cheg325 HW1 Q1

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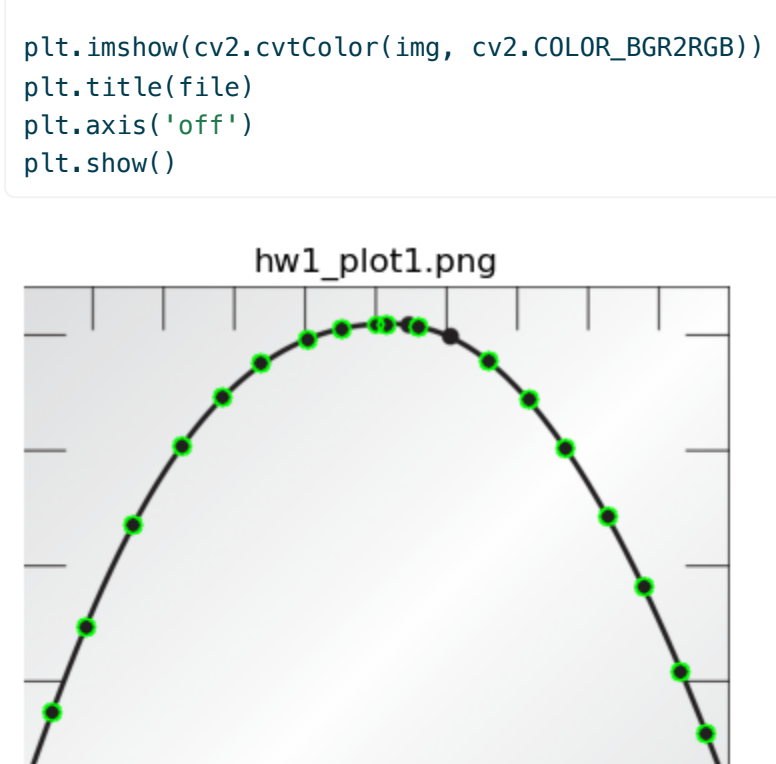
we need to do a few things to get this data read in from computer vision - find the coordinates for the circles in the plot - find the horizontal line - subtract the horizontal line from the y values - convert x and y pixels into the right values - plot the figure from the text to verify it looks identical

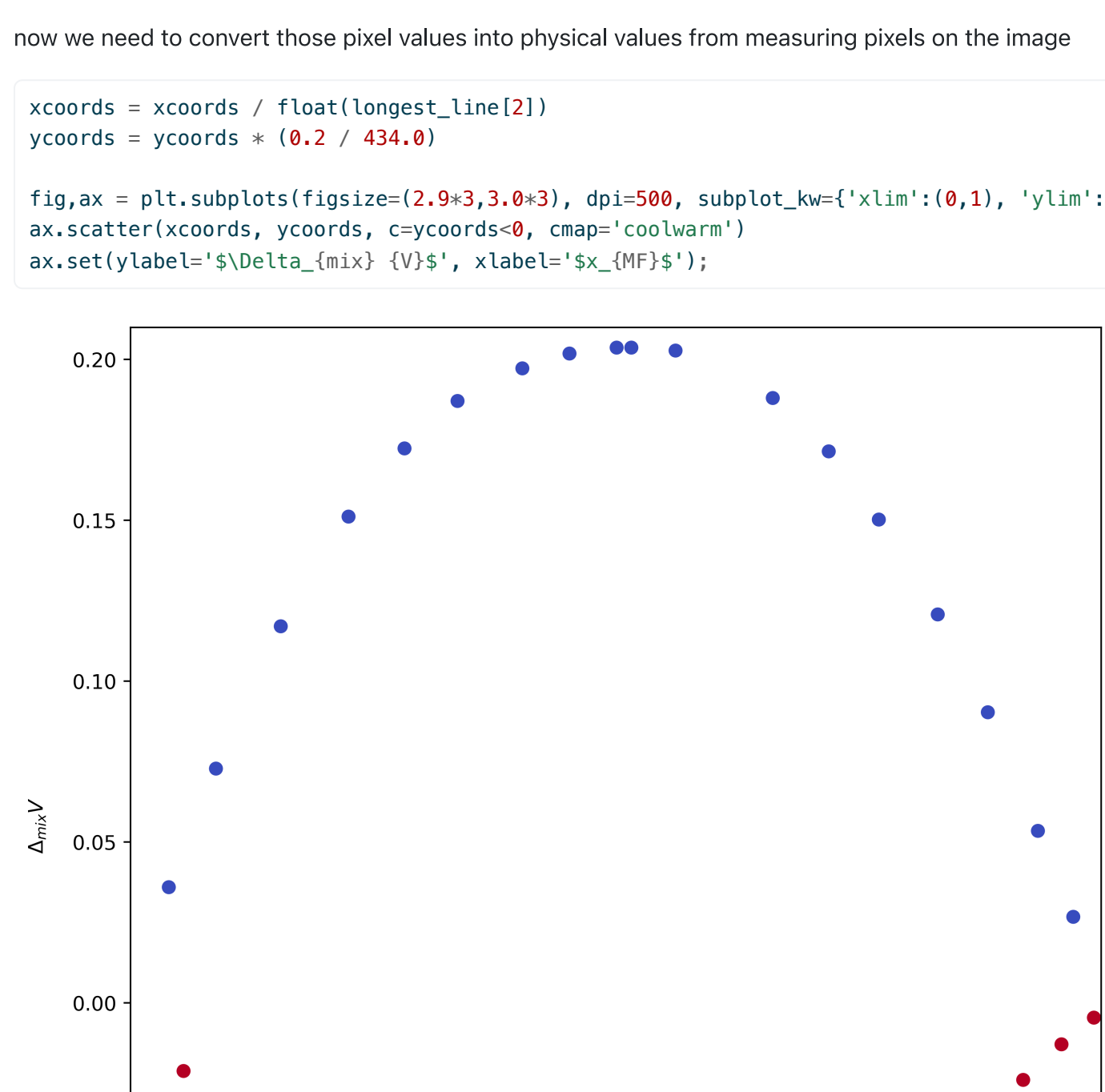
I will use a hough transform to find the circles in the image, and another to find the line. since the image is computer generated finding the shapes will be extremely easy and the parameters will likely not have to be tuned at all to get fantastic results.

```
import numpy as np
import matplotlib.pyplot as plt
import cv2
from glob import glob

file = glob("*.png")[0]
img = cv2.imread(file)
gray = cv2.cvtColor(img, cv2.COLOR_BGR2GRAY)
circles = cv2.HoughCircles(gray, cv2.HOUGH_GRADIENT, dp=1, minDist=3,
                           param1=200, param2=20, minRadius=1, maxRadius=20)

edges = cv2.Canny(gray, 50, 150, apertureSize=3)
lines = cv2.HoughLinesP(edges, 1, np.pi/180, threshold=100, minLineLength=100, maxLineGap
longest_line = None
max_length = 0

if lines is not None:
    for line in lines:
        x1, y1, x2, y2 = line[0]
        if abs(y1 - y2) < 5 and y1 > 50 and y1 < 500:  # near-horizontal line thats not a
            length = abs(x2 - x1)
            if length > max_length:
                max_length = length
                longest_line = (x1, y1, x2, y2)
    if longest_line:
        cv2.line(img, (longest_line[0], longest_line[1]), (longest_line[2], longest_line[
        cv2.putText(img, 'y=0 line', ((longest_line[0] + longest_line[2]) // 2, longest_l
                    cv2.FONT_HERSHEY_SIMPLEX, 0.8, (255, 0, 0), 1, cv2.LINE_AA)

xcoords, ycoords = [],[]
if circles is not None:
    circles = np.uint16(np.around(circles))
    for i, circle in enumerate(circles[0, :]):
        x, y = circle[0], circle[1]
        cv2.circle(img, (x, y), circle[2], (0, 255, 0), 2)

        y_0 = longest_line[1]
        y = y_0 - y
        xcoords.append(x)
        ycoords.append(y)

xcoords, ycoords = np.array(xcoords), np.array(ycoords)

plt.imshow(cv2.cvtColor(img, cv2.COLOR_BGR2RGB))
plt.title(file)
plt.axis('off')
plt.show()
```



now we need to convert those pixel values into physical values from measuring pixels on the image

```
xcoords = xcoords / float(longest_line[2])
ycoords = ycoords * (0.2 / 434.0)

fig,ax = plt.subplots(figsize=(2.9*3,3.0*3), dpi=500, subplot_kw={'xlim':(0,1), 'ylim':(-
ax.scatter(xcoords, ycoords, c=ycoords<0, cmap='coolwarm')
ax.set(ylabel='$\Delta_{mix} {V}$', xlabel='$x_{MF}$');
```



now we need to split this up into two data sets–one for each mixture. anything greater than zero is the ethanol mixture and anything below zero is the methanol mixture

```
indices = np.argsort(xcoords)
x_sorted, y_sorted = xcoords[indices], ycoords[indices]

x_mfe, y_mfe = x_sorted[y_sorted > 0], y_sorted[y_sorted > 0]
x_mfm, y_mfm = x_sorted[y_sorted < 0], y_sorted[y_sorted < 0]
```

for MF + methanol mixture first

note the naming convention there `x_mfm` is `x_mf` in the `methanol` mixture

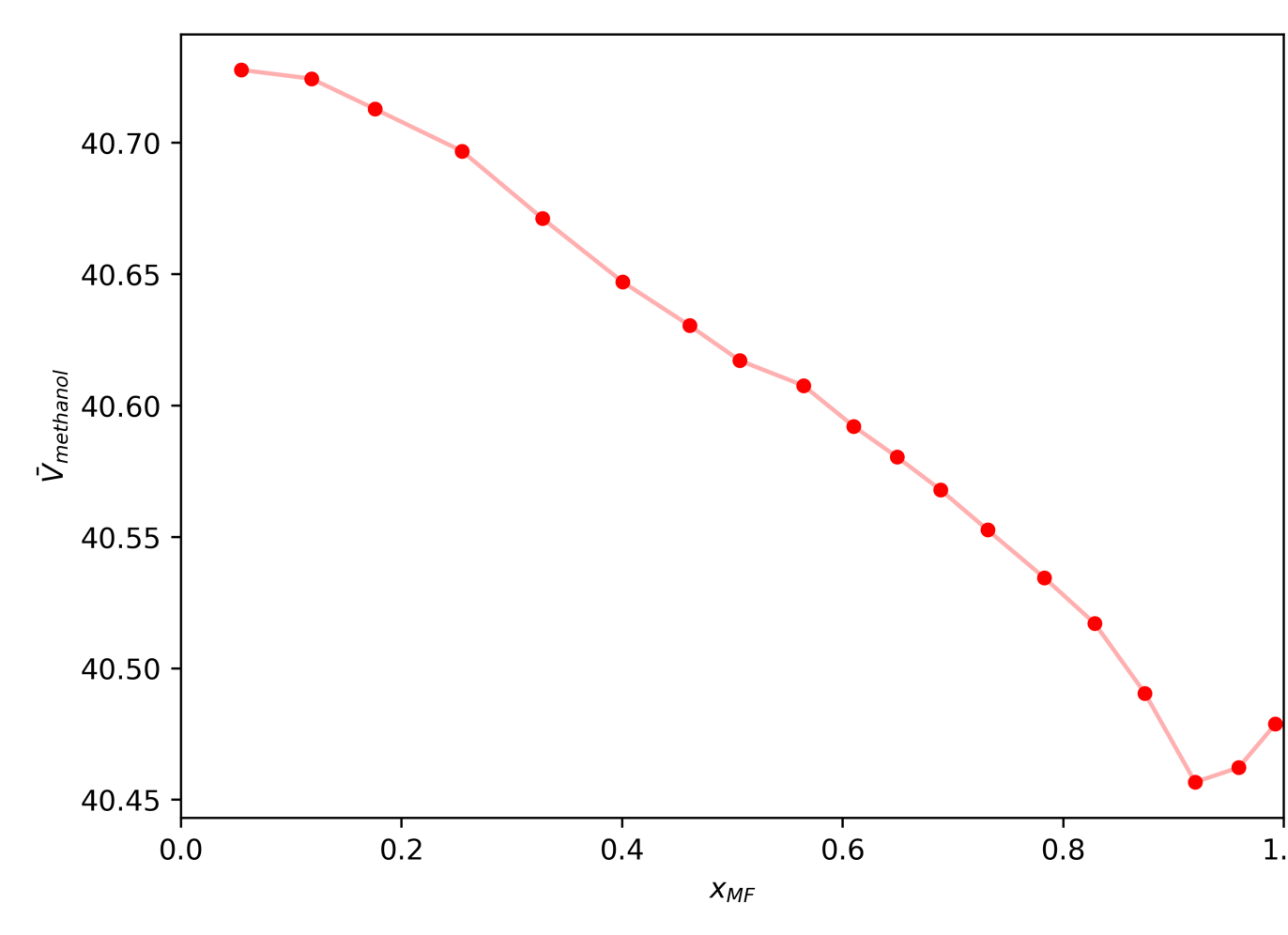
also the 0.06278 needs to be unit converted!

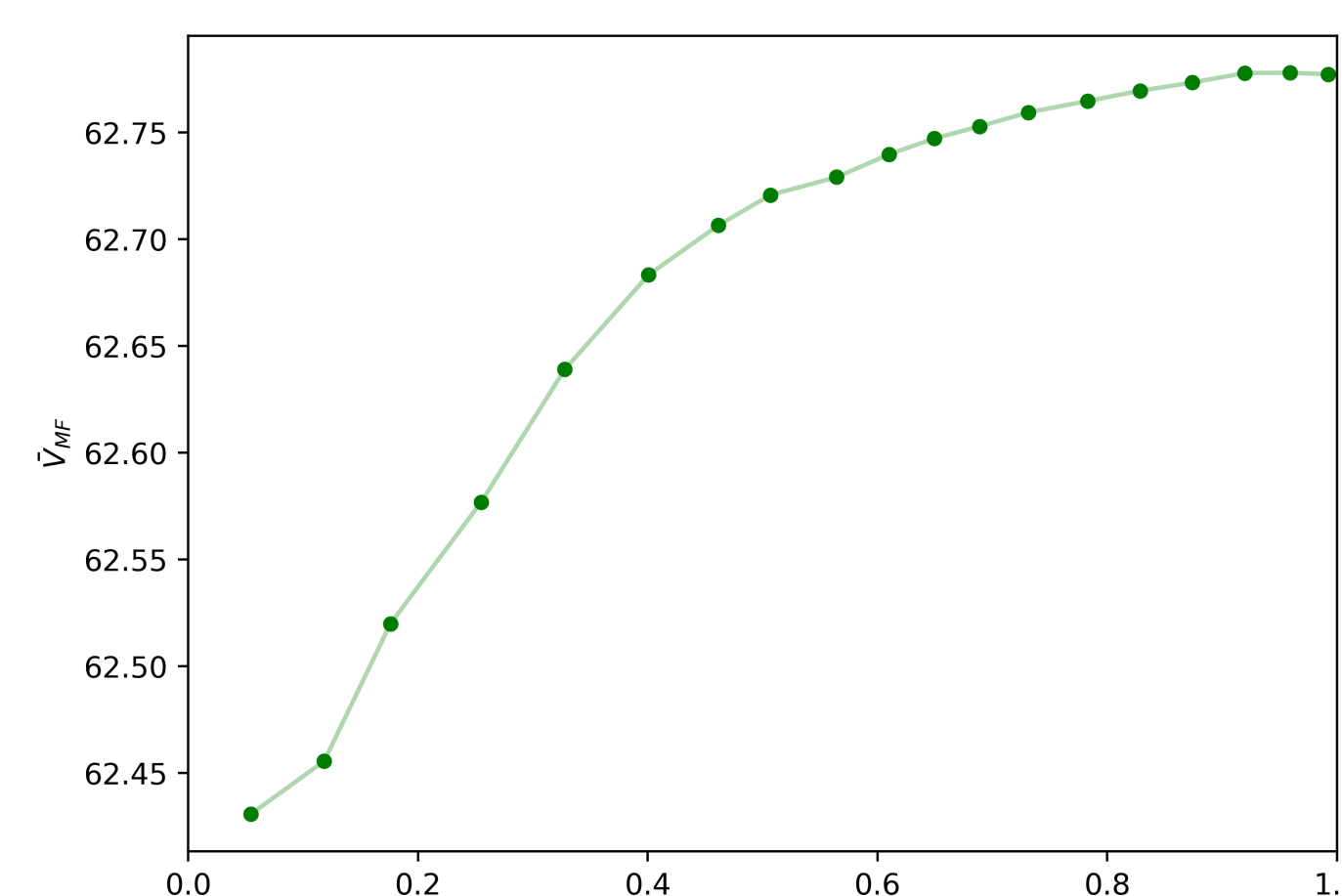
```
vmf = 0.06278 * 1000
vm = 0.04073 * 1000

vmix = y_mfm
dydx = np.gradient(y_mfm) / np.gradient(x_mfm)

pmv_m = vmix - (x_mfm * dydx) + vm
pmv_mf = vmix + ((1-x_mfm) * dydx) + vmf
```

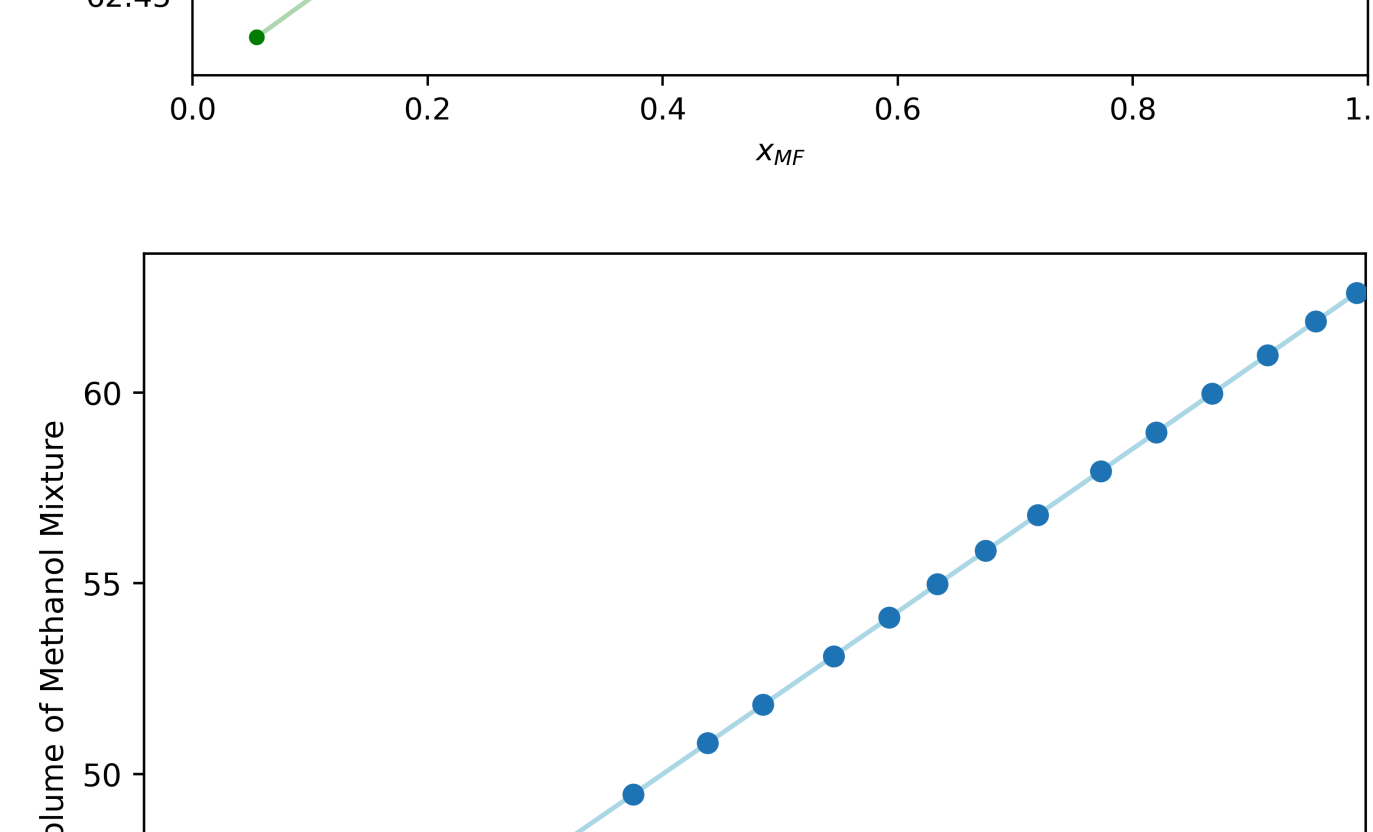
```
import pandas as pd
df = pd.DataFrame({
    'partial molar volume methanol': pmv_m,
    'partial molar volume methyl-formate': pmv_mf
}, index=x_mfm)
df.index.name = 'x_MF'
df
```

	partial molar volume methanol	partial molar volume methyl-formate
x_MF		
0.054628	40.727762	62.430691
0.118361	40.724424	62.455553
0.176024	40.712857	62.519908
0.254932	40.696857	62.576793
0.327769	40.671244	62.638996
0.400607	40.647051	62.683247
0.461305	40.630434	62.706465
0.506829	40.617124	62.720716
0.564492	40.607636	62.729092
0.610015	40.592113	62.739727
0.649469	40.580408	62.747210
0.688923	40.567890	62.752862
0.731411	40.552685	62.759426
0.783005	40.534435	62.764749
0.828528	40.517097	62.769555
0.874052	40.490553	62.773379
0.919575	40.456695	62.777844
0.959029	40.462258	62.777984
0.992413	40.478806	62.777277

```
dpi=500
fig,ax = plt.subplots(figsize=(7,5),dpi=dpi, subplot_kw={'xlabel':"$x_{MF}$", 'ylabel':"$
ax.scatter(x_mfm, pmv_m, c='red', s=18)
ax.plot(x_mfm, pmv_m, zorder=10, c='red', alpha=0.3);

fig,ax = plt.subplots(figsize=(7,5),dpi=dpi, subplot_kw={'xlabel':"$x_{MF}$", 'ylabel':"$
ax.scatter(x_mfm, pmv_mf, c='green', s=18)
ax.plot(x_mfm, pmv_mf, zorder=10, c='green', alpha=0.3);

fig,ax = plt.subplots(figsize=(7,5),dpi=dpi, subplot_kw={'xlabel':"$x_{MF}$", 'ylabel':"M
V = x_mfm * pmv_mf + (1-x_mfm) * pmv_m
ax.plot(x_mfm, V, c='lightblue')
ax.scatter(x_mfm, V, zorder=10);
```





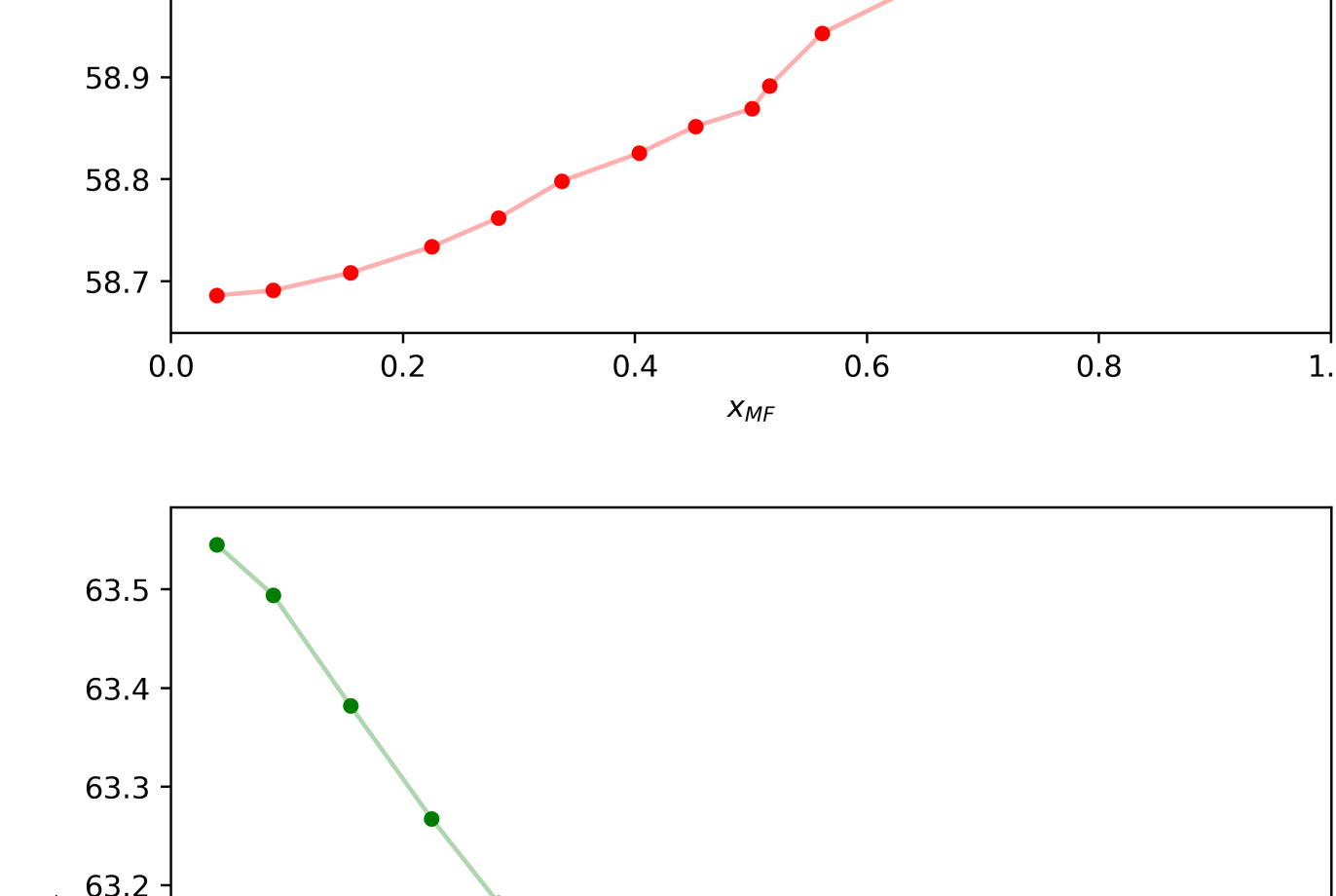


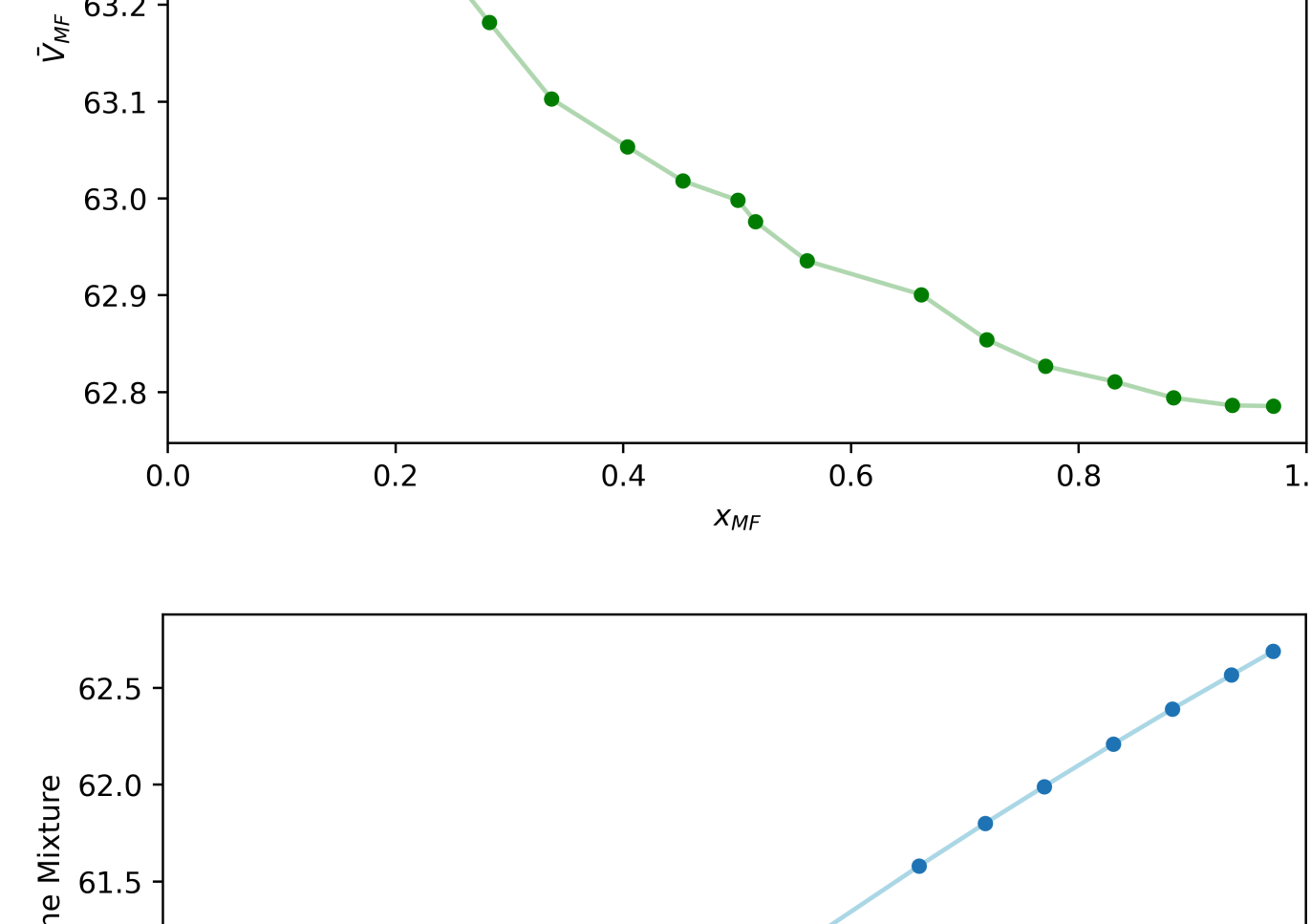
now for the ethanol mixture

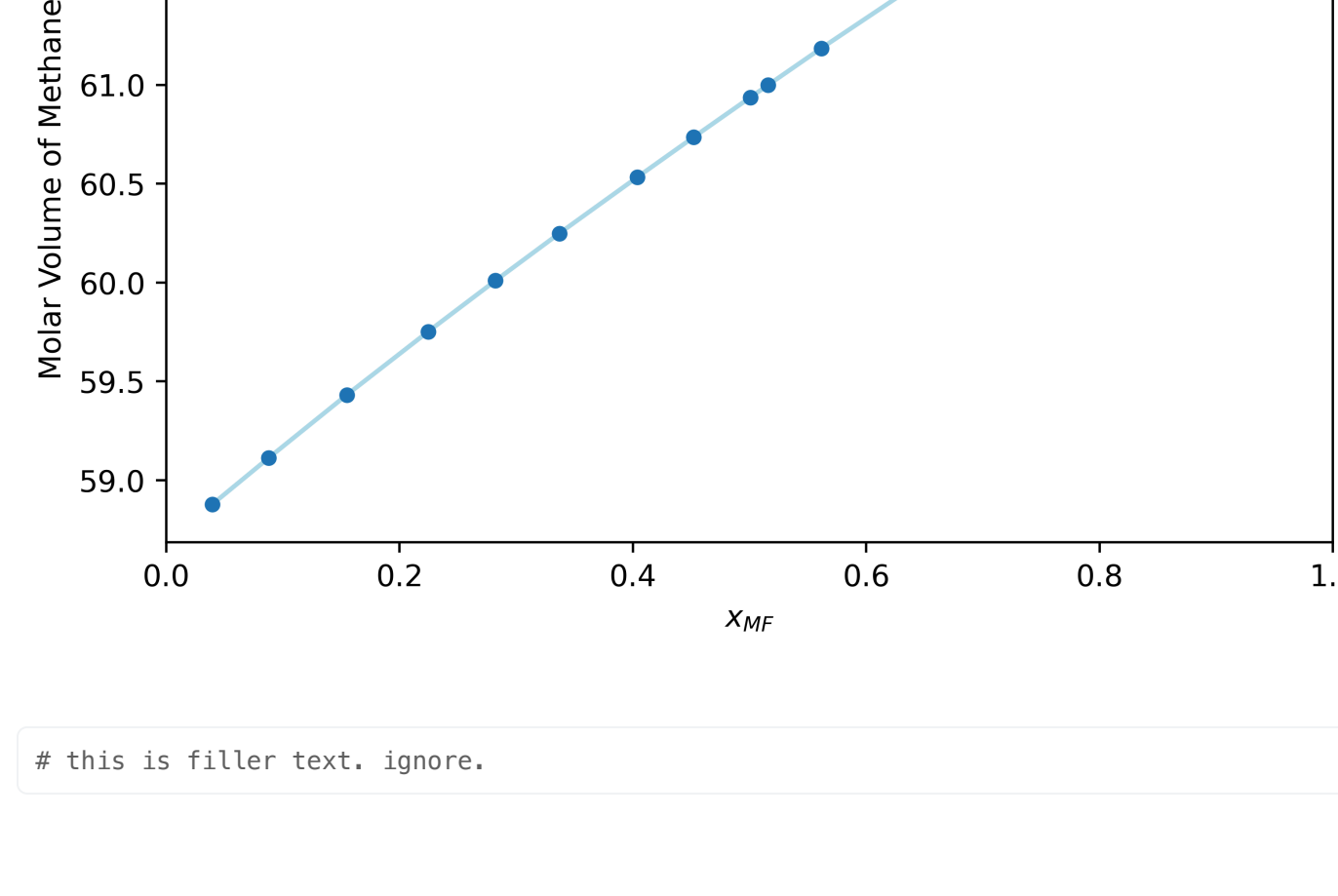
```
vmf = 0.06278 * 1000
ve = 0.05868 * 1000

vmix = np.array(y_mfe)
dydx = np.gradient(y_mfe) / np.gradient(x_mfe)

pmv_e = vmix - (x_mfe * dydx) + ve
pmv_mf = ( (vmix - (1-x_mfe)*(pmv_e - ve)) / x_mfe ) + vmf

df = pd.DataFrame({
    'partial molar volume ethanol': pmv_e,
    'partial molar volume methyl-formate': pmv_mf
}, index=x_mfe)
df.index.name = 'x_MF'
df
```

	partial molar volume ethanol	partial molar volume methyl-formate
x_MF		
0.039454	58.685991	63.545207
0.088012	58.690914	63.494189
0.154780	58.708264	63.381895
0.224583	58.733720	63.267558
0.282246	58.762003	63.182105
0.336874	58.798041	63.103030
0.403642	58.825622	63.053490
0.452200	58.851803	63.018234
0.500759	58.869203	62.998126
0.515933	58.891521	62.976336
0.561457	58.943153	62.935597
0.661608	58.999390	62.900826
0.719272	59.100200	62.854334
0.770865	59.178219	62.826793
0.831563	59.244379	62.810876
0.883156	59.346170	62.794137
0.934750	59.408873	62.786309
0.971168	59.419478	62.785568

```
dpi = 500
fig,ax = plt.subplots(figsize=(7,5),dpi=dpi, subplot_kw={'xlabel':"$x_{MF}$", 'ylabel':"$
ax.scatter(x_mfe, pmv_e, c='red', s=18)
ax.plot(x_mfe, pmv_e, zorder=10, c='red', alpha=0.3);

fig,ax = plt.subplots(figsize=(7,5),dpi=dpi, subplot_kw={'xlabel':"$x_{MF}$", 'ylabel':"$
ax.scatter(x_mfe, pmv_mf, c='green', s=18)
ax.plot(x_mfe, pmv_mf, zorder=10, c='green', alpha=0.3);

fig,ax = plt.subplots(figsize=(7,5),dpi=dpi, subplot_kw={'xlabel':"$x_{MF}$", 'ylabel':"M
V = x_mfe * pmv_mf + (1-x_mfe) * pmv_e
ax.plot(x_mfe, V, c='lightblue')
ax.scatter(x_mfe, V, zorder=10, s=18);
```








```
# this is filler text. ignore.
```