

SRM Institute of Science and Technology

Faculty of Engineering and Technology

Department of Chemical Engineering

Course Code & Title: **15CH305J Computational Techniques in Chemical Engineering**

Course Strategy Description

Course description:

To acquire computational techniques to solve chemical engineering problems by using computers

Compulsory/Elective course: Compulsory for B.Tech. Chemical Engineering

Credit hours: 3 credits

Course coordinator(s): Dr. K. Suresh, Associate Professor, Department of Chemical Engineering

Instructor(s):

Name of the instructor	Room number	Email (@ktr.srmuniv.ac.in)	Consultations (day order/periods)
Dr. K. Suresh	PGA 204	suresh.k	Day – 1: 5 and 6
Dr. Ashish Kapoor	PGA 202	ashishkapoor.o	Day – 3: 6 and 7

Relationship to other courses

Course category: Professional core

Prerequisite: 15MA206 and 15CH209

Co-requisite: Nil

Text book(s) and/or required materials:

1. Steven C. Chapra and Raymond P. Canale, Numerical Methods for Engineers, sixth Edn., McGraw Hill
2. Ismail Tosun, Modeling in Transport Phenomena – A Conceptual Approach, 2ndEdn., Elsevier Publications 2007

Reference book(s):

3. Y.V.C. Rao, “Chemical Engineering Thermodynamics”, Universities Press (India) Private Limited, 1997.
4. Robert E. Treybal, Mass Transfer Operations, 3rd Edition, McGraw Hill, 1980
5. H. Scott Fogler, Elements of Chemical Reaction Engineering, 4th Edition, Prentice Hall International Series
6. Warren L. McCabe, Julian, C. Smith and Peter Harriott, “Unit Operation of Chemical Engineering”, 7thEdn., McGraw Hill International Edition, New York, 2005.
7. H. K. Versteeg and W. Malalasekera, An introduction to computational fluid dynamics – The finite volume method, Longman Group Ltd 1995.

Class schedule: C Slot; two 50 minutes lecture sessions and two 50 minutes lab sections per week, for 15 – 16 weeks

DAY ORDER: HOUR	TIMING
DAY - 3: 6 AND 7	12.30 PM – 2.15 PM
DAY - 4: 4	10.40 AM – 11.30 PM
DAY - 5: 10	4.05 PM – 4.55 PM

Instructional Objectives (IOs) and Student Outcomes (SOs)

S.No.	Instructional Objectives	Student Outcomes				
		a				
1.	Understand the conservation of mass and energy equation	a				
2.	Familiarize the Algebraic Transcendental Equation, Linear Simultaneous Algebraic equations, Numerical Integration, Ordinary Differential Equations and Partial Differential Equations	a		d	e	k
3.	Apply computational techniques to Chemical Engineering problems.			d		k
4.	Provide the training to develop SCILAB program for solving the Chemical Engineering problems				e	

Teaching plan

Session	Topics	L / T	Text book/chapter	IOs	SOs	Problem solving (Y/N)
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UNIT I: NUMERICAL SOLUTION OF ALGEBRAIC TRANSCENDENTAL EQUATION		6				
1	Review of iterative methods: Bisection, Regula-Falsi and Newton-Raphson methods	1	[1] chapter -5.2,5.3 and 6.2	2	a, e, k	Y
2-4	Phase equilibrium problems and Equation of State	1/2	[3] chapter -11.2, 11.3	3	a	Y
5	Determination of Bubble and Dew points	1	[3] chapter -11.4	3	a, e, k	Y
6	Case studies: Roots of Equations: Non-ideal gas laws and Minimum reflux ratio	1	[1] chapter- 8.1	3	a, e, k	Y
UNIT II: NUMERICAL SOLUTION OF LINEAR SIMULTANEOUS ALGEBRAIC EQUATION		6				
7	Review of Gauss-Siedel iteration method, Gauss Elimination method and Cramer's rule	1	[1] chapter- 9.1, 9.2 and 11.2	2	a, e, k	N
8	Material and energy balance concept	1	[2] chapter- 1	1	a, k	N
9-10	Single stage and multiple stage extraction operations	1/1	[4] chapter – 10	1-3	a, e, k	Y
11	Cascade continuous stirred tank reactors	1	[2] chapter – 6.2	1-3	a, e, k	Y
12	Single and multiple effect evaporators	1	[6] chapter – 5	1-3	a, e, k	Y
UNIT III: NUMERICAL INTEGRATION		6				
13	Review of Trapezoidal rule and Simpson's rule	1	[1] chapter – 21.1 and 21.2	2	a, e, k	N
14	Determination of drying time from batch drying data	1	[4] chapter – 12	2,3	a, e	N

15-16	Determination of single and cascade plug flow reactor size	1/1	[5] chapter – 2.5	1-3	a, e	Y
17	Determination of batch kinetics from batch reactor data	1	[5] chapter 3.2	1-3	a, e, k	Y
18	Curve fitting and linear regression in heat conduction problems	1	[2] chapter – 1.4	2,3	a, e, k	Y
UNIT IV: NUMERICAL SOLUTION OF ORDINARY DIFFERENTIAL EQUATION		6				
19	Review of Taylor series, Euler's method and Runge-Kutta method	1	[1] chapter 25.1, 25.2 and 25.3	2	a, e, k	N
20	Unsteady state of mixing tank	1	[1] Chapters 2.1	1-3	e, k	Y
21	Concentration profile in a batch reactor using different numerical methods for solving the ODE	1	[1] Chapters 28.1	1-3	e, k	Y
22-23	Heat conduction problems	1/1	[2] Chapters 2.2	1-3	a, e, k	Y
24	Concentration profile along the reactor length in isothermal Plug Flow Reactor (PFR)	1	[5] Chapters 28.1	1-3	e, k	Y
UNIT V: NUMERICAL SOLUTION OF PARTIAL DIFFERENTIAL EQUATION		6				
25	Numerical methodology for solving the partial differential equation	1	[1] Chapters 30.1 and 30.2	2	a, e, k	N
26	Unsteady state one dimensional heat transfer problem	1	[7] Chapters 8.3	1-3	e, k	Y
27-28	Steady state two-dimensional heat transfer problems	1/1	[1] Chapters 30.5	1-3	e, k	Y
29-30	Unsteady state one dimensional mass transfer problem	1/1	[1] Chapters 32.1	1-3	a, e, k	Y

Evaluation methods

S.NO.	Test	Topics covered	Marks	Test/Exam duration (min)
1.	Cycle test – I	Unit I and II	15	100
2.	Cycle test – II	Unit III, IV and V	25	180
3.	Surprise test	Questions from any units	5	20
4.	Assignment	Questions from any units	5	-
5.	Final exam	All the units	50	180

S.No.	Write programs using SCILAB for solving	Contact hours	IOs	SOs	Text book/chapter
1	Linear Algebraic Equations: Gauss Seidel method	2	4	e	1
2	Linear Algebraic Equations: Gauss Elimination method	2	4	e	1,2
3	Polynomial root finding techniques: Newton Raphson Method	2	4	e	1,5
4	Bubble point and dew point using thermodynamics iteration method	2	4	e	1,3
5	Numerical Integration: Trapezoidal rule and Simpson 1/3 rule	2	4	e	1,5
6	Ordinary Differential Equation: Euler's method	2	4	e	1,5
7	Partial Differential Equation: Finite difference method	2	4	e	1,7
8	Ordinary Differential Equation: R-K Method	2	4	e	1,5

Surprise test

The surprise test will not be announced. The questions for this test will be covered until the previous class.

Home assignments

A few units will have home assignment. All the assignments should be submitted on or before the last date of submission.

Teaching Methodology

Chalk and talk for the entire course

Prepared by: Dr. K. Suresh, Associate Professor, Department of Chemical Engineering

Dated:

Revision no.:

Date of revision:

Revised by:

Course Coordinator

Academic Coordinator

HoD/Chemical