Program Name : **Diploma in Chemical Engineering**

Program Code : **CH**

Semester : **Fifth**

Course Title : **Numerical Methods in Chemical Engineering (Elective)**

Course Code : **22515**

1. RATIONALE

The numerical methods give the solution of applied problems when ordinary analytical methods fail. The increasing importance of numerical methods has led to enhanced demand for courses dealing with the techniques of numerical analysis in the area of chemical engineering. It is therefore clear that engineering would be incomplete without an adequate understanding of numerical methods. The students should gain ability which enables them to select the appropriate numerical technique to solve a given engineering problem.

2. COMPETENCY

The aim of this course is to help the student to attain the following industry identified competency through various teaching learning experiences:

- **Apply Numerical methods to solve chemical engineering problems.**

3. COURSE OUTCOMES (COs)

The theory, practical experiences and relevant soft skills associated with this course are to be taught and implemented, so that the student demonstrates the following industry oriented COs associated with the above mentioned competency:

a) Use SCILAB to visualize data and to solve problems.
b) Use Gaussian elimination and Gauss-Seidel iteration methods to solve linear systems equations in chemical processes.
c) Calculate Numerical Integration applying the Trapezoidal Rule, Simpson's Rule used in chemical processes.
d) Use Bisection and Newton-Raphson methods to find approximate roots of algebraic equation for given chemical processes.
e) Apply numerical methods to solve ordinary differential equations related to chemical processes.

4. TEACHING AND EXAMINATION SCHEME

Teaching Scheme			Credit (L+T+P)	Examination Scheme											
				Theory							Practical					
L	T	P		Paper Hrs.	ESE		PA		Total		ESE		PA		Total	
					Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min
3	-	2	5	3	70	28	30*	00	100	40	25@	10	25	10	50	20

(*): Under the theory PA, Out of 30 marks, 10 marks are for micro-project assessment to facilitate integration of COs and the remaining 20 marks is the average of 2 tests to be taken during the semester for the assessment of the cognitive domain UOs required for the attainment of the COs.

***Legends:** **L**-Lecture; **T** – Tutorial/Teacher Guided Theory Practice; **P** - Practical; **C** – Credit, **ESE** - End Semester Examination; **PA** - Progressive Assessment*

5. COURSE MAP (with sample COs, PrOs, UOs, ADOs and topics)

This course map illustrates an overview of the flow and linkages of the topics at various levels of outcomes (details in subsequent sections) to be attained by the student by the end of the course, in all domains of learning in terms of the industry/employer identified competency depicted at the centre of this map.

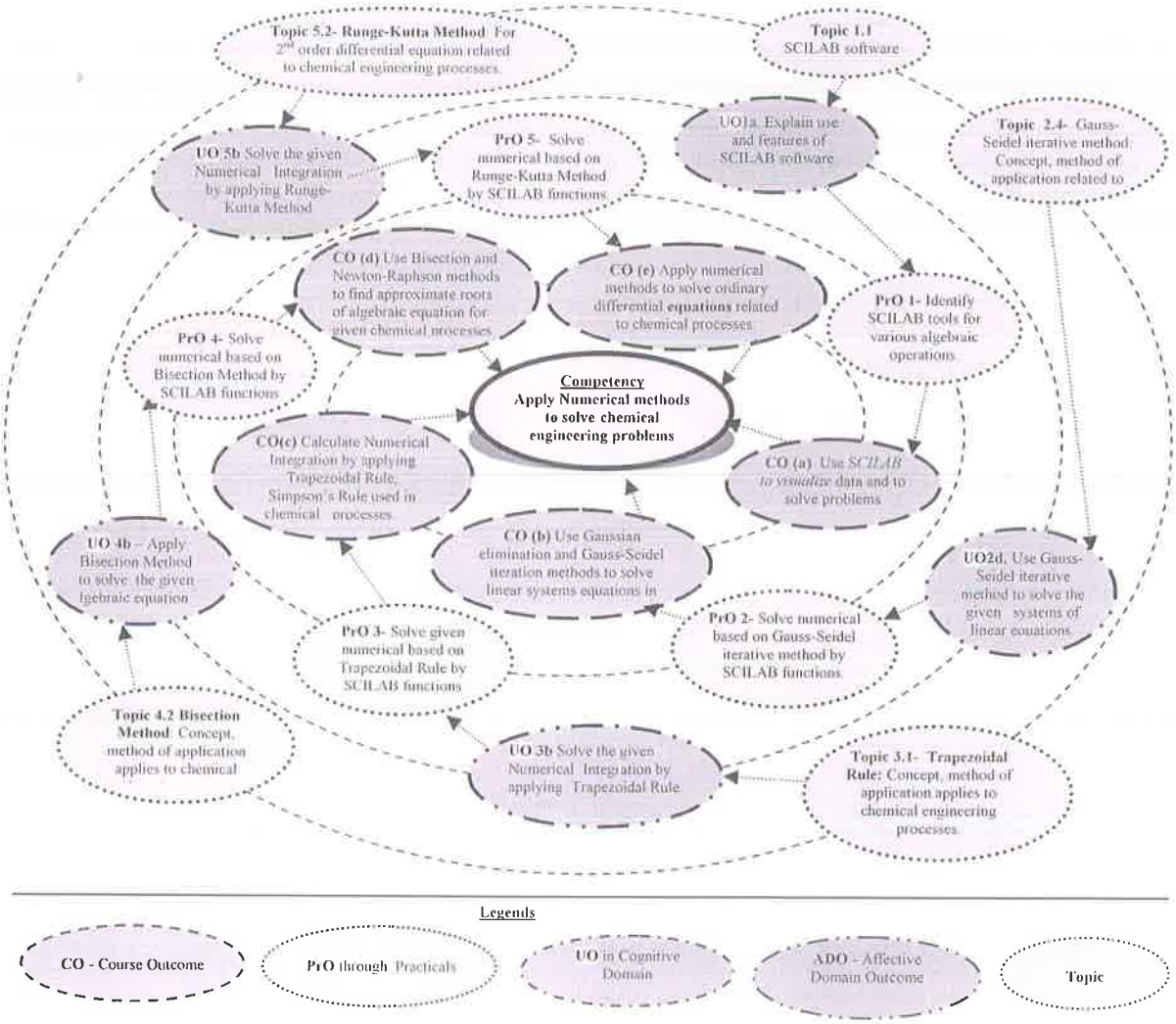

Figure 1 - Course Map

6. SUGGESTED PRACTICALS/ EXERCISES

The practicals in this section are PrOs (i.e. sub-components of the COs) to be developed and assessed in the student for the attainment of the competency:

S. No.	Practical Outcomes (PrOs)	Unit No.	Approx. Hrs. Required
1.	Show starting and exiting sessions of SCILAB software.	I	02 *
2.	Identify major tools within or accessible from the desktop of SCILAB software.	I	02 *
3.	Identify SCILAB tools for various algebraic operations	I	02 *
4.	Develop structure code in SCILAB.	I	02 *
5.	Solve numerical based on Gauss elimination method by SCILAB functions for simple chemical engineering applications	II	02

S. No.	Practical Outcomes (PrOs)	Unit No.	Approx. Hrs. Required
6.	Solve numerical based on Matrix Inversion by SCILAB functions for simple chemical engineering applications	II	02 *
7.	Solve numerical based on Gauss-Seidel iterative method by SCILAB functions for simple chemical engineering applications	II	02 *
8.	Solve numerical based on Gauss-Jordan method by SCILAB functions for simple chemical engineering applications	II	02*
9.	Solve given numerical based on Trapezoidal Rule by SCILAB functions for simple chemical engineering applications	III	02
10.	Solve numerical based on Simpson's 1/3 Rule by SCILAB functions for simple chemical engineering applications	III	02 *
11.	Solve numerical based on Bisection Method by SCILAB functions.	IV	02 *
12.	Solve numerical based on Regula-Falsi Method by SCILAB functions for simple chemical engineering applications	IV	02
13.	Solve numerical based on Newton –Raphson Method by SCILAB functions for simple chemical engineering applications	IV	02 *
14.	Solve numerical based on Runge-Kutta Method by SCILAB functions for simple chemical engineering applications	V	02 *
15.	Solve numerical based on Euler's Method by SCILAB functions for simple chemical engineering applications	V	02
16.	Solve numerical based on Taylor's Series by SCILAB functions for simple chemical engineering applications	V	02 *
	Total		**32**

Note

i. A suggestive list of PrOs is given in the above table. More such PrOs can be added to attain the COs and competency. A judicial mix of minimum 12 or more practical need to be performed, out of which, the practicals marked as '' are compulsory, so that the student reaches the 'Precision Level' of Dave's 'Psychomotor Domain Taxonomy' as generally required by the industry.*

ii. The 'Process' and 'Product' related skills associated with each PrO is to be assessed according to a suggested sample given below:

S. No.	Performance Indicators	Weightage in %
1.	Identify major tools within or accessible from the desktop of SCILAB software.	10
2.	Develop structure code in SCILAB relevant to chemical engineering processes.	20
3.	Solve given Numerical related to chemical processes by various numerical methods.	50
4.	Interpretation of result and conclusion.	10
5.	Submission of report in time.	10
Total		**100**

The above PrOs also comprise of the following social skills/attitudes which are Affective Domain Outcomes (ADOs) that are best developed through the laboratory/field based experiences:

a. Practice good housekeeping.

b. Work as a leader/a team member.
c. Follow ethical Practices.

The ADOs are not specific to any one PrO, but are embedded in many PrOs. Hence, the acquisition of the ADOs takes place gradually in the student when s/he undertakes a series of practical experiences over a period of time. Moreover, the level of achievement of the ADOs according to Krathwohl's 'Affective Domain Taxonomy' should gradually increase as planned below:

- 'Valuing Level' in 1st year
- 'Organizing Level' in 2nd year
- 'Characterizing Level' in 3rd year.

7. MAJOR EQUIPMENT/ INSTRUMENTS REQUIRED

The major equipment with broad specification mentioned here will usher in uniformity in conduct of experiments, as well as aid to procure equipment by authorities concerned.

S. No.	Equipment Name with Broad Specifications	PrO. No.
1	Computer system (Any computer system with basic configuration)	All
2	Any SCILAB software	

8. UNDERPINNING THEORY COMPONENTS

The following topics are to be taught and assessed in order to develop the sample UOs given below for achieving the COs to attain the identified competency. More UOs could be added.

Unit	Unit Outcomes (UOs) (in cognitive domain)	Topics and Sub-topics
Unit –I Introduction to SCILAB software	1a. Explain use and features of SCILAB software. 1b. Apply SCILAB software to solve various numerical methods for the given simple chemical engineering applications	**1.1 SCILAB software** **1.2** Application of numerical methods and solutions of equations (algebraic – differential -integral) using SCILAB software.
Unit–II Numerical solution of a System of linear equations	2a. Solve the given simple problem based on linear equation for the given simple chemical engineering applications 2b. Use Gaussian elimination method to solve the given systems of linear equations for the given simple chemical engineering applications 2c. Apply Matrix Inversion to solve given systems of linear equations for the given simple chemical engineering applications. 2d. Use Gauss-Seidel	2.1 **Linear equations.** 2.2 **Gauss elimination method** (Direct Method): Concept, method of application related to chemical engineering processes. 2.3 **Matrix Inversion:** Concept, method related to chemical engineering processes. 2.4 **Gauss-Seidel iterative method:** Concept, method of application related to chemical engineering processes. 2.5 **Gauss-Jordan method:** Concept, method of

Unit	Unit Outcomes (UOs) (in cognitive domain)	Topics and Sub-topics
	iterative method to solve given systems of linear equations for the given simple chemical engineering applications. 2e. Apply Gauss-Jordan method to solve given systems of linear equations for the given simple chemical engineering applications.	application related to chemical engineering processes.
Unit– III Numerical Integration	3a. Employ the concept of Numerical Integration for the given simple chemical engineering applications. 3b. Solve given Numerical Integration by applying Trapezoidal Rule for the given simple chemical engineering applications. 3c. Apply Simpson's 1/3 Rule to solve given Numerical Integration for the given simple chemical engineering applications. 3d. Use Simpson's 3/8 Rule to solve given Numerical Integration for the given simple chemical engineering applications.	**3.1 Numerical Integration Method** **3.2 Trapezoidal Rule:** Concept, method of application applies to chemical engineering processes. **3.3 Simpson's 1/3 Rule:** Concept, method of application applies to chemical engineering processes. **3.4 Simpson's 3/8 Rule:** Concept, method of application applies to chemical engineering processes.
Unit IV- Numerical solution of Algebraic equation	4a. Determine the Roots of given Algebraic equation for the given simple chemical engineering applications. 4b. Apply Bisection Method to solve given algebraic Equation for the given simple chemical engineering applications. 4c. Use Regula-Falsi Method to solve given algebraic equation for the given simple chemical engineering application. 4d. Apply Newton –Raphson Method to solve given algebraic equation for the given simple chemical engineering application.	**4.1 Concept of Algebraic equation** **4.2 Bisection Method**: Concept, method of application applies to chemical engineering processes. **4.3 Regula-Falsi Method:** Concept, method of application applies to chemical engineering processes. **4.4 Newton –Raphson Method:** Concept, method of application applies to chemical engineering processes.
Unit-V Numerical solution of Ordinary differential equation	5a. Employ the concept of Ordinary differential equation for the given for simple chemical engineering application. 5b. Solve given Numerical Integration by applying	**5.1 Concept of Ordinary differential equation.** **5.2 Runge-Kutta Method**: For 2nd order differential equation related to chemical engineering processes.

Unit	Unit Outcomes (UOs) (in cognitive domain)	Topics and Sub-topics
	Runge- Kutta Method for the given simple chemical engineering application. 5c. Calculate given Numerical Integration by applying Euler's Method for the given simple chemical engineering application. 5d. Calculate given numerical Integration by applying Taylor's Series for the given simple chemical engineering application.	**5.3 Euler's Method:** Error estimate for the Euler's method, Modified Euler's method applies to chemical engineering processes. **5.4 Taylor's Series**: For 2^{nd} order and 4^{th} order differential equation related to chemical engineering processes.

Note: To attain the COs and competency, above listed UOs need to be undertaken to achieve the 'Application Level' and above of Bloom's 'Cognitive Domain Taxonomy'

9. SUGGESTED SPECIFICATION TABLE FOR QUESTION PAPER DESIGN

Unit No.	Unit Title	Teaching Hours	Distribution of Theory Marks			
			R Level	U Level	A Level	Total Marks
I	Introduction to SCILAB software	08	04	04	04	12
II	Numerical solution of a System of linear equations	10	02	04	04	10
III	Numerical Integration	10	02	04	10	16
IV	Numerical solution of Algebraic equation	10	04	06	06	16
V	Numerical solution of Ordinary differential equation	10	04	06	06	16
Total		**48**	**16**	**24**	**30**	**70**

Legends: *R=Remember, U=Understand, A=Apply and above (Bloom's Revised taxonomy)*
Note*: This specification table provides general guidelines to assist student for their learning and to teachers to teach and assess students with respect to attainment of UOs. The actual distribution of marks at different taxonomy levels (of R, U and A) in the question paper may vary from above table.*

10. SUGGESTED STUDENT ACTIVITIES

Other than the classroom and laboratory learning, following are the suggested student-related ***co-curricular*** activities which can be undertaken to accelerate the attainment of the various outcomes in this course: Students should conduct following activities in group and prepare reports of about 5 pages for each activity, also collect/record physical evidences for their (student's) portfolio which will be useful for their placement interviews:

a) Prepare journal based on practical performed in laboratory.
b) Undertake micro-projects.
c) List down the SCILAB tools for various algebraic operations.
d) Prepare a chart of structure code in SCILAB relevant to chemical engineering processes.

e) Give seminar on relevant topics.

11. SUGGESTED SPECIAL INSTRUCTIONAL STRATEGIES (if any)

These are sample strategies, which the teacher can use to accelerate the attainment of the various outcomes in this course:

a) Massive open online courses (***MOOCs***) may be used to teach various topics/sub topics.
b) ***'L' in item No. 4*** does not mean only the traditional lecture method, but different types of teaching methods and media that are to be employed to develop the outcomes.
c) About ***15-20% of the topics/sub-topics*** which is relatively simpler or descriptive in nature is to be given to the students for ***self-directed learning*** and assess the development of the COs through classroom presentations (see implementation guideline for details).
d) With respect to item No.10, teachers need to ensure to create opportunities and provisions for ***co-curricular activities***.
e) Guide student(s) in undertaking micro-projects.
f) Demonstrate students thoroughly before they start doing the practice.
g) Encourage students to refer different websites to have deeper understanding of the subject.
h) Observe continuously and monitor the performance of students in Lab.

12. SUGGESTED MICRO-PROJECTS

Only one micro-project is planned to be undertaken by a student that needs to be assigned to him/her in the beginning of the semester. In the first four semesters, the micro-project are group-based. However, in the fifth and sixth semesters, it should be preferably be ***individually*** undertaken to build up the skill and confidence in every student to become problem solver so that s/he contributes to the projects of the industry. In special situations where groups have to be formed for micro-projects, the number of students in the group should ***not exceed three.***

The micro-project could be industry application based, internet-based, workshop-based, laboratory-based or field-based. Each micro-project should encompass two or more COs which are in fact, an integration of PrOs, UOs and ADOs. Each student will have to maintain dated work diary consisting of individual contribution in the project work and give a seminar presentation of it before submission. The total duration of the micro-project should not be less than ***16 (sixteen) student engagement hours*** during the course. The student ought to submit micro-project by the end of the semester to develop the industry oriented COs.

A suggestive list of micro-projects are given here. Similar micro-projects could be added by the concerned faculty:

a) Ideal and Non-ideal Gas Laws- Case study
b) Integration to Determine the Total Quantity of Heat- Case study.
c) Steady- State Analysis of a system of Reactors -Case study
d) One-Dimensional Mass Balance of a Reactor- Case study.

13. SUGGESTED LEARNING RESOURCES

S. No.	Title of Book	Author	Publication
1	Introductory Methods of Numerical Analysis.	Sastry S.S.	PHI Learning, New Delhi-110001, ISBN-81-203-1266-X
2	Numerical Methods for Engineers.	Chapra, Steven C., Canale Raymond P.	McGraw Hill Publishing Company Limited, New Delhi, 2005. ISBN

S. No.	Title of Book	Author	Publication
			13: 9781259027444
3	Numerical Methods	Jain , M.K., Jain R.K., Iyengar,S.R.K.	New Age International(P) Limited, Publishers, , New Delhi, 2014, /ISBN 13: 9788122433234
4	Introduction to SCILAB	Nagar, Sandeep	Independently Published, 2016. ISBN:152015111X,9781520151113
5	Scilab from Theory to Practice - I. Fundamentals	Roux, Philippe	Scilab Enterprises, ISBN-#2822702934

14. SUGGESTED SOFTWARE/LEARNING WEBSITES

a) www.tutorialpoint.com (Important website)
b) https://www.scilab.org/resourses/documentation/books
c) www.scilab.en.softonic.com
d) www.scilab.org >file>introscilab
e) www.scilab.org/en/download/latest