



# ARSD College, University of Delhi

## Model Course Handout/Lesson Plan

Course Name : B.Sc. Industrial Chemistry						
Semester	Course Code	Course Title	Lecture (L)	Tutorial (T)	Practical (P)	Credit (C)
VI	Course Code: CHEMISTRY -SEC-1	IT Skills For Chemists	2			2
Teacher/Instructor(s)		Dr. Preeti Chaudhary				
Session		2021-22				

### Objectives:

The objective of this course is to introduce the students to fundamental mathematical techniques and basic computer skills that will help them in solving chemistry problems. It aims to make the students understand the concept of uncertainty and error in experimental data. It acquaints the students with different software for data tabulation, calculation, graph plotting, data analysis and document preparation.

### Course Learning Outcomes:

By the end of the course, the students will be able to:

- Become familiar with the use of computers
- Use software for tabulating data, plotting graphs and charts, carry out statistical analysis of the data.
- Solve chemistry problems and simulate graphs.
- Prepare documents that will incorporate chemical structure, chemical equations, mathematical expressions from chemistry.

### Lesson Plan:

Unit No.	Learning Objective	Lecture No.	Topics to be covered
1	Unit 1 Mathematics	1	Fundamentals, mathematical functions, polynomial expressions, logarithms, the exponential function.
		2	Units of a measurement, interconversion of units, constants and variables, equation of a straight line, plotting graphs.
		3	Uncertainty in experimental techniques: Displaying uncertainties, measurements in chemistry, decimal places, significant figures, combining quantities.
		4	Uncertainty in measurement: types of uncertainties, combining uncertainties
		5	Statistical treatment. Mean, standard deviation, relative error

		6	Data reduction and the propagation of errors. Graphical and numerical data reduction. Numerical curve fitting: the method of least squares (regression).
		7	Algebraic operations on real scalar variables (e.g. manipulation of van der Waals equation in different forms). Roots of quadratic equations analytically and iteratively (e.g. pH of a weak acid).
		8	Numerical methods of finding roots (Newton-Raphson, binary –bisection, e.g. pH of a weak acid not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions).
		9	Differential calculus: The tangent line and the derivative of a function, numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations)
		10	Numerical integration (Trapezoidal and Simpson's rule, e.g. entropy/enthalpy change from heat capacity data)
2	Unit 2	11	Introductory writing activities: Introduction to word processor and structure drawing (ChemSketch) software.
		12	Incorporating chemical structures, chemical equations, expressions from chemistry
		13	Bragg's law, van der Waals equation, into word processing documents.
		14	Maxwell-Boltzmann distribution law,
3	Unit 3	15	Handling numeric data: Spreadsheet software (Excel/LibreOffice Calc), creating a spreadsheet, entering and formatting information,
		16	basic functions and formulae, creating charts, tables and graphs Incorporating tables and graphs into word processing documents.
		17	Simple calculations, plotting graphs using a spreadsheet
		18	Planck's distribution law, radial distribution curves for hydrogenic orbitals
		19	Gas kinetic theory- Maxwell-Boltzmann distribution curves as function of temperature and molecular weight
		20	Spectral data, pressure-volume curves of van der Waals gas (van der Waals isotherms), data from phase equilibria studies. Graphical solution of equations
4	Unit 4	21	Numeric modelling: Simulation of pH metric titration curves.
		22	Excel functions LINEST and Least Squares.
		23	Numerical curve fitting, linear regression (rate constants from concentration- time data, molar extinction coefficients from absorbance data)
		24	Numerical differentiation (e.g. handling data from potentiometric)
		25	handling data from pH metric titrations, pKa of weak acid
		26	integration (e.g. entropy/enthalpy change from heat capacity data)
5	Unit 5	27	Statistical analysis

		28	Gaussian distribution and Errors in measurements and their effect on data sets.
		29	Descriptive statistics using Excel.
		30	Statistical significance testing: The t test. The F test. Presentation graphics.

#### Evaluation Scheme:

No.	Component	Duration	Marks
1.	Internal Assessment		12
	• Quiz		
	• Class Test		
	• Attendance		
	• Assignment		
2.	End Semester Examination	2 hr	38

#### Detail of course

##### Unit 1

Mathematics Fundamentals, mathematical functions, polynomial expressions, logarithms, the exponential function, units of a measurement, interconversion of units, constants and variables, equation of a straight line, plotting graphs. Uncertainty in experimental techniques: Displaying uncertainties, measurements in chemistry, decimal places, significant figures, combining quantities. Uncertainty in measurement: types of uncertainties, combining uncertainties. Statistical treatment. Mean, standard deviation, relative error. Data reduction and the propagation of errors. Graphical and numerical data reduction. Numerical curve fitting: the method of least squares (regression). Algebraic operations on real scalar variables (e.g. manipulation of van der Waals equation in different forms). Roots of quadratic equations analytically and iteratively (e.g. pH of a weak acid). Numerical methods of finding roots (Newton-Raphson, binary – bisection, e.g. pH of a weak acid not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions). Differential calculus: The tangent line and the derivative of a function, numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations). Numerical integration (Trapezoidal and Simpson's rule, e.g. entropy/enthalpy change from heat capacity data).

##### Unit 2

Introductory writing activities: Introduction to word processor and structure drawing (ChemSketch) software. Incorporating chemical structures, chemical equations, expressions from chemistry (e.g. Maxwell-Boltzmann distribution law, Bragg's law, van der Waals equation, etc.) into word processing documents.

##### Unit 3

Handling numeric data: Spreadsheet software (Excel/ LibreOffice Calc), creating a spreadsheet, entering and formatting information, basic functions and formulae, creating charts, tables and graphs Incorporating tables and graphs into word processing documents. Simple calculations, plotting graphs using a spreadsheet (Planck's distribution law, radial distribution curves for hydrogenic orbitals, gas kinetic theory- Maxwell-Boltzmann distribution curves as function of temperature and molecular weight), spectral data, pressure-volume curves of van der Waals gas (van der Waals isotherms), data from phase equilibria studies. Graphical solution of equations

##### Unit 4

Numeric modelling: Simulation of pH metric titration curves. Excel functions LINEST and Least Squares. Numerical curve fitting, linear regression (rate constants from concentration- time data, molar extinction coefficients from absorbance data), numerical differentiation (e.g. handling data from potentiometric and pH metric titrations, pKa of weak acid), integration (e.g. entropy/enthalpy change from heat capacity data)

##### Unit 5

Statistical analysis: Gaussian distribution and Errors in measurements and their effect on data sets. Descriptive statistics using Excel. Statistical significance testing: The t test. The F test. Presentation graphics.

<b>Suggested Books:</b>
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1. McQuarrie, D.A. (2008), Mathematics for Physical Chemistry University Science Books.
2. Steiner, E.(2008),The Chemical Maths Book Oxford University Press.
3. Yates, P.(2007),Chemical calculations, CRC Press.
4. Harris,D.C.(2007),Quantitative Chemical Analysis. Freeman, Chapters 3-5.
5. Levie, R. de. (2001), How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge Univ. Press.
6. Venit, S.M. (1996), Programming in BASIC: Problem solving with structure and style. Jaico Publishing House.