta: 0.30524933
```

These can be fed into aspen by noticing  $A_{12} = \alpha$  and  $A_{21} = \beta$

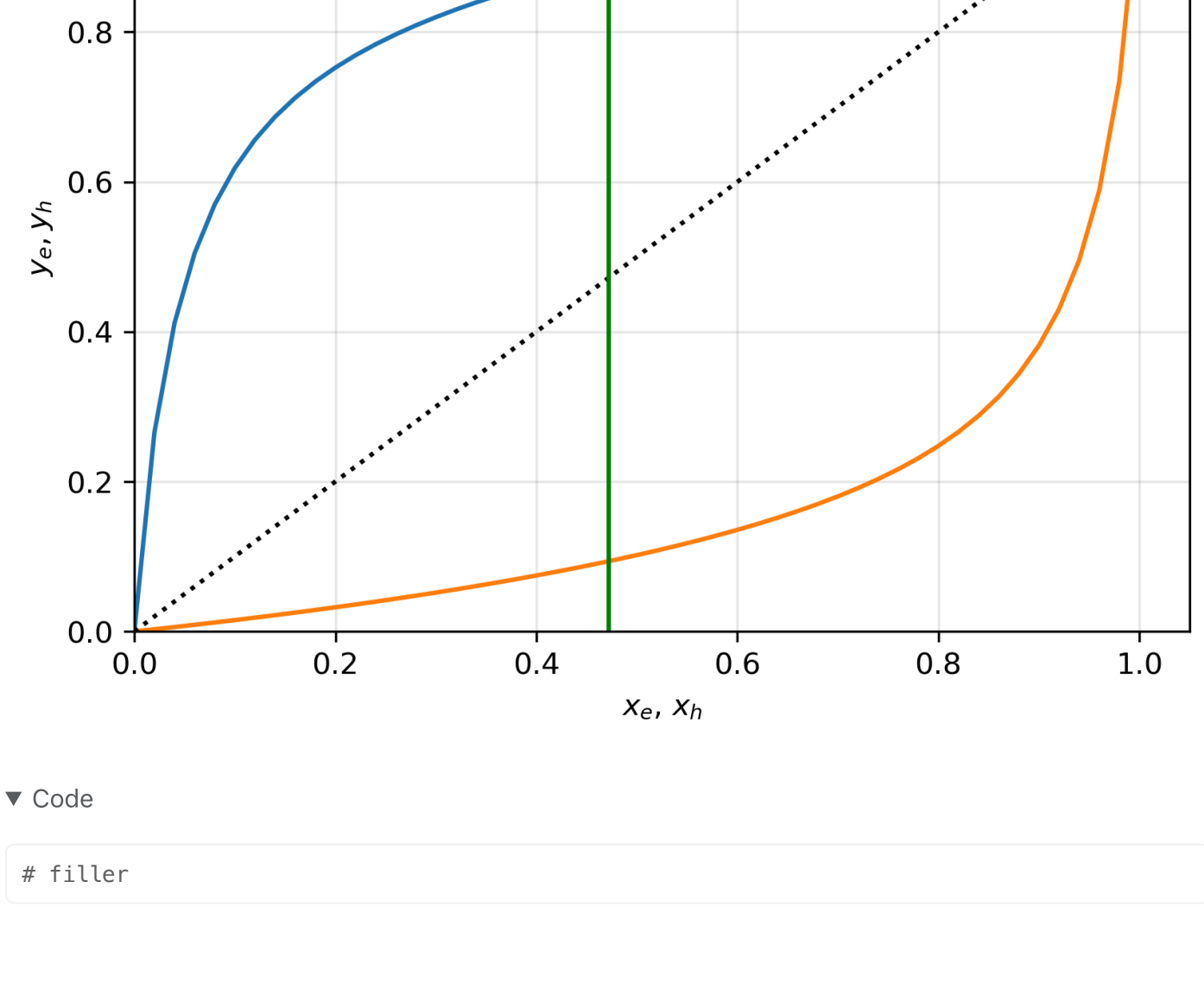


image

▼ Code

```
generate_report('vanlaar.tsv')
```

```
----- vapor composition -----
ethyl bromide: 0.8895
n-heptane: 0.1105
sum: 1.0000
----- pressure -----
0.4224 bar
```



image

▼ Code

```
# filler
```