DE LA SALLE UNIVERSITY – MANILA
COLLEGE OF SCIENCE
Mathematics Department

SYLLABUS

COURSE CODE	MTH673M/D
COURSE TITLE	Mathematics of Chemical Reaction Network
CLASS DAY & TIME	
ROOM	
NAME OF FACULTY	
COURSE CREDIT	3 Units
CONTACT NO. (DEPT)	(02) 536-0270, (02) 524-4611 loc. 420/413
TERM/SCHOOL YEAR	

COURSE DESCRIPTION

The mathematical theory of chemical reaction networks is unique in several ways: it has had good coverage in high impact science journals such as PNAS, Nature and Science, was pioneered and sustained by chemists and chemical engineers over decades until mathematicians started applying it to biological systems over a decade ago and is now emerging as a valuable contribution to Synthetic Biology. Most recently, the application of the "reaction kinetics" paradigm to ecology, epidemiology and the social sciences (via evolutionary game theory) has been proposed. The field has experienced tremendous growth in the last five years, with over 200 research papers in journals in mathematics, biology, chemistry and chemical engineering, physics and computer science.

The entirely new course intends to provide a comprehensive introduction to both the "classical" results (mainly developed by chemical engineers 1972 – 2000) and new developments in the field (since its application to biology in 2001). Important network properties such as multistationarity (existence and number of equilibria), persistence (non-extinction of species) and robustness have been successfully studied using a combination of methods from linear algebra/matrix theory, graph theory, ordinary differential equations/dynamical systems and most recently, algebraic geometry.

PREREQUISITES: Lecturer's consent to be based on the student's knowledge of linear algebra/matrix theory, fundamentals of graph theory and ordinary differential equations. Topological concepts needed, will be covered in short tutorials within the course.

COURSE OBJECTIVES

The students will:

1. Appreciate the"classical"results (mainly developed by chemical engineers 1972 – 2000) and new developments in the field (since its application to biology in 2001).
2. Identify network properties such as multistationarity (existence and number of equilibria), persistence (non-extinction of species) and robustness.
3. Apply mathematical concepts to biological/ecological systems.
4. Seek opportunities for research with mathematical, computational or biological application focus.
5. Exhibit values like:
    - cooperation through group study;
    - honesty by claiming credit only for the work he has done;
    - zeal and seriousness of intent to learn by participating actively in class discussion, doing his homework

regularly and consulting his mentor;
- patience, perseverance and diligence by solving assigned exercises completely including the difficult ones;
- faith by doing what is right and giving his best in performing any assigned task;
- show concern for the community through sharing of know-how and resources during group discussion;
- self-reliance by being able to solve problems independently.

Topic/Subtopic	Learning Strategies/ Activities	Week/Meeting
1. Mathematics of Chemical Reaction Networks: From Chemical Engineering to Systems Biology and beyond	Lecture-Discussions Problem Solving Use of ERNEST Toolbox and CRNToolboxV2.3	Weeks 1
2. Fundamentals of Chemical Reaction Networks (CRN) 2.1 Definitions and notation 2.2 Inflow and outflow reactions in a CRN 2.3 The Linear Algebra and Geometry of a CRN 2.4 The Stoichiometric Compatibility Classes (SCCs) of a CRN 2.5 The deficiency of a CRN and a linkage class 2.6 The Stoichiometric Cone of a CRN 2.7 Characteristics of weakly reversible networks and some supersets 2.8 Subnetworks and Embedded Networks 2.9 Morphisms of reaction networks 2.10 A second associated graph: Species-Reaction graph	Lecture-Discussions Problem Solving Use of ERNEST Toolbox and CRNToolboxV2.3	Weeks 1-2
3. **A Structural View of Positive Vectors in $\mathbf{R}^R$** 3.1 The dual role of positive vectors of $\mathbf{R}^R$ in current CRNT 3.2 Linear maps associated with a positive vector in $\mathbf{R}^R$ 3.3 Structure Theorem for k-Laplacian Kernel 3.4 The k-deficiency function and its properties 3.5 A graph-theoretic excursion: The Matrix Tree Theorem	Lecture-Discussions Problem Solving Use of ERNEST Toolbox and CRNToolboxV2.3	Weeks 3-4
4. **A Structural View of Positive Vectors in $\mathbf{R}^R$** 4.1 The dual role of positive vectors of $\mathbf{R}^R$ in current CRNT 4.2 Linear maps associated with a positive vector in $\mathbf{R}^R$ 4.3 Structure Theorem for k-Laplacian Kernel 4.4 The k-deficiency function and its properties 4.5 A graph-theoretic excursion: The Matrix Tree Theorem	Lecture-Discussions Problem Solving Use of ERNEST Toolbox and CRNToolboxV2.3	Weeks 5-6
5. Deficiency-Oriented Theory for Generalized Mass Action Kinetics (GMAK) Systems 5.1 Introduction 5.2. Computation of positive solutions of binomial equations 5.3 Kinetic Order Deficiency of a GMAK system	Lecture-Discussions Problem Solving Use of ERNEST Toolbox and CRNToolboxV2.3	Weeks 7-8

Topic/Subtopic	Learning Strategies/ Activities	Week/Meeting
5.4 Complex-balanced equilibria of GMAK systems 5.5 Birch´s Theorem and Deficiency Zero Theorem for GMAK systems 5.6 Translation of MAK Systems to GMAK Systems 5.7 Novel Results for Deficiency Zero MAK Systems 5.8 The Deficiency One Theorem for MAK systems 5.9 The Deficiency One, Advanced and Higher Deficiency Algorithms for MAK systems 5.10 Small MAK systems 5.11 The Main Conjectures of CRNTfor MAK systems		
6. **Injectivity and Concordance of Chemical Kinetic Systems** 6.1 Evolution of Injectivity Theory 6.2 Injective networks 6.3 An extended Jacobian determinant criterion (JDC) for injectivity 6.4 Computational aspects of the JDC 6.5 Injectivity in closed networks 6.6 Networks with all steady states degenerate 6.7 Injectivity in networks and their fully open extentions 6.8 Injectivity Theory in Power Law Systems 6.9 Injectivity Theory for Influence Specifications (Z- Injectivity) 6.10 Injectivity Theory for SM kinetics 6.11 Weakly Monotonic Kinetics and Concordance 6.12 Weakly reversible concordant networks: proof of the PsC and GAC (for MAK) 6.13 Concordance and properties of the fully open extension 6.14 Consequences of discordance 6.15 Strongly concordant networks, two-way weakly monotonic and NAC Kinetics 6.16 Extensions of the main theorems to Weakly Normal (or Nondegenerate) Networks	Lecture-Discussions Problem Solving Use of ERNEST Toolbox and CRNToolboxV2.3	Weeks 9-10
7. Topological methods for Chemical Kinetic Systems 7.1 Injectivity, concordance and the Species-Reaction Graph (SRG) 7.2 Interaction graphs and system dynamics 7.3 Graph Theory connecting CRNs and monotone systems 7.4 Integrated concepts of species-reaction and interaction graphs 7.5 Homotopy methods for counting equilibria 7.6 Lifting Theorems for Multistationarity	Lecture-Discussions Problem Solving Use of ERNEST Toolbox and CRNToolboxV2.3	Weeks 11-12
ORAL PRESENTATION & WRITTEN REPORT		Week 13-14

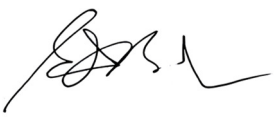
COURSE REQUIREMENTS

- Oral Report 20%
- Written Report 10%
- Problem Set 70%

SOURCES

- Feinberg M., *Complex balancing in General Kinetic Systems*. Arch. Rat. Mewch. Anal. 49 (1972) 187-194.
- Feinberg M, Horn FJM. *Chemical mechanism structure and the coincidence of the stoichiometric and kinetic subspaces*. Arch. Rational Mech. Anal. 66 (1977): 83-97
- Feinberg M, Horn FJM. *Dynamics of open chemical systems and the algebraic structure of the underlying reaction network*. Chemical Engineering Science 29 (1977): 775-787.
- Feinberg M. *Mathematical aspects of mass action kinetics. Chemical Reactor Theory: A Review* (L. Lapidus, N. Amundson, Eds. Prentice Hall 1977, pp 1-78.
- Feinberg M. *Lectures on Chemical Reaction Networks,* Univesity of Wisconsin 1979.
- Feinberg M. *Chemical oscillations, multiple equilibria, and reaction network structure*. In Warren E. Stewart, W. Harmon Ray, and Charles C. Conley, editors, *Dynamics and Modeling of Reactive Systems*, pages 59–130. Academic Press, New York, 1980.
- Feinberg M. *Chemical reaction network structure and the stability of complex isothermal reactors: I.The deficiency zero and deficiency one theorems*. Chemical Engineering Science 42 (1987) 2229-2268.
- Feinberg M. *Necessary and sufficient conditions for detailed balancing in mass action systems of arbitrary complexity*. Chemical Engineering Science 44 (1989): 819-1827.
- Feinberg M. *Some recent results in chemical reaction network theory. In Patterns and Dynamics in Reactive Media* (eds. R. Aris, D.G. Aronson and H. Swinney). IMA Volumes in Mathematics and its Applications, V. 37, 43-70, Springer Verlag, Berlin 1991.
- Feinberg M. *The existence and uniqueness of steady states for a class of chemical reaction networks*." Archive for Rational Mechanics and Analysis 132 (1995): 311-370.
- Feinberg M. *Multiple steady states for chemical reaction networks of deficiency one*. Archive for Rational Mechanics and Analysis 132 (1995): 371-406.
- Feinberg M. *A guide to the Chemical Reaction Network Toolbox Version 2.2a*. Available online at http://crnt.engineering.osu.edu/CRNTWin
- Feliu E, Wiuf C. *Enzyme-sharing as a cause of multi-stationarity in signalling systems*. J. R. Soc. Interface 9 (2012): 1224-1232.
- Feliu E, Wiuf C. *Variable Elimination in Chemical Reaction Networks with Mass Action Kinetics*. SIAM J. Appl. Math. 72 (2012) (4): 959-981.
- Feliu E, Wiuf C. *An Algebraic Approach to Signaling Cascades with n Layers*. Bull. Math. Biol. 74 (2012): 45 – 72.
- Feliu E, Wiuf C. *Preclusion of switch behaviour in networks with mass-action kinetics*. Applied Mathematics and Computation 219 (2012): 1449-1457.

Noted by:



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