ROLL NO – 13CHE1066

Q1- Algorithm on how to determine the constants m and n for nitrogen gas.

* To find m, n we need to find the value of α.
* We can get the value of α from the Peng – Robinson Equation of State. For that we need to find the parameters Psat, ρsat, and Tsat to calculate v (molar volume).
* To fit m and n values, we need to calculate α at different temperatures (T). For that, we assume different range of temperatures from 298.16K to around 1000K.
* Then by writing the loop, calculate the value of Psat from the equation given at the temperatures given above.
* Then by writing the loop, calculate the value of ρsat from the equation given at the temperatures given above from Psat equation given.
* Now, we know that**- ρsat =n/v** (ρsat – Molar Density, v- Molar Volume). Assume n to be 1 so, v=1/ ρsat. So writing the loop, calculate v at the temperatures given.
* Now we form an array of [Psat, v, Tsat], we gat Psat and v at Tsat.
* Now we define the function of Peng – Robinson EOS. Also calculate values of a, b, σ and ε as they all are constant (Which are the function of R, Tc and Pc).
* Substitute Psat =P, Tguess (T) molar volume (v) in the EOS, the unknown quantity which remains is the value of α. So define a function to determine α at different temperature as given above. Create an array of values of α at those temperatures.
* Then form an array of Tr as it is a function of T and Tc (which is known).
* Then from the array of [α, Tr], we can get the equations in terms of m and n.
* So at various guess temperatures we can get the α values and thus we can get n equations in terms of m and n. So, considering two equations in two variable (m, n) we can determine the values of m and n.
* Plot the graph of alpha versus temperature.
* Now use fit curve function to fit the function and find the error estimation using predicted values and check whether the data which is predicted is under 95 % confident level interval or not.
* Similar algorithm can be done to calculate m and n for oxygen gas.