R407 A SpecificHeat Characterization V1

March 24, 2020

```
[1]: #Import the necessary libraries
     import math as math
     import numpy as np
     import pandas as pd
     import pickle
     import itertools
     from CoolProp.CoolProp import PropsSI
     import matplotlib.pyplot as plt
     from scipy.optimize import curve_fit
     from sklearn import linear_model
     from pandas import DataFrame
     from mpl_toolkits.mplot3d import Axes3D
     from pandas import ExcelWriter
     from IPython.core.interactiveshell import InteractiveShell
     import statsmodels.formula.api as sm
     InteractiveShell.ast_node_interactivity = "all"
     %matplotlib inline
[2]: # Iteration parameters
```

```
fluid = 'R407A.mix'

P_min_kPa = 100 #Minimum pressure in kPa we will be evaluating

P_max_kPa = 3000 #Maximum pressure in kPa we will be evaluating

T_min_K = -30+273 #Minimum temp

T_max_K = 60+273 #Max temp

n = 2900 #Number of samples we will collect

m = 180

P_kPa = np.linspace(P_min_kPa, P_max_kPa, n) #The array of the pressures we_u

will be evaluating

T_K = np.linspace(T_min_K, T_max_K, m) # This is the array of temperatures_u

divided into m spaces

Spec = [] # create a list

combo = list(itertools.product(P_kPa,T_K)) # assign to combo the combination of_u

pressures and arrays
```

```
[3]: # This step is only for extraction of data, if there is already a ' xxxx.p' _{\square} _{\longrightarrow} file, then it is not necesary to load data again
```

```
#Test values to make sure there was a coherent answer according to R407a
     → tables, since those are mostly experimental tests
     # the function C fro propsSi calculates the Mass specific constant pressure
     \rightarrow specific heat in [J/kq/K]
     \#print("Specific heat at 333K and 3000 kPa :", PropsSI('C', 'T', 273+60, 'P', \square)
     →3000*1000, 'REFPROP::R407a.mix'), "J/kq/K") #Maxi
     #print("Specific heat at 243K and 100 kPa :", PropsSI('C', 'T', 273-30, 'P', __
     →100*1000, 'REFPROP::R407a.mix'), "J/kg/K") # Minimi
     #for i in combo: # extract data from propsi, use only if library (coolprops) is \Box
      → loaded and functioning
      # [p,t]=i
       # try:
              Spec.append(PropsSI('C', 'P', p*1000, 'T', t, 'REFPROP::R407a.mix')) #_
      →use the function PropsSI to
             # get the specific heat according to pressure defined and temperature
      →defined, the pressure array has 2900 points
             #according to 3000 kPa - 100 kPa Range - the temperature similarly has I
     \hookrightarrow 90 points
        # except:
              Spec.append(0) # we don't know if there is values in all the spaces, __
      →or the extent of the ProposSI Function
             # What happened above is to make sure or assess if there is data in the \Box
      → file that will adjust ot our workspace
[4]: #print(Spec) # This is Specific heat, I have used the variable Spec because it
      →wass easy to start with and have a reference
[5]: # run this only when you want to extract data again from propsi, if there is \Box
     →already a SpecificHeat.p file; there is no need to run
     #pickle.dump(Spec, open( "SpecificHeat.p", "wb" ) ) # save values from propsi_
      →in file so we don't have to run each time
[3]: X, Y = np.meshgrid(T_K,P_kPa)
[4]: Spec = pickle.load(open("SpecificHeat.p", "rb")) # load values from file
[4]: PropsSI('C','P',1162*1000,'T',264, 'REFPROP::R407a.mix')
[4]: 1358.0620567466892
[5]: X.shape
     Y.shape
```

```
Y
[5]: (2900, 180)
[5]: (2900, 180)
[5]: array([[ 100.
                               100.
                                                100.
               100.
                               100.
                                                100.
            [ 101.00034495,
                               101.00034495,
                                                101.00034495, ...,
               101.00034495, 101.00034495,
                                                101.00034495],
            [ 102.00068989, 102.00068989,
                                                102.00068989, ...,
               102.00068989, 102.00068989,
                                               102.00068989],
            [ 2997.99931011, 2997.99931011, 2997.99931011, ...,
              2997.99931011, 2997.99931011,
                                               2997.99931011],
            [ 2998.99965505, 2998.99965505,
                                              2998.99965505, ...,
              2998.99965505, 2998.99965505,
                                               2998.99965505],
            [ 3000.
                              3000.
                                               3000.
              3000.
                              3000.
                                               3000.
                                                            ]])
[6]: Z = np.split(np.array(Spec), 2900)
     Z = np.array(Z)
     Z.shape
[6]: (2900, 180)
[7]: # plotting of raw data to visualize the behaviour and see Cp (propsSI) outputs
     from mpl_toolkits.mplot3d import Axes3D # import libraries for drawing in 3D
     import matplotlib.pyplot as plt
     from matplotlib import cm
     from matplotlib.ticker import LinearLocator, FormatStrFormatter
     # this is a graph of the data we are dealing with
     %matplotlib inline
     threedee = plt.figure().gca(projection='3d')
     threedee.scatter(X,Y, Z)
     threedee.set_xlabel('Pressure (kPa)')
     threedee.set ylabel('Temp. (K)')
     threedee.set_zlabel('Cp(J/kg/K)')
     plt.show()
     #fig = plt.figure()
     #ax = fig.gca(projection='3d')
     \#surf = ax.plot\_surface(X, Y, Z, cmap=cm.coolwarm, linewidth=0, 
     →antialiased=False)# plot the plot will give two distinc surfaces with an
     \rightarrow area in between
     \#ax.set\_xlabel('T(K)', fontsize = 14)
     \#ax.set\_ylabel('P(kPa)', fontsize = 14)
```

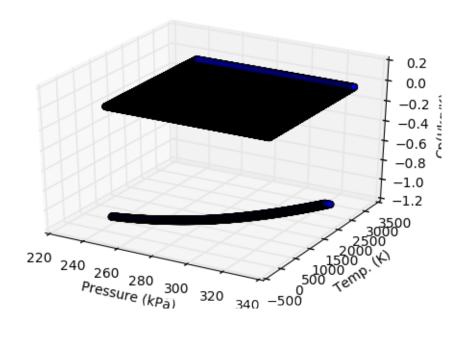
$\#ax.set_zlabel('C'(kJ/kg/K)', fontsize = 14)$

[7]: <mpl_toolkits.mplot3d.art3d.Path3DCollection at 0x7fa8af4bb518>

[7]: <matplotlib.text.Text at 0x7fa8af4f8860>

[7]: <matplotlib.text.Text at 0x7fa8af50c390>

[7]: <matplotlib.text.Text at 0x7fa8af512d68>



```
[8]: shf= pd.DataFrame.from_records( combo, columns= ['Pressure', 'Temperature'])
shf = shf.assign(Cp = Spec)
len (shf)
```

[8]: 522000

[9]: shf.head(3)

```
[9]:
        Pressure
                  Temperature
                                        Ср
           100.0
                   243.000000
                               770.671210
     0
     1
           100.0
                   243.502793
                                770.801452
     2
           100.0
                   244.005587
                                770.950061
```

[10]: Mask = (shf>0)

[11]: shf [Mask]

[11]:		Pressure	Temperature	Ср
	0	100.0	243.000000	770.671210
	1	100.0	243.502793	770.801452
	2	100.0	244.005587	770.950061
	3	100.0	244.508380	771.116277
	4	100.0	245.011173	771.299379
	5	100.0	245.513966	771.498686
	6	100.0	246.016760	771.713552
	7	100.0	246.519553	771.943363
	8	100.0	247.022346	772.187539
	9	100.0	247.525140	772.445528
	10	100.0	248.027933	772.716807
	11	100.0	248.530726	773.000880
	12	100.0	249.033520	773.297272
	13	100.0	249.536313	773.605537
	14	100.0	250.039106	773.925246
	15	100.0	250.541899	774.255994
	16	100.0	251.044693	774.597393
	17	100.0 100.0	251.547486	774.949075
	18 19		252.050279	775.310689
	20	100.0 100.0	252.553073 253.055866	775.681900 776.062390
	21	100.0	253.558659	776.451853
	22	100.0	254.061453	776.849999
	23	100.0	254.564246	777.256549
	24	100.0	255.067039	777.671239
	25	100.0	255.569832	778.093814
	26	100.0	256.072626	778.524031
	27	100.0	256.575419	778.961659
	28	100.0	257.078212	779.406474
	29	100.0	257.581006	779.858264
	•••	•••	•••	•••
	521970	3000.0	318.418994	NaN
	521971	3000.0	318.921788	NaN
	521972	3000.0	319.424581	NaN
	521973	3000.0	319.927374	NaN
	521974	3000.0	320.430168	NaN
	521975	3000.0	320.932961	NaN
	521976	3000.0	321.435754	NaN
	521977	3000.0	321.938547	NaN
	521978	3000.0	322.441341	NaN
	521979	3000.0	322.944134	NaN
	521980	3000.0	323.446927	NaN
	521981	3000.0	323.949721	NaN
	521982	3000.0	324.452514	NaN
	521983	3000.0	324.955307	NaN
	521984	3000.0	325.458101	NaN

```
521986
                3000.0
                                             NaN
                         326.463687
      521987
                3000.0
                         326.966480
                                             NaN
                3000.0
      521988
                         327.469274
                                             {\tt NaN}
      521989
                3000.0
                         327.972067
                                             NaN
      521990
                3000.0
                         328.474860
                                             NaN
      521991
                3000.0
                         328.977654
                                             NaN
      521992
                3000.0
                                             NaN
                         329.480447
      521993
                3000.0
                         329.983240
                                             NaN
      521994
                3000.0
                         330.486034
                                             NaN
      521995
                3000.0
                         330.988827
                                             NaN
      521996
                3000.0
                         331.491620
                                             NaN
      521997
                3000.0
                         331.994413
                                             NaN
      521998
                3000.0
                         332.497207
                                             NaN
      521999
                3000.0
                         333.000000
                                             NaN
      [522000 rows x 3 columns]
[12]: groupingtest = shf.loc[shf['Cp']>0]
      #len(shf.loc[shf['Cp']>0])
      groupingtest.head(2)
[12]:
         Pressure
                   Temperature
                                         Ср
            100.0
                    243.000000 770.671210
            100.0
                    243.502793 770.801452
      1
 []: #writer = pd.ExcelWriter('pandas_simplecp.xlsx', engine='xlsxwriter')
      #shf.loc[shf['Cp']<0].to_excel(writer, sheet_name='Sheet1')
      #writer.save()
[13]: negatives = shf.loc[shf['Cp']<0]
      positives = shf.loc[shf['Cp']>0]
[14]: # Plot the extracted data from propsi
      print(shf.head());
      threedee = plt.figure().gca(projection='3d')
      threedee.scatter(positives['Temperature'],positives['Pressure'],
       →positives['Cp'])
      threedee.set xlabel('Temp. (K)')
      threedee.set_ylabel('Pressure (kPa)')
      threedee.set_zlabel('Cp (J/kg/k)')
      plt.show()
        Pressure Temperature
                                        Ср
     0
           100.0
                   243.000000 770.671210
```

NaN

521985

3000.0

100.0

100.0

1

243.502793 770.801452

244.005587 770.950061

325.960894

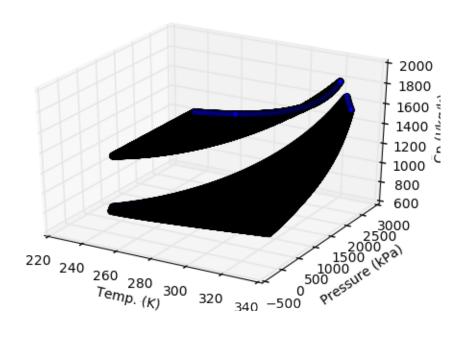
```
3 100.0 244.508380 771.116277
4 100.0 245.011173 771.299379
```

[14]: <mpl_toolkits.mplot3d.art3d.Path3DCollection at 0x7fa8a542aac8>

[14]: <matplotlib.text.Text at 0x7fa8a5bb22e8>

[14]: <matplotlib.text.Text at 0x7fa8a5bb7dd8>

[14]: <matplotlib.text.Text at 0x7fa8a5bc87f0>



[]: # Time to separate the characterization!! :)

Regression model for Mix (acording to saturated caracterization)

0.0.1 Characterization model for latent heat portion liquid portion

```
threedee.set_ylabel('Pressure (kPa)')
threedee.set_zlabel('Cp (J/kg/K)')
plt.show()
```

```
[15]: Pressure Temperature Cp

9360 152.017937 243.0 -1.109744e+08

9540 153.018282 243.0 -1.109744e+08

9720 154.018627 243.0 -1.109744e+08

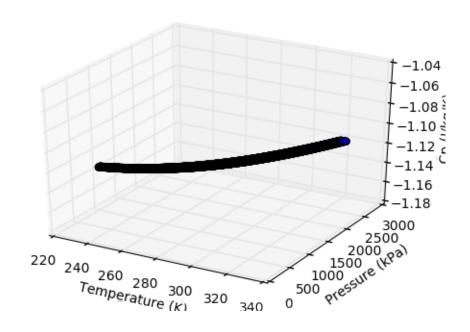
9900 155.018972 243.0 -1.109744e+08
```

[15]: <mpl_toolkits.mplot3d.art3d.Path3DCollection at 0x7fa8a41e6dd8>

[15]: <matplotlib.text.Text at 0x7fa8a5bdd2e8>

[15]: <matplotlib.text.Text at 0x7fa8a65ccba8>

[15]: <matplotlib.text.Text at 0x7fa8a41b6470>



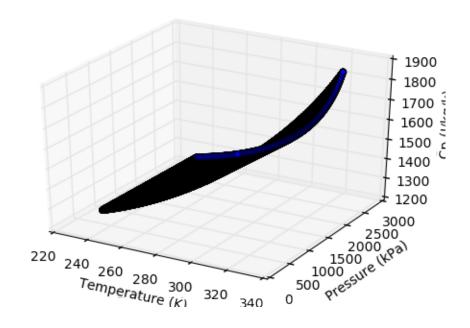
[]: # Due to the results, it is clear that propsSI for the latent portion of the specific heat data, is throwing a value that does not match with the sphysical phenomena.

The value for the portion should be instead in [J/mol] or [J/kg] since it is a rise described as the mass or molar latent heat at constant temperature # Therefore, this portion of the characterization will be performed in a seperate krunchy book

0.1 Characterization model Specific Heat for liquid portion

[16]: <matplotlib.text.Text at 0x7fa8ab3ba358>

[16]: <matplotlib.text.Text at 0x7fa8ab3ab940>



```
[17]: Liquid_positives = Liquid_positives.assign(Temp_sq = Liquid_positives['Temperature']**2)#1.56

Liquid_positives = Liquid_positives.assign(Press_sq = Liquid_positives['Pressure']**2) #1.4

Liquid_positives.head(3)
```

```
Pressure Temperature
[17]:
                                   Cp Temp_sq
                                                Press_sq
    17820 199.034150
                    243.0 1310.394142 59049.0 39614.592750
                       243.0 1310.390232 59049.0 40013.799051
    18000 200.034495
    18180 201.034840 243.0 1310.386321 59049.0 40415.006733
[39]: resultLiquid = sm.ols(formula="Cp ~ Temperature + Pressure + Temp_sq", __
    →data=Liquid positives).fit()
    forecastLiquid = resultLiquid.
     →predict(Liquid_positives[['Temperature', 'Pressure', 'Temp_sq']])
    ErrorLiquid = pd.DataFrame({'Error': forecastLiquid-Liquid_positives.Cp})
    print(resultLiquid.params)
    print(resultLiquid.summary())
    ErrorLiquid.describe()
    Intercept 5006.961681
               -30.457731
    Temperature
    Pressure
                -0.008074
                 0.063061
    Temp sq
    dtype: float64
                         OLS Regression Results
    _______
    Dep. Variable:
                                  R-squared:
                                                           0.991
                              Ср
                             OLS Adj. R-squared:
    Model:
                                                           0.991
                                                      9.083e+06
                  Least Squares F-statistic:
    Method:
                  Wed, 13 Dec 2017 Prob (F-statistic):
19:12:34 Log-Likelihood:
    Date:
                                                           0.00
                                                    -9.0782e+05
    Time:
    No. Observations:
                           249026 AIC:
                                                        1.816e+06
                           249022 BIC:
    Df Residuals:
                                                        1.816e+06
    Df Model:
    Covariance Type: nonrobust
    ______
                 coef std err t P>|t| [0.025
                                                          0.975]
    ______
   Intercept 5006.9617 3.377 1482.485 0.000 5000.342 5013.581
Temperature -30.4577 0.024 -1249.461 0.000 -30.506 -30.410
              -0.0081 3.47e-05 -232.643
    Pressure
                                        0.000
                                                 -0.008
                                                           -0.008
             0.0631 4.39e-05 1437.625 0.000 0.063
    Temp sq
    ______
    Omnibus:
                        133221.287 Durbin-Watson:
                                                           0.155
                            0.000 Jarque-Bera (JB): 2791171.881
    Prob(Omnibus):
    Skew:
                            2.127 Prob(JB):
                                                            0.00
                          18.840 Cond. No.
                                                         1.39e+07
    ______
```

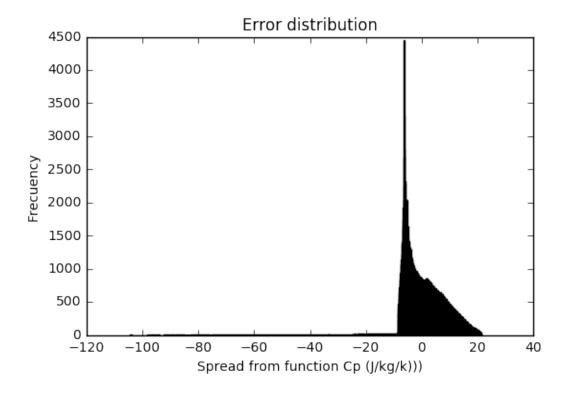
Warnings:

[1] Standard Errors assume that the covariance matrix of the errors is correctly

specified.

[2] The condition number is large, 1.39e+07. This might indicate that there are strong multicollinearity or other numerical problems.

```
[39]:
                   Error
      count 2.490260e+05
     mean -4.790373e-10
      std
            9.267901e+00
     min
          -1.045214e+02
     25%
          -5.547611e+00
      50%
          -1.018039e+00
      75%
           5.538027e+00
     max
            2.151780e+01
[40]: plt.hist(ErrorLiquid.Error, bins = 1500); # histogram of error distribution
      plt.title('Error distribution')
      plt.xlabel('Spread from function Cp (J/kg/K)))')
      plt.ylabel('Frecuency')
[40]: (array([ 1., 1., 0., ..., 29., 23., 14.]),
      array([-104.52140613, -104.43737999, -104.35335385, ...,
                                                               21.34974705,
                              21.51779932]),
                21.43377318,
      <a list of 1500 Patch objects>)
[40]: <matplotlib.text.Text at 0x7fa892b5efd0>
[40]: <matplotlib.text.Text at 0x7fa8930e70b8>
[40]: <matplotlib.text.Text at 0x7fa892e48eb8>
```



1 Result for liquid portion CpLiquid = $aT^2+bT+cP+f[J/kg/K]$

1.0.1 R2 = 0.991

a is the parameter for $Temp_sq: 0.063061$

b is the parameter for Temperature : -30.457731

c is the parameter for Pressure : -0.008074

f is the Intercept: 5006.961681

2 Result for liquid portion CpLiquid = bT+cP+f

2.0.1 R2 = 0.916

b is the parameter for Temperature : 4.558210

c is the parameter for Pressure: -0.002865

f is the Intercept: 165.200746

3 Result for liquid portion CpLiquid = bT+f

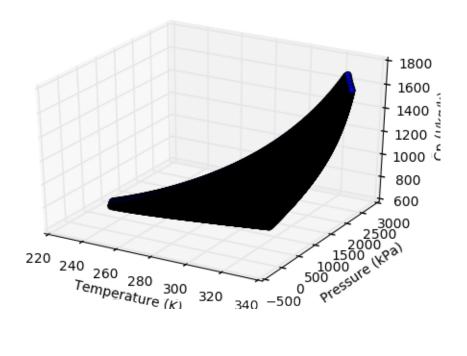
3.0.1 R2 = 0.916

b is the parameter for Temperature : 4.525411

f is the Intercept: 169.546153

3.1 Characterization model for Specific Heat for Vapor portion

- [24]: <mpl_toolkits.mplot3d.art3d.Path3DCollection at 0x7fa8a9d74ac8>
- [24]: <matplotlib.text.Text at 0x7fa8aa20a518>
- [24]: <matplotlib.text.Text at 0x7fa8aa0aaef0>
- [24]: <matplotlib.text.Text at 0x7fa8aa033358>



```
[25]: Vapor_positives.head(3)
[25]:
         Pressure Temperature
                                         Ср
            100.0
                    243.000000 770.671210
      0
      1
            100.0
                    243.502793 770.801452
      2
            100.0
                    244.005587 770.950061
[34]: Vapor_positives = Vapor_positives.assign(Temp_sq =__
       \hookrightarrow Vapor_positives['Temperature']**2)#1.56 as a suggestion, overall it is
       \rightarrow reasonable
      Vapor_positives = Vapor_positives.assign(Press_sq =_
       →Vapor_positives['Pressure']**2) #1.4
[35]: resultVapor = sm.ols(formula="Cp ~ Temperature + Pressure ", __
       →data=Vapor_positives).fit()
      forecastVapor = resultVapor.predict(Vapor_positives[['Pressure','Temperature']])
      ErrorVapor = pd.DataFrame({'Error': forecastVapor-Vapor_positives.Cp})
      print(resultVapor.params)
      print(resultVapor.summary())
      ErrorVapor.describe()
     Intercept
                     887.750263
```

OLS Regression Results

-0.381473

0.276162

Temperature Pressure

dtype: float64

Dep. Variable: R-squared: 0.937 Model: OLS Adj. R-squared: 0.937 Method: Least Squares F-statistic: 1.206e+06 Date: Wed, 13 Dec 2017 Prob (F-statistic): 0.00 Time: 19:10:22 Log-Likelihood: -8.3675e+05 No. Observations: 163429 AIC: 1.673e+06 Df Residuals: 163426 BIC: 1.674e+06

Df Model: Covariance Type: nonrobust

Error

=========								
	coef	std err	t	P> t	[0.025	0.975]		
Intercept Temperature	887.7503 -0.3815 0.2762	1.788	496.464 -62.475	0.000	884.246 -0.393	891.255 -0.370 0.277		
Pressure	0.2762	0.000	1307.812 ======	0.000 =====	0.276	0.277		
Omnibus:		41533.	631 Durbi	n-Watson:		0.177		
Prob(Omnibus):		0.0	000 Jarqu	e-Bera (JB):		169829.334		
Skew:		1.:	209 Prob(JB):		0.00		
Kurtosis:		7.3	369 Cond.	No.		1.88e+04		

Warnings:

- [1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
- [2] The condition number is large, 1.88e+04. This might indicate that there are strong multicollinearity or other numerical problems.

```
[35]:
     count 1.634290e+05
     mean 4.501923e-13
     std 4.048774e+01
     min -2.775680e+02
     25% -1.836774e+01
     50%
          3.330836e+00
     75%
          2.282027e+01
            8.744900e+01
     max
[33]: plt.hist(ErrorVapor.Error, bins = 150); # histogram of error distribution
     plt.title('Error distribution')
     plt.xlabel('Spread from function Cp (J/kg/k)))')
     plt.ylabel('Frecuency')
```

```
[33]: (array([ 3.00000000e+00,
                               4.00000000e+00, 4.0000000e+00,
               4.00000000e+00, 5.00000000e+00, 6.00000000e+00,
               6.00000000e+00,
                               6.00000000e+00,
                                                6.00000000e+00,
```

```
7.0000000e+00,
                  8.0000000e+00,
                                     1.00000000e+01,
1.0000000e+01,
                  1.20000000e+01,
                                     1.4000000e+01,
1.20000000e+01,
                  1.20000000e+01,
                                     1.4000000e+01,
1.50000000e+01,
                  1.4000000e+01,
                                     1.60000000e+01,
2.10000000e+01,
                  2.00000000e+01,
                                     2.00000000e+01,
2.00000000e+01,
                  2.3000000e+01,
                                     2.30000000e+01,
2.30000000e+01,
                  2.60000000e+01,
                                     2.60000000e+01,
2.60000000e+01,
                                     3.10000000e+01,
                  3.20000000e+01,
3.10000000e+01,
                  3.70000000e+01,
                                     3.4000000e+01,
3.60000000e+01,
                  3.60000000e+01,
                                     3.90000000e+01,
4.00000000e+01.
                  4.50000000e+01,
                                     4.50000000e+01,
4.60000000e+01,
                  5.0000000e+01,
                                     4.9000000e+01,
5.00000000e+01,
                  5.60000000e+01,
                                     5.50000000e+01,
5.90000000e+01,
                  6.3000000e+01,
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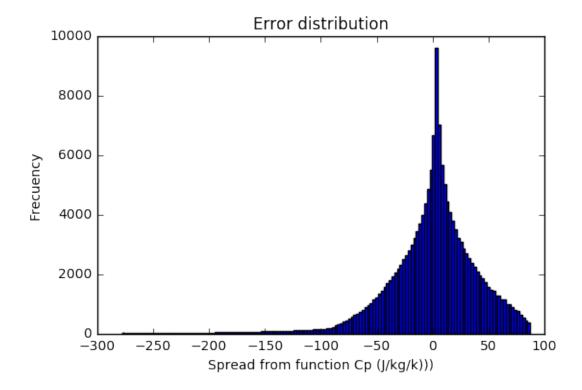
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4 Result for Vapor portion $CpVapor = aT^2+bT+cP+f$

 $4.1 \quad [\mathrm{J/kg/K}]$

4.1.1 R2 = 0.939

a is the parameter for Temp_sq: -0.017369

b is the parameter for Temperature: 9.963247

c is the parameter for Pressure: 0.278669

f is the Intercept: -645.880275

5 Result for Vapor portion CpVapor = bT+cP+f

5.0.1 R2 = 0.937

b is the parameter for Temperature: -0.381473

c is the parameter for Pressure : 0.276162

f is the Intercept: 887.750263

```
[]: #Spec.append(PropsSI('C','P', p*1000,'T',t, 'REFPROP::R407a.mix')) # test
#in case there is a need to export data to excel
#writer = pd.ExcelWriter('pandas_simpledensity.xlsx', engine='xlsxwriter')
#Liquid_df.to_excel(writer, sheet_name='Sheet1')
#writer.save()
```