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Name: 1) Satish ch14btech11014 2) Chandrakanth ch14btech11016
3) Abhilash ch14btech11017 4) Ram Prasad ch14btech11003 5) Ravi Teja ch14btech11007

12.4 (***Fitting of Langmuir isotherm and determination of heat of adsorption***)[2] Ray and Box (*Ind. Eng Chem.*, *42*(1950) 1315) reported the following data on equilibrium adsorption of propane on activated carbon at three different temperatures.

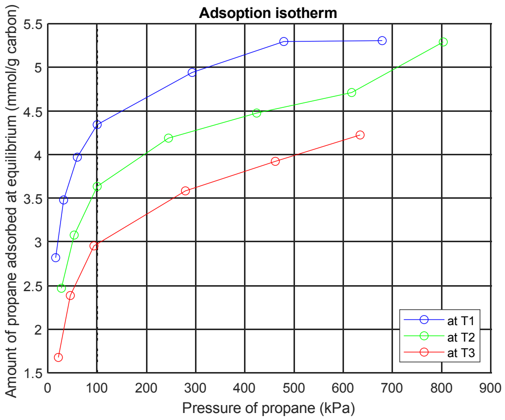
T = 310.9 K		338.7 K		366.5 K	
p (kPa)	q (mmol/g)	p (kPa)	q (mmol/g)	p (kPa)	q (mmol/g)
15.6	2.819	27.2	2.469	21.07	1.677
31.74	3.48	53.2	3.078	45.33	2.386
59.6	3.97	99.97	3.635	93.34	2.954
99.97	4.342	244.8	4.188	279.2	3.584
293	4.94	424	4.475	461.9	3.922
479.2	5.294	617.1	4.71	634.3	4.244
679.1	5.304	803.2	5.289		

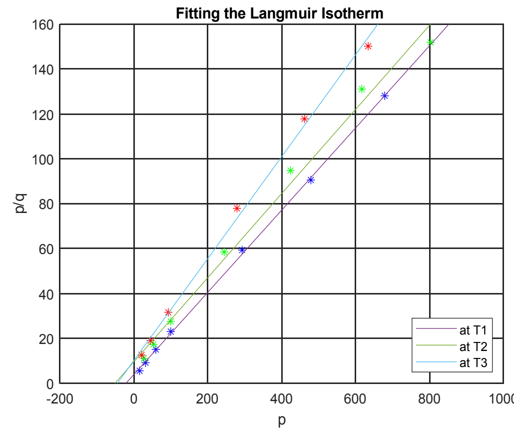
(*Contd.*)

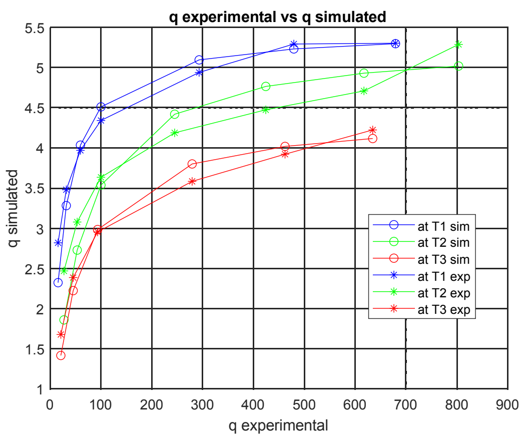
Fit the data using Langmuir isotherm and get the correlation coefficients. Determine the isosteric heat of adsorption.

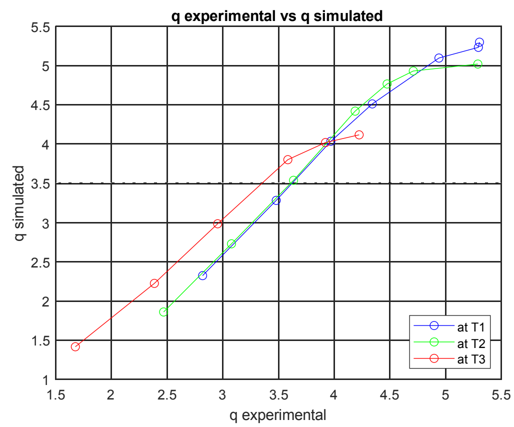
Create the following analysis for calculation of heat of adsorption.

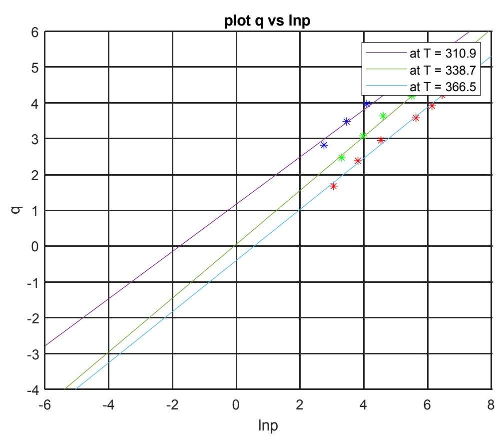
1. Plot the adsoption isotherms (q vs p) at three different temperatures from experimental observations.
2. Assume Langmuir isotherm to be valid for the above experimental data and fit the theroitical model to the experimental data. Use the straight-line form and show the plot of p/q vs p and the fitted line in the plot for three temperatures.
3. Plot the theoretical q and experimental q as a function of p for the three temperatures, as shown in the following figures.
4. Plot the theoretical q (Y-axis) vs experimental q (X axis) for three temperatures.
5. Plot q vs lnP for three temperatures.
6. For constant loading of propane, q, plot lnP vs 1/T. [for q=1.5, q=2.5, q=3.5].
7. Calculate the average slope for calculation of isosteric heat of adsorption.

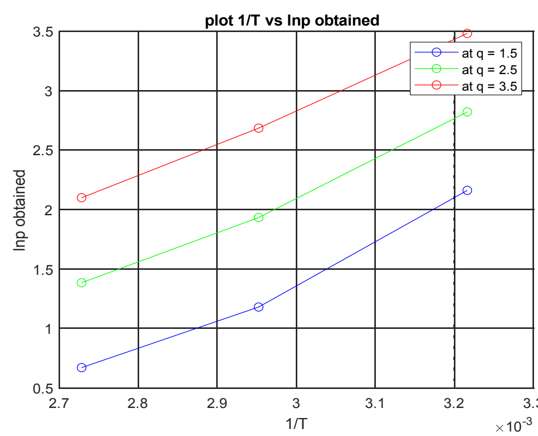












Determination of heat of adsorption **from Clausius-Clayperon equation:**

```
% delta_H_iso = -R*((T)^2)*d(lnp)/dT = -R*d(lnp)/d(1/T)

%Fitting of Langmuir isotherm and determination of heat of adsorption

%At T = 310.9K
p1 = [15.6 31.74 59.6 99.97 293 479.2 679.1];      %kPa
q1 = [2.819 3.48 3.97 4.342 4.94 5.294 5.304];     %mmol/g
y1 = p1./q1;
x1 = p1;
```

```
lnp1 = …..);

%At T = 338.7K
p2 = [27.2 53.2 99.97 244.8 424 617.1 803.2];      %kPa
q2 = [2.469 3.078 3.635 4.188 4.475 4.71 5.289];    %mmol/g
y2 = p2./q2;
x2 = p2;
lnp2 = …..;

%At T = 366.5K
p3 = [21.07 45.33 93.34 279.2 461.9 634.3];        %kPa
q3 = [1.677 2.386 2.954 3.584 3.922  4.224];       %mmol/g
y3 = p3./q3;
x3 = p3;
lnp3 = ….;

%plotiing p vs q
figure(1)
f1 = plot(p1, q1, 'bo-'); grid on; hold on;
f2 = plot(p2, q2, 'go-'); grid on; hold on;
f3 = plot(p3, q3, 'ro-'); grid on; hold on;
xlabel('Pressure of propane (kPa)');
ylabel('Amount of propane adsorbed at equilibrium (mmol/g carbon)');
title('Adsorption isotherm');
legend([f1, f2, f3],'at T1','at T2','at T3');

% Langmuir isotherm
%------ q = (qm*k*p)/(1+k*p)
%------ p/q = 1/k*qm + (1/qm)*p
%------ y = c + m*x
%------ m =1/qm
%------ c = 1/k*qm

% fitting a straight line through the points
P1 = polyfit(x1, y1,1);
…………………………….
…………………………….

figure(2)
plot(x1,y1,'b*'); grid on; hold on;
………………………………………………
………………………………………………
xlabel('p'); ylabel('p/q');
title('Fitting the Langmuir Isotherm');

% plotting the fitted curve
syms x
b1 = fplot(m1*x+c1);
…………………………….
……………………………
legend([b1, b2, b3],'at T1','at T2','at T3');
```