Q1 - Process Dynamics, Modelling & Control - Student Number: 209581412

```
%Variable Dictionary

%Pval                Raw Data Values for Pressure
%Tval                Raw Data Values for Temperature
%P                   Pressure Value Changed Units to atm
%P_evap              Flash Evaporator Pressure
%T                   Temperature Value Changed Units to Kelvins
%T_evap              Flash Evaporator Temperature
%A_PDO               Antoine Coefficient A for 1,3 - Propandiaol
%B_PDO               Antoine Coefficient B for 1,3 - Propandiaol
%C_PDO               Antoine Coefficient C for 1,3 - Propandiaol
%A_H2O               Antoine Coefficient A for Water
%B_H2O               Antoine Coefficient B for Water
%C_H2O               Antoine Coefficient C for Water
%A_Gly               Antoine Coefficient A for Glycerol
%B_Gly               Antoine Coefficient B for Glycerol
%C_Gly               Antoine Coefficient C for Glycerol
%P_sat_PDO           Saturation Pressure for 1,3 - Propandiaol
%P_sat_H2O           Saturation Pressure for Water
%P_sat_Gly           Saturation Pressure for Glycerol
%k_PDO               Vapour-Liquid Equilibrium Ratio for 1,3 - Propandiaol
%k_H2O               Vapour-Liquid Equilibrium Ratio for Water
%k_Gly               Vapour-Liquid Equilibrium Ratio for Glycerol
%molfrac_PDO         Mole Fraction of 1,3 - Propandiaol
%molfrac_H2O         Mole Fraction of Water
%molfrac_Gly         Mole Fraction of Glycerol
%Alpha               Vapour-Feed Ratio
%x_total             Total Liquid Phase Mole Fraction
%x_PDO               Liquid Phase Mole Fraction of 1,3 - Propandiaol
%x_H2O               Liquid Phase Mole Fraction of Water
%x_Gly               Liquid Phase Mole Fraction of Glycerol
%y_total             Total Vapour Phase Mole Fraction
%y_PDO               Vapour Phase Mole Fraction of 1,3 - Propandiaol
%y_H2O               Vapour Phase Mole Fraction of Water
%y_Gly               Vapour Phase Mole Fraction of Glycerol

%Question 1A
clear all
clc

global molfrac_PDO molfrac_H2O molfrac_Gly k_PDO k_H2O k_Gly
%Raw Data Values
Pval = readvars('Vapour_pressure_data.xlsx','Range','B6:B28'); % Atm
Tval = readvars('Vapour_pressure_data.xlsx','Range','A6:A28'); % C

P = Pval./750; % bar
T = Tval + 273.15; % K

Coeff_Guess(1) = 1;
Coeff_Guess(2) = 1400;
Coeff_Guess(3) = 250;
%Non-Linear function fit
```

```
Coeff = nlinfit(T,P,@(Coeff,T) Q1AFunct(Coeff,T),Coeff_Guess);
%Antoine Coefficients for 1,3 - Propandiaol
A_PDO = Coeff(1);
B_PDO = Coeff(2);
C_PDO = Coeff(3);

fprintf('Coefficient A = %f\n', A_PDO)
```

```
Coefficient A = 4.743261
```

```
fprintf('Coefficient B = %f\n', B_PDO)
```

```
Coefficient B = 1948.631342
```

```
fprintf('Coefficient C = %f\n', C_PDO)
```

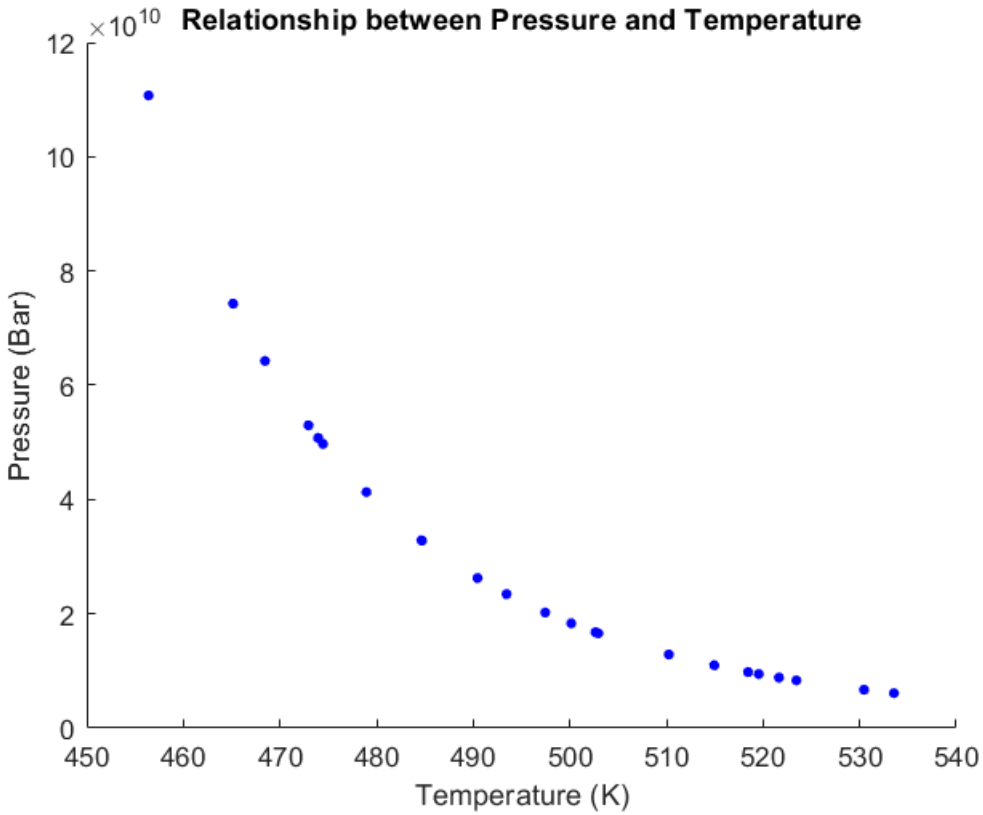
```
Coefficient C = -147.144282
```

```
%Equation used to find the Antoine coefficients
P = 10.^(A_PDO +(B_PDO./(C_PDO + T))); %bar

hold on

plot(T,P,'b.','markersize',13);
xlabel('Temperature (K)');
ylabel('Pressure (Bar)');
title('Relationship between Pressure and Temperature');

hold off
```



```
%Question 1B
A_PDO = Coeff(1);
B_PDO = Coeff(2);
C_PDO = Coeff(3);
%Antoine Coefficients for Water
A_H2O = 3.55959;
B_H2O = 643.748;
C_H2O = -198.043;
%Antoine Coefficients for Glycerol
A_Gly = 13.6485;
B_Gly = 302.1804;
C_Gly = -181.7567;
%Converting the temperature from degrees to kelvin whilst keeping pressure
%units the same
T_evap = (185 + 273.15); %K
P_evap = (2.75); %bar
%Calculating Saturation Pressure of the components
P_sat_PDO = 10^(A_PDO - (B_PDO./(T_evap + C_PDO))); %bar
P_sat_H2O = 10^(A_H2O - (B_H2O./(T_evap + C_H2O))); %bar
P_sat_Gly = 10^(A_Gly - (B_Gly./(T_evap + C_Gly))); %bar
%Calculating Vapour-Liquid ratio using Equation 2
k_PDO = P_sat_PDO./P_evap;
k_H2O = P_sat_H2O./P_evap;
k_Gly = P_sat_Gly./P_evap;
%Mole fractions of the components
molfrac_PDO = 0.015;
molfrac_Gly = 0.01;
molfrac_H2O = 1 - molfrac_PDO - molfrac_Gly;
%Finding the root of the function with Alphaas the variable
x_total = @(Alph)(molfrac_PDO)./(1 + Alph*(k_PDO - 1)) + (molfrac_H2O)./(1 + Alph*(k_H2O - 1))
%Alpha value as a fraction
Alpha = fzero(x_total,0.9);
%Alpha value as a percentage
Alpha_Percent = Alpha*100;
fprintf('Alpha = %f\n', Alpha_Percent)
```

```
Alpha = 99.154837
```

```
x_PDO = (molfrac_PDO)./(1 + Alpha*(k_PDO - 1))
```

```
x_PDO = 0.7779
```

```
x_H2O = (molfrac_H2O)./(1 + Alpha*(k_H2O - 1))
```

```
x_H2O = 0.2221
```

```
x_Gly = (molfrac_Gly)./(1 + Alpha*(k_Gly - 1))
```

```
x_Gly = 7.7236e-15
```

```
%Which all adds up to 1 as there are all liquid mole fractions and cannot exceed 1
x_total = x_PDO + x_H2O + x_Gly;
%Now to calculate the Vapour mole fractions
y_PDO = k_PDO * x_PDO
```

```
y_PDO = 0.0085
```

```
y_H2O = k_H2O * x_H2O
```

```
y_H2O = 0.9814
```

```
y_Gly = k_Gly * x_Gly
```

```
y_Gly = 0.0101
```

```
%the same principle applies to the vapurs phase aswell as the liquid
y_total = y_PDO + y_H2O + y_Gly;
```

```
function P = Q1AFunct(Coeff,T)

A = Coeff(1);
B = Coeff(2);
C = Coeff(3);

P = 10.^(A - (B./(C + T))); %bar

end
```