TO: Faculty of the Schools of Engineering

FROM: Faculty of the School of Chemical Engineering

SUBJECT: New Graduate Level Course

The Faculty of the School of Chemical Engineering has approved the following new course effective Fall 1996. Approval of the Faculty of the Schools of Engineering is requested for ChE 633.

## CHE 633, PROBABILISTIC METHODS IN CHEMICAL ENGINEERING

### A. COURSE DESCRIPTION

Semester 1, Class 3, Lab 0, Credit 3
Prerequisite: ChE 630 or equivalent

Introduction to probability; random variables and stochastic processes; Ito calculus, stochastic differential equations; Brownian dynamics; and Bridge processes. Applications to chemical engineering systems, Master equations and application of system size expansion concepts to non-equilibrium processes, stochastic point processes, population balance and the theory of fluctuations.

### B. REASON

The purpose of this course is to develop from basic concepts of probability and stochastic processes the facility to formulate models of stochastic systems encountered in chemical engineering. It will also probe into computational techniques for solving stochastic differential equations as well as Monte Carlo simulation methods.

APPROVED FOR THE FACULTY
OF THE SCHOOLS OF ENGINEERING
BY THE COMMITTEE ON
FACULTY RELATIONS

CFR Minutes 864

Date 11/25/96

Chairman R. Neal House

G. V. Reklaitis, Head
School of Chemical Engineering

# SUPPORTING DOCUMENTATION

1. **Justification:**
The need for stochastic methods has grown considerably in chemical engineering in the last two decades. Newer areas of application not only require statistical modeling techniques but involve essentially fluctuating systems for which stochastic modeling is indispensable. The required background is normally not available from advanced courses in probability and stochastic processes often too mired in measure-theoretic treatments to be comprehensible to engineers. Also not available are applications to nurture appreciation of the effectiveness of stochastic methods in engineering which will be the strong supporting feature of this course. This course has been offered as CHE 697R three times and has been well received. Enrollment was 12, 7, and 3 in the Fall of 1993, Spring of 1987, and Spring of 1985, respectively. The course will be offered again in the Fall of 1996.

2. **Level:** Graduate.

3. **Prerequisites:** CHE 630 or equivalent

4. **Course Instructors:** D. Ramkrishna

5. **Course Outline:**

INTRODUCTION:

Stochastic systems in chemical engineering. Systems driven by environmental "noise" and those with internal noise. Examples. Basic concepts of probability. **(1 week)**

RANDOM VARIABLES AND DISTRIBUTION FUNCTIONS:

Discrete and continuous random variables. Distribution functions and probability densities. Expectations. Poisson and Gaussian random variables. The Central limit theorem. Limits of sequences of random variables. **(2 weeks)**

STOCHASTIC PROCESSES:

Definition of a stochastic process. Markov processes. The Chapman-Kolmogorov equation. General processes including Levy flights. Examples of Markov processes. The Wiener, Poisson and Ornstein-Uhlenbeck, and Random telegraph processes. Martingales and Semi-Martingales. **(3 weeks)**

STOCHASTIC DIFFERENTIAL EQUATIONS:

Ito calculus and stochastic integration. Ito and Stratonovich integrals. Solution of stochastic systems. The Fokker-Planck equation. Boundary crossing probabilities. Ito's formula and transformation of Ito systems. Application to chemical engineering systems driven by "external" noise. **(4 weeks)**

MASTER EQUATIONS AND JUMP PROCESSES:

Description of particulate systems by the Master equation. Macroscopic deterministic laws via van Kampen's system size expansion. Modeling of systems with internal noise. **(3 weeks)**

STOCHASTIC POINT PROCESSES & POPULATION BALANCE:

Statistical treatment of populations. Population balance for large and small populations. Theory of fluctuations. **(2 weeks)**

**6. Text:**

"Handbook of Stochastic Methods,"
by C. G. Gardiner, Springer Verlag, 1994.

"Stochastic Processes in Physics & Chemistry,"
by N. G. Van Kampen, North Holland, 1981.

Plus several others for collateral reading.