COLUMBIA UNIVERSITY

IN THE CITY OF NEW YORK
DEPARTMENT OF CHEMICAL ENGINEERING

17 December 2020

MEMORANDUM FOR: Chemical Engineers of CHEN E4330

SUBJECT: CHEN E4330 Advanced Chemical Kinetics Course Syllabus

1. **CHEN E4330 Advanced Chemical Kinetics**
   3.0 pts

Prerequisites: Undergraduate Chemical Kinetics, Mass transport, or Kinetics S2E Module.
Course Description: Reaction kinetics, molecular view of reaction kinetics, reactions in liquid, reactions at surfaces, diffusion-reaction systems. Applications to the design of batch and continuous reactors. Special topics in kinetics and reactor design.

2. **Instructor:**
   Dr. Robert G. Bozic LTC USA(Ret)
   818 Mudd Building
   212-854-9637, rb2335@columbia.edu

   Teaching Assistant
   Name: to be determined
   Email: to be determined

3. **Class Hours:** Tuesday (08:40 AM – 09:55 PM) and Thursday (08:40 AM -09:55 PM)

4. **Classroom/Computer Room:** See the Directory of Classes website for classroom and/or online designation / Mudd 251

5. **Textbook and Materials (required, suggested, and supplemental):**

a. Textbook (Required):

Folger, H.S. *Elements of Chemical Reaction Engineering 5th Edition*, Prentice Hall, Upper Saddle River, N.J. 2016. ISBN-13: 9780133887518. Unless you are very strong in programming (Matlab, Python, or Mathematica etc.) Students are encouraged to purchase a version of Fogler that includes Polymath software. Polymath contains simple-to-learn Ordinary Differential Equation (ODE) and non-linear equation solvers. Educational versions of Polymath were listed as available $20 (4 mo. license), $30 (12 mo. license), or $39 (perpetual-use license). Students can purchase and download this software from: www.polymath-software.com/fogler/ (Note: Polymath is only available for Windows, and not Mac computers) Fogler's 5th Ed. website: http://umich.edu/~elements/5e/ (Esposito, CHEN E4330 Spring 2020 Syllabus).

Textbook (Suggested):

Houston, Paul L., *Chemical Kinetics and Reaction Dynamics, 2nd Edition*, Dover Publishing, 2006. ISBN-13: 9780486453347(highly recommended textbook)

b. **Materials (Required):**

1.CHEN E4330 Courseworks web site at https://courseworks.columbia.edu/ Accessed 19 Nov 2020.

c. Materials (Supplemental)

1.Computer programs, reference books, and internet sites:

ASPEN Plus. Chemical Engineering Computer software licensed to Columbia University Computers in Mudd 251 (also called 251 ET). (See the CUIT web site for remote access available: https://cuit.columbia.edu/computer-lab-technologies Accessed 19 Nov 2020)

Atkins, Peter and Julio de Paula, *Physical Chemistry 11th Edition*, Oxford University Press. Oxford, U.K. 2018, ISBN-13: 9780198769866 (molecular kinetics)

Beer, David *A Guide to Writing as an Engineer, 2nd Edition*, John Wiley & Sons, Inc. Hoboken, NJ. 2005. ISBN-13: 978-0471430742 (technical writing).

Crowl, Daniel A. and Joseph F. Louvar, *Chemical Process Safety" Fundamentals with Applications 4th Edition*, Prentice Hal New York 2019: ISBN-13: 978-0134857770, (reactor safety)

Higham, Desmond J. and Higham, Nicholas J. *Matlab Guide 2nd Edition*, SIAM: Philadelphia, 2005, ISBN-13: 978-0898715781 (Matlab)

Masel, Richard I., *Principles of Adsorption and Reaction on Solid Surfaces*, John Wiley and Sons Inc., New York, 1996. ISBN-13: 978-0-471-30392-3: (surface reactions)

Peters, Max S. and Klaus D. Timmerhause, *Plant Design and Economics for Chemical Engineers 5th edition*, McGraw-Hill, New York 2003, ISBN-13: 978-0071240444 (process diagrams. symbols, and design, HAZOps)

Rawling, James Blake and Ekerdt, John G., *Chemical Reactor Analysis and Design Fundamentals 1st Edition*, Nob Hill Publishing, 2002. ISBN-13: 978-0615118840.
Sandler, S. *Chemical, Biochemical, and Engineering Thermodynamics 4th Edition*, Wiley, New York, 2006. ISBN-13: 978-0471661740 (chemical equilibrium)

Seider, Warren D., Seader, J.D. Lewin, Daniel R, and Soemantri Widagdo *Product and Process Safety Design Principles, Synthesis, Analysis, and Evaluation, 3rd Edition*, New York: Wiley 2009: ISBN-13:978-0470-04895-5, (design and cost estimation)

Steinfeld, Francisco, and Hase, *Chemical Kinetics and Dynamics 2nd Edition*, Prentice Hall, 1998. ISBN-13: 978-0137371235

2.Other supplemental material will be posted on the course works web page throughout the course.

6. Course Objectives:

a. Understand kinetic rate expressions and how to design experiments to determine them.
b. Develop computer skills for mathematical modeling of reactive systems, with the understanding that these skills can be broadly applied to a wide range of real-world problems.
c. Develop problem-solving methodologies and creative thinking skills for the design and optimization of continuous and batch reactors.
d. Gain exposure to advanced topics in kinetics and reactor design relevant to graduate-level research and industry, with an emphasis on opportunities to engineer more sustainable chemical and energy conversion systems.

7.Classroom Procedures:

a. Lesson Schedule and Calendar. CHEN E4330 is a 13-week course consisting of 26 regular class hours (75 minutes each class).

1. The schedule of classes follows. ***(****Schedule subject to change)*

Week 1	Course overview, review of undergrad concepts.	Notes, Fogler 1
Week 2	Chemical equilibrium	Notes
Week 3	Rate laws / classical kinetics	Fogler Ch. 3.1-3.3, Houston Ch 2
Week 4	Analyzing rate data, multiple reactions	Fogler Ch. 7.1-7.4, 8.1-8.4
Week 5	Surface reactions	Notes, Fogler 10.1-10.3
Week 6	**Midterm 1 (Tuesday 16 February 2021)** Surface reactions and catalysis	Notes, Fogler 10.1-10.3

Week 7	Molecular kinetics: collision theory, Potential Energy Surfaces (PES)	Notes, Fogler Prof. Ref. R3.1, R3.2, Houston Ch 1, 3
	Spring Break - No Class	
Week 8	Molecular kinetics: Activated Complex Theory (ACT)	Notes, Fogler Prof. Ref. R3.1, R3.2, Houston Ch 1, 3
Week 9	Introductory reactor design concepts	Notes, Fogler Ch. 2,4
Week 10	**Midterm 2 (Tuesday 23 March 2021)** pressure drop /Packed Bed Reactors (PBRs)	Fogler Ch. 4, 5.5
Week 11	non-isothermal reactors	Fogler Ch. 11, 12.1-12.5
Week 12	Kinetics and mass transport	Fogler Ch. 14, 15
Week 13	Advanced reactor design concepts.	Notes, parts of Fogler Ch. 6, 12, 16
Exam Week	Final Exam. Location is To Be Announced (TBA) at the SSOL web site: https://ssol.columbia.edu/	

MEMORANDUM FOR: Chemical Engineers of CHEN E44330
SUBJECT: CHEN E4330 Advanced Chemical Kinetics Course Syllabus

2. Calendar: (As of 17 December 2020)

Spring 2021 CHEN E4330 Adv Chemical Kinetics (Source http://registrar.columbia.edu/academic-calendar/ As of 17Dec2020)

	SUNDAY	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY	SATURDAY
JANUARY	3	4	5	6	7	8	9
	10 Week 1	11	12 Lsn 1 Administration review of undergrad Folger Chap 1, **HW1 Assigned**	13	14 Lsn 2 review of undergrad Folger Chap 1	15	16
	17 Week 2	18 M.L. King Jr B-Day (No Classes)	19 Lsn 3 Chemical equilibrium **HW2 Assigned**	20	21 Lsn 4 Chemical equilibrium **HW1 Completed**	22 last day to add class	23
	24 Week 3	25	26 Lsn 5 Rate laws / classical kinetics Fogler Ch. 3.1-3.3, Houston Ch 2 **HW3 Assigned**	27	28 Lsn 6 Rate laws / classical kinetics Fogler Ch. 3.1-3.3, Houston Ch 2	29 last day to add class	30
	31 Week 4	1	2 Lsn 7 Analyzing rate data, multiple reactions Fogler Ch. 7.1-7.4, 8.1-8.4 **HW2 Completed**	3	4 Lsn 8 Analyzing rate data, multiple reactions Fogler Ch. 7.1-7.4, 8.1-8.4	5	6
FEBRUARY	7 Week 5	8	9 Lsn 9 Surface reactions Fogler 10.1-10.3 **HW4 Assigned**	10	11 Lsn 10 Surface reactions Fogler 10.1-10.3 **HW3 Completed**	12	13
	14 Week 6	15	16 Lsn 11 **Midterm 1**	17	18 Lsn 12 Surface reactions and catalysis Fogler 10.1-10.3	19	20
	21 Week 7	22	23 Lsn 13 Molecular kinetics: collision theory, potential e Fogler Prof. Ref. R3.1, R3.2, Houston Ch 1, 3 **HW5 Assigned**	24	25 Lsn 14 Molecular kinetics: collision theory, potential energy surfaces (PES) Fogler Prof. Ref. R3.1, R3.2, Houston Ch 1, 3	26	27
	28 Spring Recess	1 Spring Recess	2 Spring Recess	3 Spring Recess	4 Spring Recess	5 Spring Recess	6 Spring Recess
MARCH	7 Week 8	8	9 Lsn 15 Molecular kinetics: Activated complex theory (Fogler Prof. Ref. R3.1, R3.2, Houston Ch 1, 3 **HW4 Completed**	10	11 Lsn 16 Molecular kinetics: Activated complex theory (ACT Fogler Prof. Ref. R3.1, R3.2, Houston Ch 1, 3	12	13
	14 Week 9	15	16 Lsn 17 Introductory reactor design concepts Fogler Ch. 2,4 **HW6 Assigned**	17	18 Lsn 18 Introductory reactor design concepts Fogler Ch. 2,4 **HW5 Completed**	19	20
	21 Week 10	22	23 Lsn 19 **Miidterm 2**	24	25 Lsn 20 pressure drop / PBRs Fogler Ch. 4, 5.5	26	27
APRIL	28 Week 11	29	30 Lsn 21 non-isothermal reactors Fogler Ch. 11, 12.1-12.5 **HW7 Assigned**	31	1 Lsn 22 non-isothermal reactors Fogler Ch. 11, 12.1-12.5	2	3
	4 Week 12	5	6 Lsn 23 Kinetics and mass transport Fogler Ch. 14, 15	7	8 Lsn 24 Kinetics and mass transport Fogler Ch. 14, 15 **HW6 Completed**	9	10
	11 Week 13	12	13 Lsn 25 Advanced reactor design concepts. Notes, parts of Fogler Ch. 6, 12, 16	14	15 Lsn 26 Advanced reactor design concepts. Notes, parts of Fogler Ch. 6, 12, 16 **HW7 Completed**	16 Study/Exam Days	17
	18	19 Study/Exam Days	20 Study/Exam Days	21 Study/Exam Days	22 Study/Exam Days	23 Study/Exam Days	24
	25	26	27 Commencement	28 Commencement	29 Commencement	30	1

- b. *What you should to bring to class:* Yourself, a calculator, writing implement, a notebook, textbook, computer lab top as desired.

- c. *What **not** to bring to class*: ***Anything that would disturb others around you.***

- d. ***Be on time for class** and actively participate*. Being on time for class means that you are seated, ready to take notes, solve problems, listen to lecture, and take other classroom instructions prior to the start time. This standard is adopted in order to provide the best class experience possible. Walking into class after the class start time disrupts the class for your fellow students who are on time. You are required to be in class and seated ready to go at the start time. This can effect your grade. Class participation is part of your grade.

- e. *Web Site*. The web site for this class contains important administrative and scheduling information, and is located at the Columbia Course Works web site: I will update the site with lecture slides and links to safety articles as appropriate.

- f. *Homework Policy:* Homework will not be collected and should be completed by the completion date unless otherwise specified. For problems solved using software such as Matlab, Python, or Mathematica, knowledge of some coding is required in order to complete the homework set. If Excel was used to generate solution plots, be sure to write up (in Microsoft Word or similar software) key equations that were used to generate those plots develop your methodology used to solve the problem. Collaboration with classmates on homework is encouraged. "Copying" answers from ANY source is unacceptable and against University rules. Turning in anything that does not represent your own work and thought process is considered plagiarism and is subject to the Columbia Policy on Academic Integrity: bulletin.engineering.columbia.edu/academic-integrity-and-discipline Accessed 19 Nov 2020. Use of files from previous classes is not authorized. Students are ultimately responsible for knowing all aspects of the problems. If a student is suspected of a breach on academic integrity, the student will be referred to the university office on matters of honor and academic integrity.

- g. *Exam Policy*: You are not allowed to talk, text, email, or use any communication system with anyone during this exam. The only authorized calculator models are all TI 30-X models, all TI-36X models, all Casio fx-115 models, all Casio fx-991 models, and the HP 33s and HP 35s. If the exam is taken in the presence of anyone else, at the top of your exam, write down the names of who is sitting directly to your left and right. You are not allowed to use any cell phones, calculators, computers, or any device that allows for storage of data during the exams. Any exceptions to this policy will be announced by the instructor prior to the specific event.

- h. *Computational software*: Certain homework problems will require Matlab, Polymath, Python, Mathematica, or other comparable software to be used. If you do not know how

to program (i.e. for Matlab or Python or Mathematica), then students are recommended to learn Polymath, which contains canned solvers and is relatively easy to learn. Matlab and Mathematica are available for free download by Columbia students: https://cuit.columbia.edu/cuit/software-downloads Accessed 19 Nov 2020. If the preceding link does not work, directly contact CUIT for the software. See information on the previous page for downloading Polymath at this https://www.polymath-software.com/fogler/

8. **Course Grade:** The final grade in this course will be based on points awarded according to the following system:

25 % homework, quizzes, class attendance, and participation
The remaining 75% of the grade will be given by the *higher* of the two averages
60 % midterms + 40 % final
50 % midterms + 50 % final

12. **Office Hours:** Tuesdays and Thursdays 10:00 AM – 11:00 AM in Room 818 Mudd or online at the Zoom meeting, if classroom participation is not active. Otherwise by appointment. Email contact is the preferred method of contact for ease of recording information.

15. **Documentation:** (https://bulletin.engineering.columbia.edu/academic-integrity-and-discipline accessed 28 Mar 2020). Columbia University also provides students and faculty access to free software that helps you cite and you write your reports, namely, "endnote". The software is available for download at https://library.columbia.edu/services/citation-management.html accessed 20 Nov 2020). Using "endnote" or a similar form of software is recommended in order to keep the bibliography organized and in the correct format.
The Columbia University guidance on documentation policy is straightforward, and is also in accordance with good professional and ethical practice. The intent is simple. You must identify all outside sources of ideas that are not your own. This means that if an idea did not originate with you, you must identify the source. To do otherwise is inconsistent with the principles of the Honor Code, the Engineering Code of Ethics, and the stated goals of Columbia University. Furthermore, in the larger civilian society, failure to document an idea is illegal, and can result in loss of engineering licensure, fines, and possible incarceration.

16. Academic integrity: If a student is suspected of a breach of academic integrity, the student will be referred to the university office on matters of honor and academic integrity. As your grade is determined based on in-class examinations, it is imperative that you do your own work. Do not cheat on any exams. Students who are suspected of cheating on an exam will be reported to the School of Engineering and Applied Science for further processing which can result in dismissal from Columbia. All students are reminded of the following information from the Columbia University Web site:
"Academic integrity defines a university and is essential to the mission of education. At Columbia students are expected to participate in an academic community that honors intellectual work and respects its origins. As such, a violation of academic integrity is one of the most serious offenses a student can commit at Columbia and can result in dismissal."

(https://bulletin.engineering.columbia.edu/academic-integrity-and-discipline accessed 28 Mar 2020)

"Academic Integrity Policies and Expectations: Violations of policy may be intentional or unintentional and may include dishonesty in academic assignments or in dealing with University officials, including faculty and staff members. Moreover, dishonesty during the Dean's Discipline hearing process may result in more serious consequences" (https://bulletin.engineering.columbia.edu/academic-integrity-and-discipline accessed 28 Mar 2020)

"Common types of academic integrity violations:

-Plagiarism: the use of words, phrases, or ideas belonging to another, without properly citing or acknowledging the source

-Self-plagiarism: the submission of one piece of work in more than one course without the explicit permission of the instructors involved

-Falsification or misrepresentation of information in course work or lab work; on any application, petition, or forms submitted to the School

-Fabrication of credentials in materials submitted to the University for administrative or academic review

-Violating the limits of acceptable collaboration in course work set by a faculty member or department

-Facilitating academic dishonesty by enabling another to engage in such behavior

-Cheating on examinations, tests, or homework assignments

-Unauthorized collaboration on an assignment

-Receiving unauthorized assistance on an assignment

-Copying computer programs

-Unauthorized distribution of assignments and exams

-Lying to a professor or University officer

-Obtaining advance knowledge of exams or other assignments without permission." (https://bulletin.engineering.columbia.edu/academic-integrity-and-discipline accessed 20 Nov 2020)

17. **Welcome!** Sometimes kinetics and reactor design are referred to as the heart and soul of chemical engineering. Embrace this opportunity to expand your horizons in this part of chemical engineering as you strive to be a subject matter expert.

- Robert G. Bozic Ph.D.
- LTC USA(Ret)
- Course Director,
- CHEN E4330 Advanced Chemical Kinetics

Works Cited

ASPEN Plus. Chemical Engineering Computer software licensed to Columbia University Computers in Mudd 251 (also called 251 ET). (See the CUIT web site for remote access available: https://cuit.columbia.edu/computer-lab-technologies Accessed 19 Nov 2020)

Atkins, Peter and Julio de Paula, *Physical Chemistry 11th Edition*, Oxford University Press. Oxford, U.K. 2018, ISBN-13: 9780198769866 (molecular kinetics)

Beer, David *A Guide to Writing as an Engineer, 2nd Edition*, John Wiley & Sons, Inc. Hoboken, NJ. 2005. ISBN 0-471-430774-9. (technical writing).

CHEN E4330 Courseworks web site at https://courseworks.columbia.edu/ Accessed 19 Nov 2020.

Crowl, Daniel A. and Joseph F. Louvar, *Chemical Process Safety" Fundamentals with Applications 4th Edition*, Prentice Hal New York 2019: ISBN-13: 978-0134857770, ISBN-10: 0134857771 (New edition of the textbook 2019) Supplemental reference for reactor safety

Esposito, Daniel, CHEN E4330 Advanced Chemical Kinetics Syllabus Spring 2020, Columbia University. https://courseworks.columbia.edu/

Felder, R. M., Rousseau, R.W. and Lisa G. Bullard *Elementary Principles of Chemical Processes, 4th Edition*, Wiley, New York, 2016

Folger, H.S. *Elements of Chemical Reaction Engineering 5th Edition*, Prentice Hall, Upper Saddle River, N.J. 2016. ISBN13: 9780133887518, ISBN-10: 0133887510.

Higham, Desmond J. and Higham, Nicholas J. *Matlab Guide 2nd Edition*, SIAM: Philadelphia, 2005, ISBN-13: 978-0898715781 (Matlab)

Hildebrand, Francis B. *Advanced Calculus for Applications, 2nd Edition*, Prentice-Hall (1976). ISBN-13: 978-0130111890, ISBN-10: 0130111899

Houston, Paul L., *Chemical Kinetics and Reaction Dynamics, 2nd Edition*, Dover Publishing, 2006. ISBN-13: 9780486453347(highly recommended textbook)

Masel, Richard I., *Principles of Adsorption and Reaction on Solid Surfaces*, John Wiley and Sons Inc., New York, 1996. ISBN-13: 978-0-471-30392-3: (surface reactions)

Nilson, Linda B. *Teaching at its Best, A Research-Based Resource for College Instructors, 3rd Edition*, San Francisco, CA, Jossey-Bass A Wiley-Imprint, 2010. www.joseybass.com

Peters, Max S. and Klaus D. Timmerhause, *Plant Design and Economics for Chemical Engineers 5th edition*, McGraw-Hill, New York 2003, ISBN-13: 978-0071240444 (process diagrams. symbols, and design, HAZOps)

Rice, Richard G. and Duong D. Do *Applied Mathematics and Modeling for Chemical Engineers 2nd Edition*, New York, Wiley 2012. ISBN-13: 978-1118024720

Sandler, S. *Chemical, Biochemical, and Engineering Thermodynamics 4th Edition*, Wiley, New York, 2006. ISBN-13: 978-0471661740 (chemical equilibrium)

Steinfeld, Francisco, and Hase, *Chemical Kinetics and Dynamics 2nd Edition*, Prentice Hall, 1998. ISBN-13 :978-0137371235

Stewart, James, *Calculus Concepts and Contexts*, New York: Brooks/Cole Publishing. 1998, p151-164 Section 2.7, derivatives, p239-247, Section 26. Implicit Differentiation, p402 -408, Section 5.6 Integration by parts, p789-797, Section 11.5 The chain rule and implicit differentiation.

www.cuit.columbia.edu/content/mathematica accessed 19 Nov 2020)

www.bulletin.engineering.columbia.edu/academic-integrity-and-discipline accessed 20 Nov 2020

www.polymath-software.com/fogler/ Accessed 19 Nov 2020. (Polymath is only available for Windows, and not Mac) (Esposito, 2020)

www.umich.edu/~elements/5e/ Accessed 19 Nov 2020. Fogler's 5th Ed. Website, (additional resources found here)

Zill, Dennis G. and Warren S. Wright, *Advanced Engineering Mathematics 5th Edition*, Burlington, MA: Jones and Bartlett Learning LLC, 2014.