Code: **QF851**

Name: **Quimiometria e Controle Multivariado de Processos Químicos**

Name in English: **Chemometrics and Multivariate Control of Chemical Processes**

Name in Spanish: **Quimiometría y Control Multivariado de Procesos Químicos**

Type of Discipline: **Weekly**

Type of Approval: **Grade and Attendance**

Characteristic: **Regular**

Frequency: **75%**

Period Type / Offering Period: **Semester / All periods**

Requires Final Exam: **Yes**

Vectors

T	L	P	O	PE	OE	SL	WEEKS	CREDITS
2	**-**	**-**	**-**	**-**	**-**	**2**	**15**	**2**

Occurrence on curriculum:

Pre requirement:

Summary: Monitoring the state of a chemical process over time is crucial because the operator, when alerted to any unexpected changes, can take timely action.

The aim is to introduce how multivariate modeling of processes is done using Chemometrics and how monitoring and optimization are performed over time.

Program:

INTRODUCTION

CHEMOMETRICS

Exploratory Data Analysis:

PCA - Principal Component Analysis

HCA - Hierarchical Cluster Analysis

Construction of Calibration Models:

PCR - Principal Component Regression

PLS - Partial Least Squares Regression

MULTIVARIATE CONTROL OF CHEMICAL PROCESSES

Types of chemical processes:

CONTINUOUS

BATCH

MULTIVARIATE PROCESS MODELING.

Objectives:

1- Understand the relationships between different parts of the process

2- Maintain process control

3- Improve product quality

PROCESS CONTROL:

We will discuss how control chart theory can be implemented in a multivariate manner.

APPLICATIONS: Some time will be spent on REAL industry or laboratory applications.

Basic Bibliography

1) FERREIRA, M. M. C.; **Quimiometria: Conceitos, Métodos e Aplicações.** Campinas: Unicamp, 2015. 493 p
2) COSTA, A. F. B.; EPPRECHT, E. K., CARPINETTI, L. C. R. **Controle estatístico de Qualidade**, São Paulo: Atlas, 2004. 334 p
3) BAKEEV, K. A. **Process Analytical Technology**. Oxford: Blackwell Publishing Ltd, 2005. 451 p

Supplementary Bibliography

1) FERREIRA, M. M. C**. Revisitando a análise de componentes principais.** Quim. Nova 2022. http://dx.doi.org/10.21577/0100-4042.20170910. Online desde 1 de junho.
2) FERREIRA, M. M. C.; ANTUNES, A. M.; MELO, M. S.; VOLPE, P. L. O.; **Quim. Nova** 1999, 22, 724.
3) MONTGOMERY, D. C. **Introduction to Statistical Quality Control**. 5 ed. New York: John Wiley & Sons Inc, 2005. 774 p
4) MASON, R. L.; YOUNG, J. C. **Multivariate Statistical Process Control with Industrial Applications**. Chapell Hill: ASA-SIAM Series on Statistics and Applied Probability, 2002. 257 p
5) Recent articles will be indicated throughout the course.