SRM UNIVERSITY

FACULTY OF ENGINEERING AND TECHNOLOGY

SCHOOL OF CHEMICAL ENGINEERING

COURSE PLAN

Course code : CH0301 Course Title : Computational methods in Chemical Engineering

Semester : V Course Time : June 2011 – Dec 2011

Required Text Books:

1. Mickley H. S., Sherwood T.K. and Reed C.E., Applied Mathematics in Chemical Engineering, McGraw Hill, New York,1957.
2. Alan L.Myers and Warren D Seider., Introduction to Chemical Engineering and Computer Calculations, Prentice Hall, Engle Wood Cliffs (N.J), 1976.

Web resources: 1) http://www.che.iitb.ac.in/faculty/scp/CL-701-Lecture-Notes-07.pdf
2) http://ocw.mit.edu/courses/#chemical-engineering

Prerequisite :

Engineering Mathematics, Basic chemical engineering concepts, Numerical methods

Objectives

To familiarize:

1. Numerical solution of algebraic transcendental equation.
2. Solution of linear simultaneous algebraic equations.
3. Numerical integration.
4. Solution of ordinary differential equations.
5. Unsteady state heat and mass transfer problems

Assessment Details

Cycle Test-I	: 10 Marks
Cycle Test-II	: 10 Marks
Model Exam	: 20 Marks
Surprise Test	: 05 Marks

Attendance : 05 Marks

Out comes

Students who have successfully completed this course will have full understanding of the following concepts

Course Outcome	Program outcome
1. Students are able to apply numerical techniques to solve chemical engineering problems 2. This subject is useful to solve simultaneous equation by various methods 3. Students become familiar with numerical integration techniques 4. Students gain the knowledge of solving differential equation by various methods 5. Students can become familiar with unsteady state problems and its solutions	1. This subject increases the analytical thinking ability of the students 2. Students become familiar with various numerical techniques and will be able to apply it to chemical engineering problems 3. The course is useful when the students carry out research activities or when they pursue higher studies

Detailed Lesson plan

NUMERICAL SOLUTION OF ALGEBRAIC TRANSCENDENTAL EQUATION					
Session No	Topics to be covered	Time (Min)	Ref	Teaching method	Testing method
1	Introduction to iteration methods	50	1 & 2	GB	Discussion
2	Bisection method – transcendental equation	50	1 & 2	GB	Discussion
3	Regula falsi & Newton Raphson methods	50	1 & 2	GB	Discussion
4	Problems based on iteration methods	50	1 & 2	GB	Problems
5	Phase equilibrium – concepts	50	1 & 2	GB	Discussion
6	Equation of state concept and calculations	50	1 & 2	GB	Discussion
7	Dew point & bubble point calculations	50	1 & 2	GB	Problems

8	Differential distillation – an introduction	50	1 & 2	GB	Discussion
9	Minimum reflux ratio – calculations	50	1 & 2	GB	Problems
SOLUTION OF LINEAR SIMULTANEOUS ALGEBRAIC EQUATIONS					
1	Gauss method – an introduction	50	1 & 2	GB	Discussion
2	Application of Gauss method	50	1 & 2	GB	Problems
3	Gauss – siedel iteration method – concepts	50	1 & 2	GB	Discussion
4	Problems on Gauss – siedel iteration method	50	1 & 2	GB	Problems
5	Jacobi's iteration method – introduction	50	1 & 2	GB	Discussion
6	Problems on Jacobi's iteration method	50	1 & 2	GB	Problems
7	Multi effect evaporators – introduction	50	1 & 2	GB	Discussion
8	Problems in multi effect evaporators	50	1 & 2	GB	Problems
9	Application of above methods for chemical engineering problems	50	1 & 2	GB	Problems
NUMERICAL INTEGRATION					
1	Trapezoidal rule	50	1 & 2	GB	Discussion
2	Simpson's 1/3 and 3/8 rule	50	1 & 2	GB	Discussion
3	Weddle's rule – numerical integration	50	1 & 2	GB	Discussion
4	Rayleigh's equation solution – mass transfer	50	1 & 2	GB	Problems
5	NTU calculation in absorption units	50	1 & 2	GB	Problems
6	Determination of drying time-batch drying	50	1 & 2	GB	Problems
7	Determination of reactor size	50	1 & 2	GB	Problems
8	Flux determination & interpolation concepts	50	1 & 2	GB	Discussion
9	Estimation of thermodynamic properties	50	1 & 2	GB	Problems
SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS					
1	Taylor's series method	50	1 & 2	GB	Discussion
2	Euler's method for differential equations	50	1 & 2	GB	Discussion
3	Runge – Kutta method	50	1 & 2	GB	Discussion
4	Application of Runge – Kutta method	50	1 & 2	GB	Problems
5	Predictor – corrector method – introduction	50	1 & 2	GB	Discussion
6	Problems on Predictor – corrector method	50	1 & 2	GB	Problems

7	Heat conduction problems	50	1 & 2	GB	Problems
8	Problems on chemical reaction engineering	50	1 & 2	GB	Problems
9	Comparison of numerical and analytical solution	50	1 & 2	GB	Discussion
UNSTEADY STATE PROBLEMS					
1	Unsteady state process - introduction	50	1 & 2	GB	Discussion
2	Heat transfer – an introduction	50	1 & 2	GB	Discussion
3	Unsteady state heat transfer	50	1 & 2	GB	Discussion
4	Numerical methods available for solving unsteady state problems	50	1 & 2	GB	Problems
5	Boundary condition Problems in transient Heat transfer	50	1 & 2	GB	Discussion
6	Mass transfer – basic concepts	50	1 & 2	GB	Discussion
7	Unsteady state mass transfer	50	1 & 2	GB	Discussion
8	Various numerical methods available for mass transfer problems	50	1 & 2	GB	Discussion
9	Problems in unsteady state mass transfer	50	1 & 2	GB	Discussion