Lab Session 5

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AIM

The goal of the laboratory session is to estimate parameters of Antoine equation, estimate error using root mean square, and plot graph of predicted $\ln(p^{vap})$ and actual $\ln(p^{vap})$ as function of temperature.

METHOD

Graph plotting, estimation of p^{vap} and error calculations

Approach 1: First we load the data of excel file using readmatrix function.

Approach 2: Then we calculated log(P) and 1/T and stored these values in a matrix.

Approach 3: Using cvpartition function of MATLAB, the given data is divided into two sets, with 70% data in training set and rest in test set.

Approach 4: Using fitlm function, we fitted the data of training set linearly, and calculated the value of coefficients (A and B) in Antoine equation.

Antoine equation is given by: $\ln(p^{vap}) = A - (B/T)$

Approach 5: Using coefficients given by fitlm function and temperature data of test set, we estimated p^{vap}.

Approach 6: Using rms function, error is calculated of training set and test data set.

Calculation of molar volume of CO_2 and H_2

Approach 1: We first calculated molar volume using ideal gas equation,

$$V = R*T/P$$

Approach 2: Then calculated the values of unknowns in given non-dimensional expressions,

$$\beta = \frac{bP}{RT}$$

$$q = \frac{a(T)}{bRT}$$

$$\Omega = \frac{\beta Tr}{Pr}$$

$$\Psi = q\Omega T_r\, \alpha(T_r,\omega)$$

$$T_r = \frac{T}{Tc}$$

$$P_r = \frac{P}{Pc}$$

Approach 3: Using the values of unknowns and given values of known constants we applied fsolve function on the below expression:

$$f = -V + \frac{R*T}{P} + b - \frac{a(T)}{P}\frac{V-b}{(V+\varepsilon b)(V+\sigma b)}$$

RESULTS AND ANALYSIS

The following result is obtained using fitlm to find coefficient:

For CH_3OH: A=24.8968 and B=4525.8091

For H_2O: A=24.7005 and B=4941.2486

The root mean squared error on training data set:

For CH_3OH = 0.06995

For H_2O = 0.077013

The root mean squared error on test data set:

For CH_3OH = 0.082868

For H_2O = 0.079342

The following molar volume is obtained:

Using ideal gas equation:

V_{CO2} = 0.00051458

VH2 = 0.00051458

Using Redlich-Kwong equation:

V_{CO2} = 0.001122

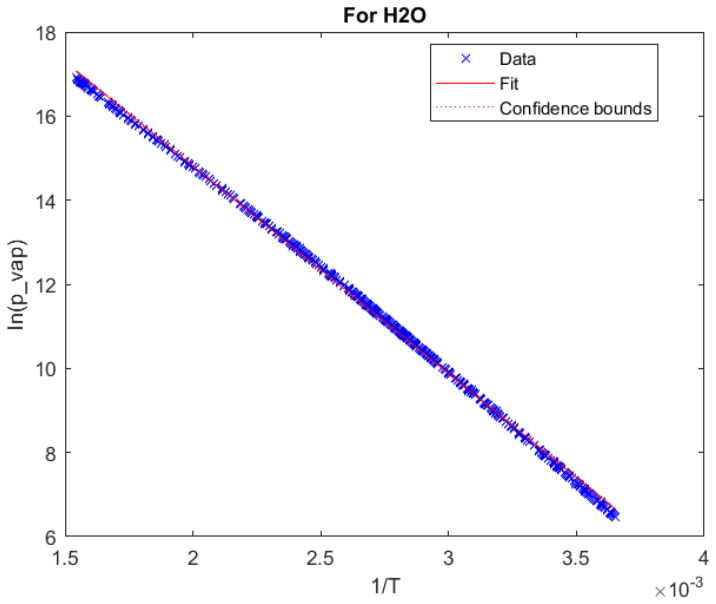
VH2 = 0.000483

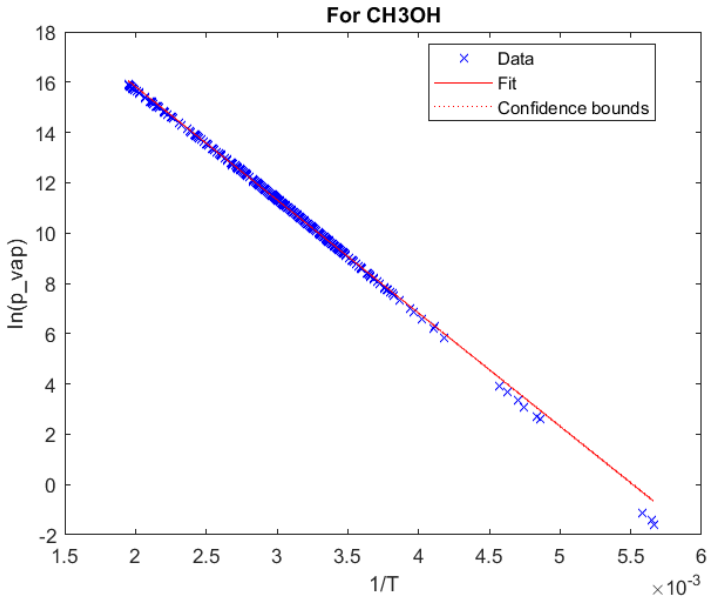
Using Peng-Robinson equation:

V_{CO2} = 0.001095

VH2 = 0.000490

The following graph is obtained:





The following command window screenshot shows the result:

```
Command Window
  For CH3OH A=24.8912 and B=4523.881
  For H2O A=24.6931 and B=4939.4125
  The test data error comes out to be 0.078374 for H2O
  The test data error comes out to be 0.066137 for CH3OH
  The trainig data error comes out to be 0.077474 for H2O
  The training data error comes out to be 0.076993 for CH3OH
  Molar volume of CO2 using ideal gas equation = 0.00051458
  Molar volume of CO2 using Redlich-Kwong equation = 0.0011225
  Molar volume of CO2 using Peng-Robinson equation = 0.001095
  Molar volume of H2 using ideal gas equation = 0.00051458
  Molar volume of  H2 using Redlich-Kwong equation = 0.00048389
  Molar volume of H2 using Peng-Robinson equation = 0.00049018
fx >>
```

CONCLUSION

The given excel data of H_2O comes out to be less scattered whereas the data of CH_3OH is scattered as confirmed from the above graph.

For CH_3OH, the error of training data set is lower than that of test data set. Similar, conclusion is also true for H_2O.

The molar volume calculated using ideal gas equation is significantly greater than those values calculated by Peng-Robinson and Redlich-Kwong equations. Also, the molar volume calculated using Redlich-Kwong equation comes closer to Peng-Robinson equation. This shows significance of such equations over ideal gas equation.

APPENDIX

The MATLAB code to solve the problem is as follows:

```
% PART A
H2O = readmatrix("data_pvap.xlsx", 'Sheet', 'H2O');
CH3OH = readmatrix("data_pvap.xlsx", 'Sheet', 'CH3OH');
H2O_T = H2O(:, 1);
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```
H2O_P = H2O(:, 2);
CH3OH_T = CH3OH(:, 1);
CH3OH_P = CH3OH(:, 2);
log_H2O_P = log(H2O_P);
log_CH3OH_P = log(CH3OH_P);

H2O = [H2O_T, H2O_P, 1./H2O_T, log(H2O_P)];
CH3OH = [CH3OH_T, CH3OH_P, 1./CH3OH_T, log(CH3OH_P)];

n_H2O = length(H2O);
n_CH3OH = length(CH3OH);

% Using cvpartition to divide into two sets
part_H2O = cvpartition(n_H2O, "HoldOut", 0.3);
H2O_training_set = H2O(training(part_H2O), :);
H2O_test_set = H2O(test(part_H2O), :);

part_CH3OH = cvpartition(n_CH3OH, "HoldOut", 0.3);
CH3OH_training_set = CH3OH(training(part_CH3OH), :);
CH3OH_test_set = CH3OH(test(part_CH3OH), :);

% Using fitlm to fit data linearly
AB_H2O_test = fitlm(H2O_test_set(:,3), H2O_test_set(:, 4));
AB_CH3OH_test = fitlm(CH3OH_test_set(:,3), CH3OH_test_set(:, 4));
AB_H2O_training = fitlm(H2O_training_set(:,3), H2O_training_set(:, 4));
AB_CH3OH_training = fitlm(CH3OH_training_set(:,3), CH3OH_training_set(:, 4));

% values of A and B after using fitlm
A_H2O = AB_H2O_training.Coefficients{1,1};
B_H2O = AB_H2O_training.Coefficients{2,1};
A_CH3OH = AB_CH3OH_training.Coefficients{1,1};
B_CH3OH = AB_CH3OH_training.Coefficients{2,1};

% Estimating p_vap using test data set and training set
test_ln_p_vap_H2O = B_H2O.*H2O_test_set(:,3)+A_H2O;
training_ln_p_vap_H2O = B_H2O.*H2O_training_set(:,3)+A_H2O;
test_ln_p_vap_CH3OH = B_CH3OH.*CH3OH_test_set(:,3)+A_CH3OH;
training_ln_p_vap_CH3OH = B_CH3OH.*CH3OH_training_set(:,3)+A_CH3OH;

% Calculation of root mean square error
err_H2O_test= rms(test_ln_p_vap_H2O-H2O_test_set(:,4));
err_H2O_training= rms(training_ln_p_vap_H2O-H2O_training_set(:,4));
err_CH3OH_test= rms(test_ln_p_vap_CH3OH-CH3OH_test_set(:,4));
err_CH3OH_training= rms(training_ln_p_vap_CH3OH-CH3OH_training_set(:,4));

% Plotting data
figure
plot(AB_H2O_training);
figure
plot(AB_CH3OH_training);


% PART B
T=483;
P=78*10^5;
R =8.31;
P_c= [7.38*10^5, 12.93*10^5];
T_c= [304.15, 33.18];
omega= [0.225, -0.22];
sigma= [1, 1+(2^0.5)];
eps = [0, 1-(2^0.5)];
```

```
omg = [0.08664, 0.0778];
shi = [0.42748, 0.45724];
P_r = P./P_c;
T_r = T./T_c;

beta = (omega.*P_r)./T_r;  %calculation of beta
b= (beta.*R*T)/P;  %calculation of b

% solving Ideal Gas equation
V_ideal = (R*T)/P;


% solving Redlich-Kwong (RK) equation
alpha_Tr_RK=T_r(1)^-0.5;
q_RK = (shi(1)*alpha_Tr_RK)./(omg(1).*T_r);
a_RK = (q_RK.*b*R*T);

f_CO2_RK = @(V) [-V+((R*T)/P)+b(1)-(a_RK(1)/P)*((V-b(1))/((V+eps(1)*b(1))*(V+sigma(1)*b(1))))];
f_H2_RK = @(V) [-V+((R*T)/P)+b(2)-(a_RK(2)/P)*((V-b(2))/((V+eps(1)*b(2))*(V+sigma(1)*b(2))))];
V_RK_CO2 = fsolve(f_CO2_RK, V_ideal );
V_RK_H2 = fsolve(f_H2_RK, V_ideal );


% solving  Peng-Robinson (PR) equation
alpha_Tr_PR= 1 + (0.37464 + 1.54226.*(omega)-0.26992.*(omega.^2)).*(1-T_r.^0.5);
q_PR = (shi(2)*alpha_Tr_PR)./(omg(2).*T_r);
a_PR = (q_PR.*b*R*T);

f_CO2_PR = @(V) [-V+((R*T)/P)+b(1)-(a_PR(1)/P)*((V-b(1))/((V+eps(1)*b(1))*(V+sigma(1)*b(1))))];
f_H2_PR = @(V) [-V+((R*T)/P)+b(2)-(a_PR(2)/P)*((V-b(2))/((V+eps(1)*b(2))*(V+sigma(1)*b(2))))];
V_PR_CO2 = fsolve(f_CO2_PR, V_ideal );
V_PR_H2 = fsolve(f_H2_PR, V_ideal );

% Printing results in command window
disp(['For CH3OH A=', num2str(A_CH3OH), ' and B=', num2str(-B_CH3OH)]);
disp(['For H2O A=', num2str(A_H2O), ' and B=', num2str(-B_H2O)]);
disp(['The error comes out to be ', num2str(err_H2O_test), ' for H2O']);
disp(['The error comes out to be ', num2str(err_CH3OH_test), ' for CH3OH']);
disp(['The error comes out to be ', num2str(err_H2O_training), ' for H2O']);
disp(['The error comes out to be ', num2str(err_CH3OH_training), ' for CH3OH']);
disp(['Molar volume using ideal = ', num2str(V_ideal)]);
disp(['Molar volume CO2 using Redlich-Kwong = ', num2str(V_RK_CO2)]);
disp(['Molar volume CO2 using Peng-Robinson = ', num2str(V_PR_CO2)]);
disp(['Molar volume H2 using ideal = ', num2str(V_ideal)]);
disp(['Molar volume H2 using Redlich-Kwong = ', num2str(V_RK_H2)]);
disp(['Molar volume H2 using Peng-Robinson = ', num2str(V_PR_H2)]);
```