ChE 205 – Computational Methods in Chemical Engineering

Homework Set #12

This homework should be turned in as a hard copy to Ms. Zhang using the Homework Cover Sheet.

Problem 1. A 20-liter storage tank with a bursting pressure rating of 3600 psi is filled with chlorine gas \( (T_c = 417.2 \text{ K}, p_c = 7.71 \times 10^6 \text{ J m}^{-3}) \). Use the Redlich-Kwong (RK) equation of state to estimate the gas pressure (psi) from the temperature \( T \) (K) and molar volume \( V \) (m\(^3\) mol\(^{-1}\)).

\[
p = \frac{RT}{V-b} - \frac{a}{T^{0.5}V(V+b)}
\]

The constants \( a \) and \( b \) can be obtained from critical data as follows.

\[
a = 0.4278R^2 T_c^{2.5} / p_c
\]

\[
b = 0.0867RT_c / p_c
\]

The universal gas constant is \( R = 8.3145 \text{ J mol}^{-1} \text{ K}^{-1} \). Unit conversions: 1 bar = 100,000 J m\(^{-3}\). 1 bar = 14.5038 psi. The following temperature readings (Celsius) were recorded over a 24-hour period in the room in which the tank is to be stored:

28.9, 27.2, 25.4, 23.7, 24.8, 29.1, 28.1, 26.4, 25.7, 27.4, 26.9

Calculate the mean temperature along with the 95% confidence interval. Based upon this uncertainty in the temperature and a 10% safety (over-design) factor for the tank bursting pressure, what is the maximum mass (kg) of chlorine that can safely be stored in the tank?

Problem 2. Consider the same temperature readings from Problem 1 along with the following sample of volume measurements (m\(^3\)):

1.47, 1.56, 1.38, 1.42, 1.35, 1.48, 1.52, 1.37, 1.45

Determine the mean volume along with its 95% confidence interval. Assuming validity of the ideal gas law determine the pressure for 0.18 kg of chlorine, and its uncertainty (Pascals).
Some Useful Statistical Formulas

**Standard deviation**

- **Standard deviation**: root mean square of deviations:
  \[
  \sigma \equiv \sqrt{\sigma^2} = \sqrt{\langle x^2 \rangle - \mu^2}
  \]

  associated with the 2nd moment of \(x_i\) distribution

- **Sample variance**: replace \(\mu\) by \(\bar{x}\)
  \[
  s^2 \equiv \frac{1}{N - 1} \sum (x_i - \bar{x})^2
  \]

  \(N - 1\) instead of \(N\) because \(\bar{x}\) is obtained from the same data sample and not independently
Definition

If our sample yields the list of numbers \( \{x_1, x_2, \ldots, x_n\} \), then the \textit{sample variance} is given by

\[
s^2 = \frac{(x_1 - \bar{x})^2 + (x_2 - \bar{x})^2 + \cdots + (x_n - \bar{x})^2}{n - 1}.
\]

The sample standard deviation \( s \) is the square root of the sample variance.

Alternate form

An easier version for computing the sample variance is

\[
s^2 = \frac{(x_1)^2 + (x_2)^2 + \cdots + (x_n)^2 - n\bar{x}^2}{n - 1}.
\]

- To make a confidence interval when we don’t know \( \sigma \), we replace \( \frac{\sigma}{\sqrt{n}} \) with our estimate \( \frac{s}{\sqrt{n}} \).
- If our sample size \( n \) is at least 30, we use the \( Z \)-curve just like last time.
- If our sample size \( n \) is less than 30, we use the \( t \)-curve for \( n - 1 \) “degrees of freedom.”
- So the only change in our procedure is to look up the numbers in a different table!