NATIONAL UNIVERSITY OF ENGINEERING
COLLEGE OF SCIENCES
CHEMISTRY PROGRAM

CQ085 – CHEMOMETRICS

I. GENERAL INFORMATION

CODE	**:**	CQ085 – Chemometrics
SEMESTER	**:**	8
CREDITS	**:**	04
HOURS PER WEEK	**:**	06 (Theory – Laboratory)
PREREQUISITES	**:**	Instrumental analytic chemistry II
CONDITION	**:**	Mandatory

II. COURSE DESCRIPTION

The chemometrics course provides students with the knowledge and skills necessary to understand and apply the appropriate chemometric techniques to solve a specific problem, in addition to interpreting the results obtained in the treatment of data using the appropriate software. The course develops the topics of Signal Processing and Analysis of Temporary Series, Pattern Recognition Techniques: Analysis of Principal Components and Cluster Analysis, Classification Techniques such as Discriminant Analysis and SIMCA, and calibration methods such as Multiple Linear Regression, Regression by Main Components and Partial Least Squares.

III. COURSE OUTCOMES

By the end this course the student will:

- Apply the basic concepts for the interpretation of the results obtained.
- Manage the necessary software for chemometric treatment of chemical data.
- Interpret the results obtained through the software.
- Develop the experimental methodology for the use of the appropriate chemometric technique.
- Solve problems of interpretation of chemical data when many variables intervene.

IV. LEARNING UNITS

1. **CHAPTER 1: SIGNAL PROCESSING / 8 HOURS**
   Signal processing / Series - time analysis.

2. **CHAPTER 2: INTRODUCTION TO THE MULTIVARIATE ANALYSIS / 4 HOURS**
   Introduction / Basic definitions / Exploratory data analysis / Recognition of supervised and unsupervised patterns / Multivariate regression.

3. **CHAPTER 3: ANALYSIS OF MAIN COMPONENTS / 8 HOURS**
   Matrices of multivariate data / Loads and scores / Eigenvalues / Graphical representations. Analysis of cases.

4. **CHAPTER 4: CLUSTER ANALYSIS / 6 HOURS**
   Similarities / Neighborhoods / Dendogram / Cases analysis.

5. **CHAPTER 5: RECOGNITION OF SUPERVISED PATTERNS / 6 HOURS**
   General principles / Discriminant analyzes / Discriminant analysis, k-nearest / SIMCA / Case analysis.

6. **CHAPTER 6: MULTIVARIATE CALIBRATION / 6 HOURS**
   Multiple Linear Regression (MLR) / Regression by principal components (RPC) / Partial Least Squares (PLS) / Validation of calibration models / Case analysis.

7. **CHAPTER 7: ADVANCED TOPICS IN CHEMOMETRY / 4 HOURS**
   Multiview analysis, Images Analysis / Artificial Neural Networks / Exposition of applications**.**

V. LABORATORIES AND PRACTICAL EXPERIENCES

Laboratory 1: Signal treatment and time series
Laboratory 2: Analysis of main components
Practice 1: Clusters analysis
Laboratory 3: Discriminant analysis
Laboratory 4: Multiple Linear Regression
Laboratory 5: PCR and PLS regression
Laboratory 6: Application exposition
Practice 2: Pattern Recognition laboratory
Practice 3: Calibration laboratory
Practice 4: Research work exposition

VI. METHODOLOGY

The subject is developed in sessions of theory and qualified practices. In the theory sessions the teacher presents the foundation of the chemometric techniques, with the mathematical notions necessary for the understanding of the subject, then solve some related problems using the necessary software to finally discuss with the students some practical applications in the field of chemistry research. In the practices, practical exercises will be left to solve with the suitable software, having the student to interpret the obtained results.

VII. EVALUATION FORMULA

Evaluation system G:
PE: Partial Exam (Weight 1)
FE: Final Exam (Weight 1)
AP: Average of Practices (Weight 1)
The final average (FA) is calculated as shown below:

$$FA = \frac{PE + FE + AP}{3}$$

Number of Practices: ten (10)

The AVERAGE OF PRACTICES (AP) is obtained in the following way: By Regulation, one (01) practice with the lowest grades and one (01) laboratory are eliminated and the AVERAGE OF PRACTICES of the eight (08) remaining grades.

VIII. BIBLIOGRAPHY

- Otto, Mathias, Chemometrics Statistics and Computer Application in Analytical Chemistry, Wiley-VCH, 1999.

- Brereton, Richard, Chemometrics Data Analysis for the Laboratory and Chemical Plant, Jhon Wiley & Sons, Ltda., 2003.

- Beebe, Kenneth, et al, Chemometrics A Practical Guide, Jhon Wiley & Sons, Ltda., 1998.