Mathematical Techniques in Chemical Engineering

1. **Course number and name:** 020TMCCS4 Mathematical Techniques in Chemical Engineering

2. **Credits and contact hours:** 6 ECTS credits, 3x1:15 contact hours

3. **Names of instructors:** Mansour Tawk

4. **Instructional materials:**
   - Course handouts
   - Solved exercises
   - References
     - Practical Methods of Optimization , Second Edition , R. Fletcher , 2000
     - Process Modelling, Identification, and Control, Ján Mikleš · Miroslav Fikar, 2007
     - Data Reconciliation , & Gross Error Detection, Shankar Narasimhan and Cornelius Jordache, 1999

5. **Specific course information**
   a. **Catalog description:**
      Reminder of the fundamental properties used in optimization. Optimization problem (mathematical programming). Derivation. Topology concept. Convexity. Analysis of convexity. Eigenvalues. One-dimensional search. Definitions and general assumptions. Method of direct search for the golden ratio. Quadratic interpolation method (Quasi-Newton). Examples. Conclusion. Theoretical aspects of unconstrained optimization. Formulation of the problem. Fundamental theorem. Conclusion. Numerical methods for unconstrained problems. Fundamental principle of descent methods. Direction of descent. Length of the descent step. Stopping test (s). First-order methods. Second order Newton method. Quasi-Newtonian methods. Generalized reduced gradient, SQP.

   b. **Prerequisites**: 020DCPCS3 Dynamics and Process Control

   c. **Required/Selected Elective/Open Elective:** Required

6. **Specific goals for the course**

   a. **Specific outcomes of instruction:**
      Master the advanced mathematical methods in chemical engineering.
      - Optimization techniques
      - Identifying the systems
      - Data reconciliation
      - Matlab Applications

b. PIs addressed by the course:

PI	1.2	2.3
Covered	x	x
Assessed	x	x

7. Brief list of topics to be covered
- Method of optimizations
- Systems identification
- Data reconciliation