# Scilab for Chemical Engineers

## TSEC - Online Certificate Course

---

# SAMPLE PROBLEMS

---

Aditya Ganesh Date: 08 - 02 - 2025

# 1 Functions

## 1.1 Basic Functions

### 1.1.1 Temperature Conversion:

Write a function `celsiusToFahrenheit(T_C)` that converts a temperature from Celsius to Fahrenheit. Additionally, write a function `fahrenheitToCelsius(T_F)` that converts from Fahrenheit to Celsius.

### 1.1.2 Pressure Calculation:

Write a function `pressureIdealGas(n, V, T)` that calculates the pressure of an ideal gas using the Ideal Gas Law: $P = \frac{nRT}{V}$. Assume $R$ (the gas constant) is 8.314 J/(mol·K).

## 1.2 Intermediate Functions

### 1.2.1 Reactor Volume Calculation:

Write a function `CSTRVolume(F, k, X)` to calculate the required volume of a Continuous Stirred-Tank Reactor (CSTR) given the feed flow rate $F$, reaction rate constant $k$, and conversion $X$ using the formula $V = \frac{F \cdot (X - X_0)}{k \cdot (1-X)}$.

### 1.2.2 Heat Exchanger Area:

Write a function `heatExchangerArea(Q, U, LMTD)` to calculate the required heat exchanger area using the formula $A = \frac{Q}{U \cdot LMTD}$, where $Q$ is the heat duty, $U$ is the overall heat transfer coefficient, and $LMTD$ is the logarithmic mean temperature difference.

### 1.2.3 Boiling Point Elevation:

Write a function `boilingPointElevation(M, k_b, m)` that calculates the boiling point elevation of a solution given the molality of the solution $m$, the ebullioscopic constant $k_b$, and the molar mass $M$ of the solute.

## 1.3 Advanced Functions

### 1.3.1 Reaction Rate Calculation:

Write a function `reactionRate(C, k, order)` that calculates the rate of a chemical reaction given the concentration $C$, the reaction rate constant $k$, and the order of the reaction.

### 1.3.2 Batch Reactor Simulation:

Write a function `batchReactor(C0, k, t)` that simulates the concentration $C$ of a reactant in a batch reactor over time $t$ using first-order kinetics and plots the concentration vs. time.

### 1.3.3 Distillation Column Calculation:

Write a function `distillationColumn(N, xD, xB, xF)` that calculates the number of theoretical stages $N$ in a distillation column using the Fenske equation, given the distillate mole fraction $xD$, bottoms mole fraction $xB$, and feed mole fraction $xF$.

# 2 Numerical Methods

## 2.1 Root finding algorithms

### 2.1.1 Bisection Method

Find the root of the function $f(x) = x^3 - 6x^2 + 11x - 6.1$ within the interval [2, 4] using the Bisection Method. (Use tolerance value of $10^{-6}$)

### 2.1.2 Newton-Raphson Method

Find the root of the function $f(x) = \cos(x) - x$ with an initial guess of $x_0 = 0.5$ using the Newton-Raphson Method.

### 2.1.3 Secant Method

Find the root of the function $f(x) = e^x - 3x^2$ with initial guesses $x_0 = 0$ and $x_1 = 1$ using the Secant Method.

### 2.1.4 Fixed-Point Iteration

Find the root of the function $f(x) = x^3 - 2x - 5$ by rewriting it as $g(x) = \sqrt[3]{2x+5}$ and using Fixed-Point Iteration with an initial guess of $x_0 = 2.0$.

## 2.2 System of linear equations

### 2.2.1 Gauss Elimination

Solve the following system of linear equations using Gauss elimination

$$\begin{bmatrix} 2 & -1 & 1 \\ 3 & 3 & 9 \\ 3 & 3 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2 \\ -1 \\ 5 \end{bmatrix} \tag{1}$$

### 2.2.2 Gauss-Seidel

Solve the following system of linear equations with Gauss-Seidel method

$$\begin{bmatrix} 4 & 1 & 2 \\ 3 & 5 & 1 \\ 1 & 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 4 \\ 7 \\ 3 \end{bmatrix} \tag{2}$$