Inconsistent results?

Load RefpropLink

In[6]:=
```
Needs["RefpropLink`"]
```

```
Found NIST REFPROP Version: 10.0.0.2
```

Define a mixture and state point.

In[18]:=
```
fg001 = "CO2;H2O;Argon;Nitrogen;Oxygen;SO2";
z001 = {0.5, 0.4, 0.04, 0.01, 0.005, 0.045};
T001 = 1 °C;
P001 = 1 atm;
```

In[22]:=
```
out001 =
 RefProp[fg001, "TP", "D QMOLE Cp Cv H E CP/CV", 30 * T001, P001, z001, SatComp → True]
```

Out[22]=
$$\{D \to 0.0645454\ \text{mol/L},\ \text{QMOLE} \to 0.625672,\ Cp \to -9.99999 \times 10^6\ \text{J/(K mol)},$$
$$Cv \to -9.99999 \times 10^6\ \text{J/(K mol)},\ H \to 14\,853.4\ \text{J/mol},\ E \to 13\,283.6\ \text{J/mol},$$
$$CP/CV \to -9.99999 \times 10^6,\ z \to \{0.5, 0.4, 0.04, 0.01, 0.005, 0.045\},$$
$$x \to \{0.000520337, 0.998317, 1.83495 \times 10^{-6}, 1.87946 \times 10^{-7}, 1.8432 \times 10^{-7}, 0.00116074\},$$
$$y \to \{0.798829, 0.0420388, 0.0639301, 0.0159827, 0.00799129, 0.0712282\}\}$$

This is a two-phase region. Note from the second composition in x that the liquid phase is mostly water. H and E are the mole-weighted average Enthalpy and Internal Energy.

In[23]:=
```
xliq = out001[[9, 2]]
```

Out[23]=
$$\{0.000520337, 0.998317, 1.83495 \times 10^{-6}, 1.87946 \times 10^{-7}, 1.8432 \times 10^{-7}, 0.00116074\}$$

In[24]:=
```
yvap = out001[[10, 2]]
```

Out[24]=
$$\{0.798829, 0.0420388, 0.0639301, 0.0159827, 0.00799129, 0.0712282\}$$

Try this using SATSPLN

In[30]:=
```
out002 = RefProp[fg001, "TP", "D QMOLE Cp Cv H E CP/CV",
   30 * T001, P001, z001, SatComp → True, iFlag → 1]
```

... RefProp: INFO: Saturation splines created sucessfully.

Out[30]=
$$\{D \to 0.0645454\ \text{mol/L},\ \text{QMOLE} \to 0.625672,\ Cp \to -9.99999 \times 10^6\ \text{J/(K mol)},$$
$$Cv \to -9.99999 \times 10^6\ \text{J/(K mol)},\ H \to 14\,853.4\ \text{J/mol},\ E \to 13\,283.6\ \text{J/mol},$$
$$CP/CV \to -9.99999 \times 10^6,\ z \to \{0.5, 0.4, 0.04, 0.01, 0.005, 0.045\},$$
$$x \to \{0.000520337, 0.998317, 1.83495 \times 10^{-6}, 1.87946 \times 10^{-7}, 1.8432 \times 10^{-7}, 0.00116074\},$$
$$y \to \{0.798829, 0.0420388, 0.0639301, 0.0159827, 0.00799129, 0.0712282\}\}$$

In[31]:= **xliq = out002[[9, 2]]**

Out[31]= $\{0.000520337, 0.998317, 1.83495 \times 10^{-6}, 1.87946 \times 10^{-7}, 1.8432 \times 10^{-7}, 0.00116074\}$

In[32]:= **yvap = out002[[10, 2]]**

Out[32]= {0.798829, 0.0420388, 0.0639301, 0.0159827, 0.00799129, 0.0712282}

Get Liquid values

In[34]:= **liqinfo = RefProp["TP", "D QMOLE Cp Cv H E CP/CV", 30 * T001, P001, xliq]**

Out[34]= $\{D \to 55.2282\ \text{mol/L}$, QMOLE $\to -9.99999 \times 10^{6}$, Cp $\to 75.4139\ \text{J/(K mol)}$,
Cv $\to 74.1927\ \text{J/(K mol)}$, H $\to 2271.41\ \text{J/mol}$, E $\to 2269.57\ \text{J/mol}$, CP/CV $\to 1.01646\}$

In[38]:= **γLiq = liqinfo[[3, 2]] / liqinfo[[4, 2]]** **(* Cp/Cv *)**

Out[38]= 1.01646

Note: This is the same value returned by the returned CP/CV value. This is also very close to the value returned by the REFPROP GUI for Liquid @ 1.0163 (not sure why there's a slight difference).

Note also that gamma only equals H/E for an ideal gas! Therefore:

In[37]:= **liqinfo[[5, 2]] / liqinfo[[6, 2]]**

Out[37]= 1.00081

This is an inaccurate ratio, especially in the Liquid region!

Get Vapor values

In[35]:= **vapinfo = RefProp["TP", "D QMOLE Cp Cv H E CP/CV", 30 * T001, P001, yvap, SatComp → True]**

Out[35]= $\{D \to 0.0404019\ \text{mol/L}$, QMOLE $\to -9.99999 \times 10^{6}$, Cp $\to 36.4756\ \text{J/(K mol)}$,
Cv $\to 27.9585\ \text{J/(K mol)}$, H $\to 22381.\ \text{J/mol}$, E $\to 19873.1\ \text{J/mol}$, CP/CV $\to 1.30463$,
x $\to$ {0.798829, 0.0420388, 0.0639301, 0.0159827, 0.00799129, 0.0712282},
y $\to$ {0.798829, 0.0420388, 0.0639301, 0.0159827, 0.00799129, 0.0712282}$\}$

In[39]:= **γVap = vapinfo[[3, 2]] / vapinfo[[4, 2]]**

Out[39]= 1.30463

This is very close to the value returned from the REFPROP GUI @ 1.3074.

Note that the compositions, x & y in the calls above are only maintained in the 2-phase region where they are in equilibrium with each other. If you remove one or the other, they will no longer maintain that equilibrium composition unless they end up in the single-phase region as happens above.

Actual Saturation Curve Values @ original composition

In[46]:=
```
satVap = RefProp["TQ", "P D H E S Cp Cv CP/CV W", 30 * T001, 1, z001, iFlag → 1]
```

... RefProp: INFO: Saturation splines created sucessfully.

Out[46]=
```
{P → 10.5664 kPa , D → 0.00419663 mol/L , H → 31 259.7 J/mol ,
 E → 28 741.9 J/mol , S → 152.212 J/(K mol) , Cp → 35.3005 J/(K mol) ,
 Cv → 26.9347 J/(K mol) , CP/CV → 1.31059, W → 310.766 m/s }
```

Note: P is not 1 atm in this case! we need to make this call at the vapor composition, not the bulk.

In[47]:=
```
satVap = RefProp["TQ", "P D H E S Cp Cv CP/CV W", 30 * T001, 1, yvap, iFlag → 1]
```

... RefProp: INFO: Saturation splines created sucessfully.

Out[47]=
```
{P → 101.325 kPa , D → 0.0404019 mol/L , H → 22 381. J/mol ,
 E → 19 873.1 J/mol , S → 130.307 J/(K mol) , Cp → 36.4756 J/(K mol) ,
 Cv → 27.9585 J/(K mol) , CP/CV → 1.30463, W → 272.834 m/s }
```

In[56]:=
```
Pout = UnitConvert[satVap[[1, 2]], atm]
```

Out[56]=
```
1. atm
```

In[57]:=
```
γSatVap = satVap[[8, 2]]
```

Out[57]=
```
1.30463
```

Now we are at the vapor composition and a pressure of 1 atm which was the intended value.
Liquid saturation state at 30 °C does not converge, but it does with PQ inputs and returns the temperature at 30 °C.

In[52]:=
```
satLiq = RefProp["PQ", "T D H E S Cp Cv CP/CV W", P001, 0, xliq, iFlag → 1]
```

... RefProp: INFO: Saturation splines created sucessfully.

Out[52]=
```
{T → 303.15 K , D → 55.2282 mol/L , H → 2271.41 J/mol ,
 E → 2269.58 J/mol , S → 7.96273 J/(K mol) , Cp → 75.4139 J/(K mol) ,
 Cv → 74.1927 J/(K mol) , CP/CV → 1.01646, W → 1512.81 m/s }
```

In[54]:=
```
Tout = UnitConvert[satLiq[[1, 2]], °C]
```

Out[54]=
```
30. °C
```

In[55]:=
```
γSatLiq = satLiq[[8, 2]]
```

Out[55]=
```
1.01646
```