CH-440 Chemometrics in Electroanalysis

Credit Hours: 3-0

Pre-requisite: Nil

Course Objectives:

This course is designed to:

1. Provide foundational knowledge of chemometrics and its application in electroanalytical chemistry.
2. Equip students with tools for data analysis, calibration, and interpretation of electrochemical measurements.
3. Develop problem-solving skills using statistical and mathematical models relevant to analytical chemistry.
4. Enhance students' ability to critically analyze experimental data using chemometric techniques.

Course Contents:

1. Introduction to Chemometrics: Definition and scope, Role of chemometrics in analytical, chemistry, Overview of electroanalysis
2. Basics of Electrochemical Techniques: Potentiometry, Voltammetry, Amperometry, Conductometry, Electrochemical sensors and electrodes
3. Data Preprocessing and Exploratory Data Analysis: Signal smoothing and baseline correction, Normalization and scaling, Principal Component Analysis (PCA), Cluster analysis
4. Calibration Methods: Classical calibration vs multivariate calibration, Linear regression and multiple linear regression (MLR), Partial least squares (PLS) and Principal component regression (PCR)
5. Experimental Design: Factorial design, Response surface methodology, Optimization of electroanalytical methods
6. Pattern Recognition and Classification: Discriminant analysis, K-nearest neighbors (KNN), Artificial neural networks (ANN) (introductory overview)
7. Case Studies in Chemometrics and Electroanalysis: Application in pharmaceutical analysis, Environmental and biosensor applications, Real-world data interpretation

Course Outcomes:

Upon successful completion of the course, students will be able to:

1. Understand and apply key chemometric methods in analyzing electrochemical data.
2. Select and implement appropriate data preprocessing techniques.
3. Design and evaluate calibration models for complex electrochemical systems.
4. Interpret multivariate datasets using statistical tools and pattern recognition techniques.
5. Utilize chemometrics for enhanced decision-making in research and industry-based electroanalytical processes.

Recommended Books (Theory):

1. "Practical Guide to Chemometrics" by Paul Gemperline
2. "Fundamentals of Analytical Chemistry" by Douglas A. Skoog
3. "Data Handling in Science and Technology – Chemometrics in Environmental Chemistry" by W. Einax "Introduction to Multivariate Calibration" by Harald Martens & Tormod Næs
4. Chemometrics: Statistics and Computer Application in Analytical Chemistry" by Matthias Otto"Electrochemical Methods: Fundamentals and Applications" by Allen J. Bard & Larry R. Faulkner