**Experimental data fitting to the thermodynamic virial equation of state, using regression**

clear

clc

%the purpose of this code is to make use of regression to model

%experimental data for the fitting of the virial equation of state

% entering of experimental data

t = [ 273.15,298.15,303.15,323.15,348.15,373.15,398.15,423.15,448.15,473.15,498.15,523.15,548.15,573.15,598.15,623.15];

B = [ -222.21,-185.8,-179.4,-156.7,-133.0,-113.6,-97.3,-83.6,-71.7,-61.5,-52.4,-44.5,-37.3,-30.9,-25.0,-19.6];

C = [10360,10600,10400,9650,8660,7720,6960,6260,5680,5290,4840,4500,4130,3860,3540,3270];

crittemp = 305.3;% critical temperature given “Introduction to Chemical Engineering Thermodynamics”, J. M. Smith, H. C. Van Ness & M. M. Abbott

redutemp = t./crittemp;% reduced temperature calculated which will be used for the model

% calculating the B values using the model. differentiate the model

% equation partially with respect to each unknown.

mat1 = ones(1,16); %values for a0 is a vector of ones

a1calc = redutemp.^-1.6; %calculate values for a1

r1=[]; %initialize a vector to store all a1 values

for n=1:1:16; %initialize a for loop to calculate all the values of a1

r1(n)=a1calc(n);

end

a2calc = redutemp.^-4.2; %calculate values for a2

r2=[]; %initialize a vector to store all a2 values

for n = 1:1:16 %initialize a for loop to calculate all the values of a2

r2(n)=a2calc(n);

end

mat2 = [mat1' r1' r2']; %a matrix containing all initial coefficients

mat3 = mat2\B'; %use the backslash operator to solve for the final coefficients

a0 = mat3(1);

a1 = mat3(2);

a2 = mat3(3);

calcB = a0+a1.\*r1+a2.\*r2; %calculated B values using the model

% calculating the C values using the model. differentiate the model

% equation partially with respect to each unknown.

mat4 = ones(1,16); %values for b0 is a vector of ones

b1calc = redutemp.^-2.8; %calculate values for b1

r3=[]; %initialize a vector to store all b1 values

for n=1:1:16; %initialize a for loop to calculate all the values of b1

r3(n)=b1calc(n);

end

b2calc = redutemp.^-3;

r4=[]; %initialize a vector to store all b2 values

for n=1:1:16; %initialize a for loop to calculate all the values of b1

r4(n)=b2calc(n);

end

b3calc = redutemp.^-6;

r5=[]; %initialize a vector to store all b3 values

for n=1:1:16; %initialize a for loop to calculate all the values of b3

r5(n)=b3calc(n);

end

b4calc = redutemp.^-10.5;

r6=[]; %initialize a vector to store all b4 values

for n=1:1:16; %initialize a for loop to calculate all the values of b4

r6(n)=b4calc(n);

end

mat5 = [mat4' r3' r4' r5' r6']; %producing a matrix with the initial coefficients

mat6 = mat5\C';

b0 = mat6(1);

b1 = mat6(2);

b2 = mat6(3);

b3 = mat6(4);

b4 = mat6(5);

calcC = b0+b1.\*r3+b2.\*r4+b3.\*r5+b4.\*r6 ; %calculated C values using the model

tempNEW = 340:1380; %new temperature values

redutempNEW=tempNEW./crittemp; %corresponding new reduced temperature values

%calculate B and C values for the new temperature range:

calcBnew = a0+a1.\*(redutempNEW).^-1.6+a2.\*(redutempNEW).^-4.2;

calcCnew = b0+b1.\*(redutempNEW).^-2.8+b2.\*(redutempNEW).^-3+b3.\*(redutempNEW).^-6+b4.\*(redutempNEW).^-10.5;

%plot graph of the experimental and model predictions for the second and

%third virial coefficients as functions of reduced temperature

figure(1);

plot(redutemp,B,'sq');

hold on

plot(redutempNEW,calcBnew);

xlabel('Reduced Temperature');

ylabel('B values');

title('Graph of the experimental and model predictions for the second virial coefficient');

legend('Experimental Values','Model Values');

figure(2);

plot(redutemp,C,'k\*');

hold on

plot(redutempNEW,calcCnew,'r');

xlabel('Reduced Temperature');

ylabel('C values');

title('Graph of the experimental and model predictions for the third virial coefficient');

legend('Experimental Values','Model Values');

%calculations for pressure

Bderiv=-1.6\*a1\*crittemp^1.6.\*tempNEW.^-2.6-4.2\*a2\*crittemp^4.2.\*tempNEW.^-5.2;

Cderiv=-2.8\*b1\*crittemp^2.8.\*tempNEW.^-3.8-3\*b2\*crittemp^3.\*tempNEW.^-4-6\*b3\*crittemp^6.\*tempNEW.^-7-10.5\*b4\*crittemp^10.5.\*tempNEW.^-11.5;

volume=(2.\*calcCnew-Cderiv.\*tempNEW)./(Bderiv.\*tempNEW-calcBnew); %see report for derivation of this equation

R=83.14; %universal gas constant

Z=1+calcBnew./volume+calcCnew./volume.^2; %virial equation of state

pressure=Z.\*R.\*tempNEW./volume;

critpressure=48.72; %critical pressure in bar

redupressure=pressure./critpressure;

%plot graph of reduced temperature vs. reduced pressure

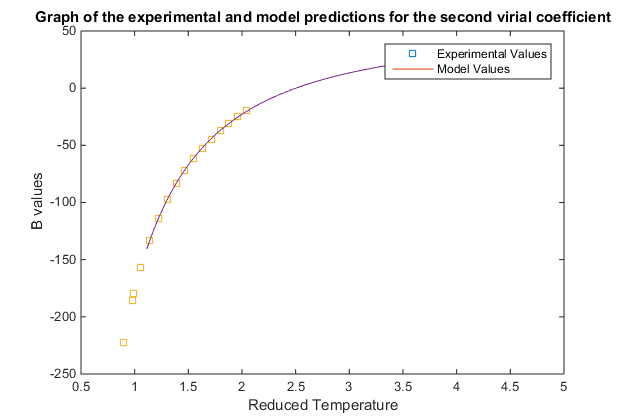
figure(3);

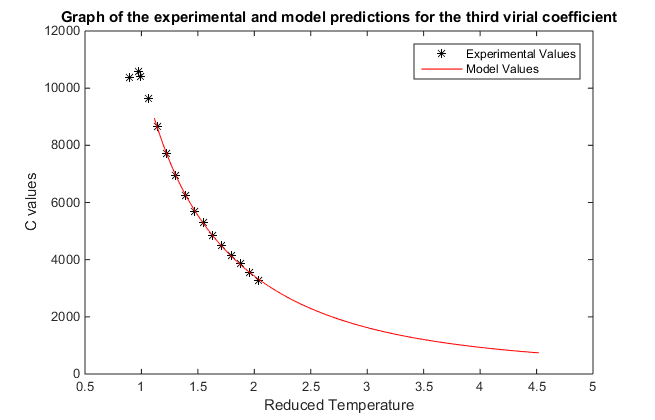
plot(redupressure,redutempNEW,'k');

xlabel('Reduced Pressure');

ylabel('Reduced Temperature');

title('Inversion Curve');

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