Problem 1. Partial molar concepts

1(a). For a mixture to be ideal, we need ΔHmix=0. However in this case ΔHmix≠0. The mixture is not ideal.

1(b). Plot molar enthalpy of mixing as a function of mole fraction of H2SO4.

In[9]:=
```
Nh2so4 = 1; MWh2so4 = 98.708;
Nh2o = {0.25, 1, 1.5, 2.33, 4, 5.44, 9, 10.1, 19, 20};
MWh2o = 18;
dHmix = -{8242, 28200, 34980, 44690, 54440, 58370, 62800, 64850, 70710, 71970};
```

In[13]:=
```
xh2so4 = Nh2so4 / (Nh2so4 + Nh2o)
```

Out[13]= $\left\{0.8, \frac{1}{2}, 0.4, 0.3003, \frac{1}{5}, 0.15528, \frac{1}{10}, 0.0900901, \frac{1}{20}, \frac{1}{21}\right\}$

In[14]:=
```
dHmix = dHmix / (Nh2so4 + Nh2o)
```

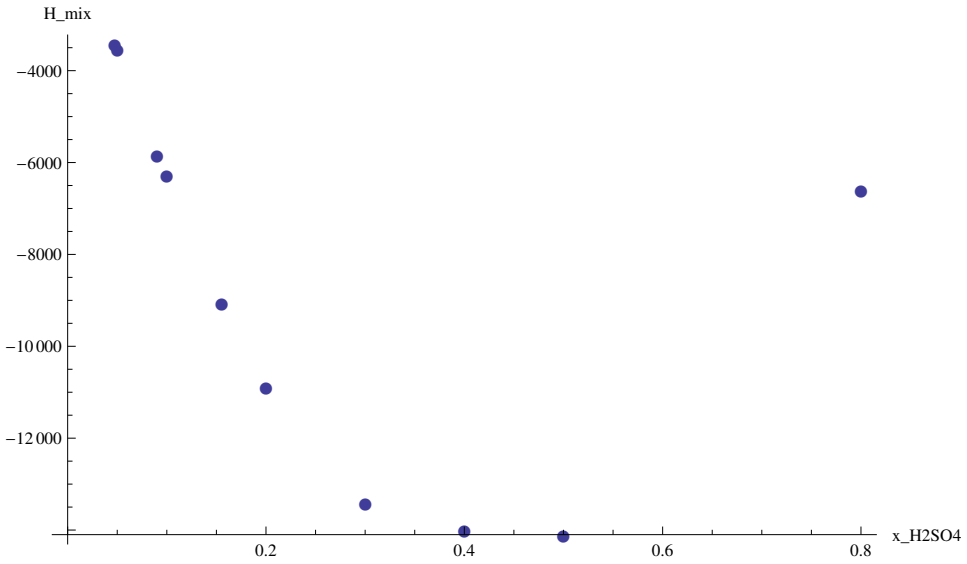
Out[14]= $\left\{-6593.6, -14100, -13992., -13420.4, -10888, -9063.66, -6280, -5842.34, -\frac{7071}{2}, -\frac{23990}{7}\right\}$

In[46]:=
```
dataset = Thread[{xh2so4, dHmix}]
```

Out[46]= $\left\{\{0.8, -6593.6\}, \left\{\frac{1}{2}, -14100\right\}, \{0.4, -13992.\}, \{0.3003, -13420.4\}, \left\{\frac{1}{5}, -10888\right\}, \{0.15528, -9063.66\}, \left\{\frac{1}{10}, -6280\right\}, \{0.0900901, -5842.34\}, \left\{\frac{1}{20}, -\frac{7071}{2}\right\}, \left\{\frac{1}{21}, -\frac{23990}{7}\right\}\right\}$

In[20]:=
```
ListPlot[%, AxesLabel → {x_H2SO4, H_mix}, PlotMarkers → {●, 10}]
```

Out[20]=



1(c) Heat evolved in mixing

In[21]:=
```
x60 = (60 / MWh2so4) / (60 / MWh2so4 + 40 / MWh2o)
```
Out[21]=
```
0.214783
```

In[22]:=
```
x25 = (25 / MWh2so4) / (25 / MWh2so4 + 75 / MWh2o)
```
Out[22]=
```
0.0573022
```

In[24]:=
```
delH = (60 / MWh2so4 + 40 / MWh2o) * (-12 000) + (25 / MWh2so4 + 75 / MWh2o) * (-3500)
```
Out[24]=
```
-49 430.7
```

1(d). Partial molar enthalpy in solution

In[25]:=
```
xh2so4 = (50 / MWh2so4) / (50 / MWh2so4 + 50 / MWh2o)
```
Out[25]=
```
0.154231
```

In[39]:=
```
xh2so4 = Nh2so4 / (Nh2so4 + Nh2o)
```
Out[39]=
$$\left\{0.8,\ \frac{1}{2},\ 0.4,\ 0.3003,\ \frac{1}{5},\ 0.15528,\ \frac{1}{10},\ 0.0900901,\ \frac{1}{20},\ \frac{1}{21}\right\}$$

In[43]:=
```
slopeofcurve = (dHmix[[7]] - dHmix[[5]]) / (xh2so4[[7]] - xh2so4[[5]])
```
Out[43]=
```
-46 080
```

In[44]:=
```
Hh2o = dHmix[[6]] - slopeofcurve * xh2so4[[6]]
```
Out[44]=
```
-1908.39
```

In[45]:=
```
Hh2so4 = dHmix[[6]] + slopeofcurve * (1 - xh2so4[[6]])
```
Out[45]=
```
-47 988.4
```

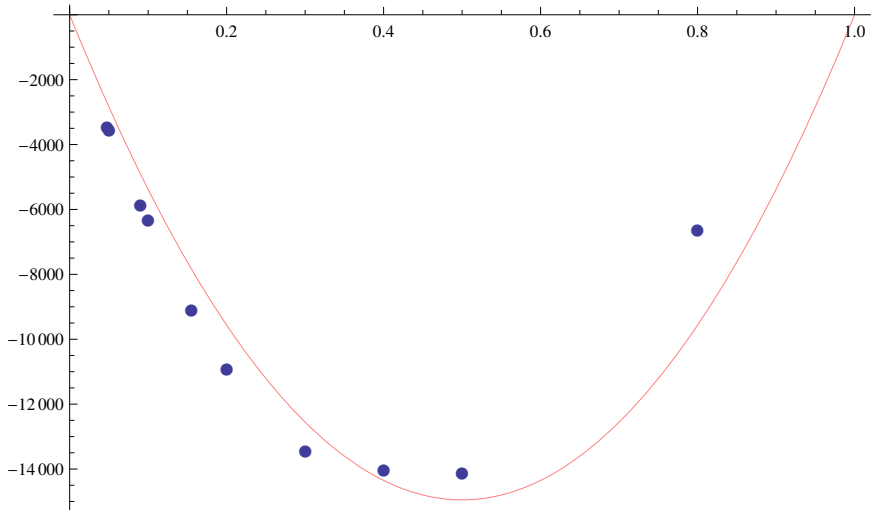
1(e). Fit to a regular solution model to estimate $\chi 12$.

In[47]:=
```
regularsoln = Fit[dataset, {x * (1 - x)}, x]
```
Out[47]=
```
-59 797.8 (1 - x) x
```

Therefore the mixing enthalpy model is -59797.8 $x_1 x_2$.

In[48]:=
```
Show[Plot[regularsoln, {x, 0, 1}, PlotStyle → Pink],
 ListPlot[dataset, AxesLabel → {x_H2SO4, H_mix}, PlotMarkers → {●, 10}]]
```

Out[48]=



Get χ from the fit:

In[49]:=
```
chi = -59 797.8 / (8.314 * 298)
```

Out[49]=
```
-24.1356
```