1. Course Information

Course Name: Mathematics for Chemists

Semester, Year & Section: Spring 2014

Location & Time: Wednesday 8:40-12:30 K-15, Friday 10:40-12:30 K-15

2. Instructor Information

Name: Mehmet Fatih Danışman

Office Address: 0-318 Chemistry

Office Hours: No office hours. Take appointment (through e-mail) before coming to my office

3. Course Description

The objective of this course is to equip the students with the basic knowledge of functions of single and multivariable, Lagrange multipliers, Newton-Raphson method, numerical integration, first order differential equations of types exact, linear, homogenous, separable, higher order differential equations with constant coefficients, partial differential equations, matrices, determinants, set of linear equations and their applications on chemical problems.

4. Course Materials & Resources

Textbook:

The Chemistry Maths Book / Steiner, E., Call no: QA37.2 .S7985 (in reserve collection). 35 copies are available in the bookstore.

Other Resources:

Books:

- **Differential Equations / Ross, Shepley L.**, Call no: QA371 .R6. This is a particularly good book for studying differential equations, with lots of nice examples with solutions.

- **Advanced Calculus / Kaplan, W.**, Call no: QA303 .K33. This book covers almost all the material in *Steiner,* in more detail.

- **Mathematical methods in the physical sciences / Mary L. Boas.** Call no: QA37 .B725 (in reserve collection). The contents of this book and the order/way they are covered are almost identical to *Steiner.* However some topics are explained in a more detailed/understandable way. You can consider this book as an alternative to the original textbook, and refer to it when you need further information.

- **Mathematical methods for scientists and engineers / Donald A. McQuarri**

www:

- **http://mathworld.wolfram.com/**

Software:

- *Mathcad*: This is a powerful and easy to use/learn math software. Since it is based on a visual input format that uses standard mathematical notation (rather than text input that many other math software, like *Mathematica*, use) it is very easy to learn how to use it. You can solve almost all of the problems that we will discuss in the class by using *Mathcad* and **I'll provide the solutions to some of the recommended questions as a *Mathcad* worksheet file.** So if you want these solutions, you should, first, have access to Mathcad, second, learn how to open and read a *Mathcad* file. ***Mathcad* is installed (or will be installed shortly) in all the computers in the chemistry computer lab**. I believe learning (or at least getting familiar with) a math software will be very beneficial for you. Particularly you can utilize Mathcad in physical chemistry, analytical chemistry and quantum chemistry courses.

5. Contents

We will start covering from Ch. 8, and you are assumed to have some knowledge of the first seven chapters of the book. Some of the rest of the chapters will be covered partially. The sections that will be covered in each of these chapters are given below in parentheses.

- Chapter 8: Complex numbers (5 hours)
- Chapter 9: Functions of several variables (9 hours)
- Chapter 10: Functions in 3 dimensions (3 hours)
- Chapter 11: First-order differential equations (5 hours)
- Chapter 12: Second-order differential equations. Constant coefficients (6 hours)
- Chapter 13: Second-order differential equations. Some special functions (5 hours)
- Chapter 14: Partial differential equations (4 hours)
- Chapter 15: Orthogonal expansions. Fourier analysis (15.1, 15.2, 15.4) (4 hours)
- Chapter 16: Vectors (4 hours)
- Chapter 17: Determinants (5 hours)
- Chapter 18: Matrices and linear transformations (18.1, 18.2, 18.3, 18.4) (4 hours)
- Chapter 19: The matrix eigenvalue problem (19.1, 19.2, 19.3) (4 hours)
- Chapter 20: Numerical methods (20.3, 20.5, 20.7) (3 hours)
- Chapter 21: Probability and statistics (21.9) (2 hours)

6. Course Policies

a. Exams and Grading Policy

Not everyone will be permitted to take the final exam. In order to be eligible for the final exam, you must attend the at least 50% of the classes. Otherwise, a) You will not be allowed to take the final examination; b) your letter grade will be assigned as "NA" in your record.

Please note that students with a "NA" grade at the end of the semester have no right for "bütünleme" according to the regulations of METU.

2 Midterm Exams (March 23, 2 pm; April 27 2pm)	30% each
Final Exam	40%
Bonus in class quizzes	5 – 10%

- Please bring your calculators and school ID's to the exam. Exam dates and locations will be posted on METU online.
- While assigning the letter grades, average grade of the class, the spread of the grades and attendances will be taken into account. This doesn't necessarily mean that the average score will get CC but rather should be considered as a "modified catalog". **inally regardless of the class average, a total score of less than 45 will fail. This does not necessarily mean that any score above 45 will pass (passing score may depend on the class average). If you try to negotiate about your grade during the grading period at the end of the term, official grading and attendance rules (see METU Academic Catalog, Article 10) will be applied.**
- Make up exam will be given, after the finals period, **only** to those students who have a **valid, officially documented excuse** (see METU Academic Catalog, Article 9). Unfortunately each term there exist some who miss the passing grade by just 1 or 2 points. At the end of this term, if you happen to be one of those, please **don't** come to my office just before the grades are submitted and ask for an extra/make up exam to raise your grade.
- **Personal statement: Grading is the worst part of teaching. Especially when one has to fail a student (due to his poor performance) who is in a critical position (family problems, personal problems, financial problems, extended period of study,…). So, those of you**

who are in critical condition please inform me at the beginning of the term about your condition, so that I can (a) advise you about what to do/ how to study if you want to pass the course, (b) talk to your academic adviser and find out how we can help you. Please do not wait till the end of the term and come to see me for negotiating about your grades during the grading period.

b. Office Hours and Communication

- If you want to see me for any course related questions/problems, please first take an appointment through e-mail (otherwise you may not find me at my office, or I may be busy). **Please include in the subject line of your e-mails "CHEM 257". E-mails without "CHEM 257" in the subject line will not be considered/replied.**
- All announcements (grades, assignments,...) will be posted on "METU Online" website (and when possible via e-mail), and you are expected to check METU Online and METU e-mail accounts regularly (weekly).

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7. University Policies

It is very important that you know and understand the university regulations regarding academic integrity, since you are expected to and should act according to these rules throughout your university life. Below I quoted the abovementioned academic integrity code.

Code of Integrity *
All students are expected to have academic integrity principle in all academic works. That is, a student must submit work only the student's own. Students shall comply with academic integrity codes and shall avoid situations likely to violate this code since academic dishonesty diminishes credit to the academic community.

Academic Dishonesty
Academic dishonesty is defined as any activity, which tends to undermine the academic integrity of the university. Academic integrity is one of the major factors that determines the image and dignity of the university. So not only academic people are responsible to maintain the duration of academic integrity, all members of the university including students should obey the rules and regulations of the university.

Academic Misconducts
Behaviour considered as misconduct or violation in academic terms are defined so:

a. Cheating

Cheating means giving or receiving any unauthorized aid in any academic exercise. It includes but is not limited to the following actions:
- *Copying from someone else's test or examination paper*
- *Using external assistance like the use of tutors, books, lecture notes and calculator in any in-class or take-home examination although it is prohibited*
- *Possessing, buying, selling, removing, receiving or using a copy or copies of any materials to be used as an instrument of academic evaluation*
- *Using another person as a substitute in an academic evaluation*
- *Working with other persons on a particular project although the instructor has required indivudial work*
- *Copying a report or homework assignment prepared by someone else or using records or laboratory results obtained by someone else as it is your work*
- *Attempting to influence or change any academic evaluation by unfair means which includes altering exam results or grades or changing anything on exam papers hiddenly while they are shown by the instructor for control and objections*

b. Plagiarism

Plagiarism means using a part or whole of a written material without proper acknowledgement of source. A student should pay attention to the originality of any material he or she uses for such situations:
- *Whenever he or she quotes another person's actual words,*
- *Paraphrases another person's words,*

- *Uses another person's idea, opinion or theory,*
- *Whenever he or she uses internet sources, borrows facts, statistics or any information which is not common knowledge.*
- *As a whole, theses, essays, term papers, and other academic project requirements must be the original work of the student who is submitting them. And while using other materials, the source should be properly and clearly defined by references.* For useful information regarding plagiarism check http://www.fbe.metu.edu.tr/Intihal/intihal.htm

3. Fabrication

Fabrication is defined as intentionally misrepresentation of any academic information or citation in order to deceive. A student must not falsify or invent any information or data in an academic exercise including, but not limited to, records or reports, laboratory results, and citations to the sources of information.

4. Interference

Interference is defined as trying to get advantage in any academic evaluation by unfair ways. This includes but is not limited to the following:

- *A student should not steal, change or destroy another student's work. This includes theft, defacement, harming or collecting all sources so as to prevent others to reach the information they contain.*
- *A student should not give or offer bribe, promise favors, make threats to any academic staff to change or affect any grade or result of any academic evaluation.*

5. Facilitating Academic Dishonesty

This means aiding or abetting others to cheat, to plagiarise or to commit any academic dishonesty. A student must not intentionally or knowingly help or attempt to help another student to commit an act of academic misconduct. It includes but is not limited to the following:

- *Giving unauthorized assistance to another or others during an academic evaluation like allowing students to copy from each other or lecture books or notes.*
- *Substituting for another student in an academic evaluation.*
- *Permitting one's academic work to be represented as the work of another.*
- *Providing any information about any academic evaluation before it takes place to a student such that that person gains an advantage for academic evaluation.*

6. Responsibility to Report Academic Dishonesty

Universities are academic entities which are devoted to innovate and transmit new knowledge for the scientific, technological, economic, cultural and social improvement of the society through scholarly research and related community services. The responsibility is to maintain an environment in which it members should behave in a good manner.

Academic Dishonesty is a serious threat to the dignity of the university. It decreases the quality of education and causes loss of confidence in terms of university premises. That's why it is the responsibility of all students to report any witnessed academic dishonesty. If one does not comply with university rules and regulations and academic misconducts stated above and if another one sees or realises this and does not report it to any academic unit, he or she will be a part of the violation committed against university's integrity.