CHEM 101 – CHEMISTRY AND THE COMPUTER   Fall 2019

Dr. Roger H. Terrill   www.chemistry.sjsu.edu/rterrill   roger.terrill@sjsu.edu

Office: DH-004B, 924-4970   Lecture: DH 503

Class Meetings / Office Hours:

Activity:	T and Th	09:30-10:20 a.m.	DH-503
Seminar:	T and Th	10:30-11:20 a.m.	DH-503
Office Hours:	T and Th	12:30-01:20 p.m. or by appointment	DH-004B
Final Exam:	W, 12/11/19	09:45-12:00 p.m. or by appointment	DH-004B

Prerequisites: Chem 55, Math 030 or 030P with grades of "C" or better; "C-" not accepted.

Text: None required. Useful resources include "Excel for Chemists" and "Numerical Recipes for Chemists" and "Excel VBA Programming for Dummies"

Lecture Notes and Activity Instructions: These will be distributed via the course website on Canvas. https://sjsu.instructure.com/

Objectives: Demonstrate competence in the use of Microsoft Excel for the archiving, analysis and tabular and visual presentation of scientific data. Demonstrate competence in solving chemical problems using Excel, Excel Visual Basic for Applications (VBA).

The above objectives fall within objectives 1-5, 8 and 10 the Chemistry Department Program Learning Objectives for the BS and BA in Chemistry.

Final Exam: The final exam will be on **Wednesday, December 11, from 945-1200** in the regular classroom. Note that this is final exam date and time for Section 2, which starts at 9:30 AM.

Grading Structure: A single letter grade will be assigned for Chem 101.

Lecture Grade: 50% of the total grade, based on exams and quizzes. Material on the exams will be based on the lecture and homework assignments.

Activity Grade: 50% of the total grade. This will be based on assignments mainly done during the activity session.

Extra Credit: None

Weights assigned to points: None

Late or missing work: No credit will be given for late or missing work

***Preliminary* plans for grading structure:**

Lecture Grade: 300 points

Midterm exam:	100 points
Final two-hour exam:	100 points
3-10 Quizzes:	100 points

Activity Grade: 300 points

15 Exercise assignments:	300 points
Approximate Total	600 points

Grading scale by *percent* of total points:

96	92	88	84	80	76	72	68	64	60	56	52	<52
A+	A	A-	B+	B	B-	C+	C	C-	D+	D	D-	F

Week	Overview of Proposed Lecture Topics	
1	**Basics of Computers and MS Office: Excel, and Word**	Processors, operations, stack, cache, storage, basic operations, file systems, file formats, numeric formats (binary, bcd, floating point). Data types in programming: Boolean, integer, float, string, etc. Representation of integers, signed integers and real numbers. ASCII text convention.
1	**Display of Quantitative Information I Textual**	Number formatting, significant figures and symbols. Table formatting. Display of units. "Paste special to preserve data." Audit trails: file names, paths, dates and conditions. Information management. Equation editor.
1	**Display of Quantitative Information II Visual**	Data import and export, graphing to scientific standards, scaling, formatting, dealing with different number formats. Use of text editor (Notepad), Binary editors and Excel.
2	**Basic Chemical Calculations**	Chemical functions: plots to extract information: Gas Laws, solubility, pH and complexation.
3	**Programming in VBA**	Syntax, basic concepts and interfacing with Excel worksheets. Making and using user-defined functions.
4	**Generalized Multivariate Least Squares Regression**	Theory and application of univariate and multivariate least squares analysis using in-spreadsheet matrix manipulation, Visual Basic and analysis tools "Linest" and "Regression"
5	**Statistical Calculations**	Excel exercises in statistics: Descriptive aspects mean, median, mode, standard deviation, confidence tests. Data Modeling by Regression
6	**Propagation of Random Uncertainty: Simulation and Theory**	Discrete distributions generated by variable input variables. Differential error propagation methods.
7	**Monte-Carlo Methods**	Error propagation by extrema and by random number generation. Calibration curve examples.
8	**Calibration Methods**	Using Excel to deal with external and internal standards, standard additions, spike recovery and quality control standards.
8	**Iteration and Data Import**	Further VBA concepts, Macro recording and adaptation.
9	**Advanced Equilibria**	Exact solutions by computational approximation. Minimization using successive convergent approximation and via the golden mean method.
10	**Spectral Fitting**	Multivariate Linear and Non-linear regression
11	**Titration Curves: Modeling and fitting**	Single and multiple equilibrium modeling of titration data: pH versus volume of titrant, pCa, pCl etc.
12	**Smoothing Methods**	Smoothing functions, moving average, triangular, Gaussian.
12	**Discrete Fourier Analysis**	Basic concepts and theorems, issues attending discrete signal processing (Nyquist theorem, aliasing etc.) signal recovery, smoothing.
13	**Diffusion Simulation**	Simulation of boundary condition problems.
14	**Cross correlation and Autocorrelation analysis**	Fourier and discrete correlation analysis for signal recovery. Examples from flow cytometry and dynamic light scattering.
15	**Molecular Mechanics / Quantum Calculations**	Introduction to the WebMO interface to Firefly molecular modeling and calculation software. Structural determination, normal modes of vibration and UV spectral prediction.

Course Requirements and Assignments:
"Success in this course is based on the expectation that students will spend, for each unit of credit, a minimum of 45 hours over the length of the course (normally three hours per unit per week) for instruction, preparation/studying, or course related activities, including but not limited to internships, labs, and clinical practica. Other course structures will have equivalent workload expectations as described in the syllabus."

Classroom Protocol:
Be polite.

Due Dates and Policy on Late Work:
I all material are submitted via Canvas, so submission after the due date will not be possible except in extenuating circumstances and by agreement with me. Exercises will typically be due before the beginning of the next activity period.

Drop Policy:
The deadline to drop classes without a W is Tuesday, September 3rd. The deadline to add is September 10th. After the regular drop period ends, only documented medical or similar emergencies will be accepted as a valid reason to drop a course. Note particularly that a change in work schedule is no longer an acceptable reason. Therefore, it is critical that you inform your employer that you have a serious commitment for your scheduled class and laboratory times during the whole semester. If your employer cannot guarantee that you can meet this obligation, then you should drop the class in order to allow someone who can fulfill this commitment to register. Also, be aware of the fact that "unsatisfactory performance in course work and protection of your GPA is not a serious and compelling reason in itself for requesting permission to drop". After the twentieth day of instruction, all petitions to drop classes or withdraw from school will be reviewed by the Director of Academic Services. Petitions are available in the Student Resource Center.

ADDENDUM TO ALL CHEMISTRY DEPARTMENT GREENSHEETS
(Except Chem 291 Sections)

Revised August 2018

University Policy

Per University Policy S16-9, university-wide policy information relevant to all courses, such as academic integrity, accommodations, etc. will be available on the Office of Graduate and Undergraduate Programs' Syllabus Information Web Page at http://www.sjsu.edu/gup/syllabusinfo/

CHEMICAL SAFETY – *all courses*

   Chem 120S is a required course for all chemistry majors and minors and a prerequisite for all Chem 180/298 research.

EMERGENCIES AND EVACUATIONS – *all courses*

   If you hear a continuously sounding alarm, or are told to evacuate by Emergency Coordinators (colored badge identification), walk quickly to the nearest stairway (end of each hall). Take your personal belongings, as you may not be allowed to immediately return. Follow instructions of Emergency Coordinators. Be quiet so you can hear. Once outside, move away from the building. Do no return to the building unless the Police or Emergency Coordinators announce that you may.

<u>DISABLED STUDENTS</u> – ***all courses***

Campus policy in compliance with the Americans with Disabilities Act: "If you need course adaptations or accommodations because of a disability, or if you need special arrangements in case the building must be evacuated, please make an appointment with me as soon as possible, or see me during office hours. Presidential Directive 97-03 requires that students with disabilities requesting accommodations must register with DRC to establish a record of their disability."

<u>ACADEMIC INTEGRITY STATEMENT</u> – ***all courses*** (from the Office of Student Conduct and Ethical Development):

"Your own commitment to learning, as evidenced by your enrollment at San José State University, and the University's Academic Integrity Policy requires you to be honest in all your academic course work. Faculty members are required to report all infractions to the Office of Student Conduct and Ethical Development. The policy on academic integrity can be found at http://sa.sjsu.edu/student_conduct.