APPLIED STOCHASTICS FOR ENGINEERING

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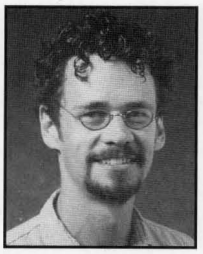

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There is an old joke that says that a statistician is someone who drowns while trying to cross a river with an average depth of three feet. But that sounds to me like the definition of a *bad* statistician. On the other hand, I have run across many otherwise *good* engineers who recognize the perils of considering only an average quantity, but have avoided probabilistic models altogether. I believe that engineers might serve themselves better in the long run by becoming good statisticians and good stochastic modelers.

There is a perceptible increase in the interest of stochastics in the chemical engineering community, evidenced by two observations: the fall 1993 AIChE meeting is slated to contain a session on "Probabilistic Models," and no less than three articles from the 1989 issues of this journal included some discussion of stochastic models in a new course description. Clearly, stochastics is playing an increasing role in chemical engineering.

Last spring our department initiated a course in introductory stochastics designed to introduce graduate students to this rapidly expanding field. Fourteen students enrolled in the course, two students audited it, and two faculty also attended regularly. The sophistication of the semester projects that were turned in suggests that the students learned a lot, and the course appeared to generate a great deal of enthusiasm.

In this article we will consider the following questions in order:

- *What is Stochastics?*
- *Why is it of interest to chemical engineers?*
- *What tools can be taught in a single semester course?*

WHAT IS STOCHASTICS?

One day in 1910, Albert Einstein had just finished working on a stochastic problem involving Brownian motion when his young son Hans Albert asked him for a *Rechenaufgabe.*[1] He thought up the following probability problem: "How long will it take til the ground is wet if it rains at the rate of 10mm/hr?" The problem is probabilistic, because rain does not fall uniformly, but rather in drops which cover (roughly) circular regions on the ground when they hit. After some portion of the ground is wet, the next drop may land completely on a dry area, completely on a wet area, or partly on each. There is no way to know where a given drop will land, so it must be treated *statistically.* Therefore, how long it takes a given portion of land to be completely wetted is not a deterministic question but a statistical one. We can find only the probability that it will take any given time to wet the ground.

Or, consider a second problem. Suppose that I take my red 1966 Volkswagen Beetle to a particular point in the salt flats in Arizona, fill it with one quart of gas, push-start it (as usual), point it north, put it in first gear, set a brick on the gas pedal, and let it go without a driver. Where will the Beetle be when it runs out of gas? If there were no wind we might be able to predict all of the forces on the Beetle and, in principle, calculate where the car will end up. But, in reality there is wind, the strength and direction of which we cannot predict. If we run the experiment many times, the Beetle will end up in a different place each time. We quickly understand that the car is subject to both random *and* deterministic forces, and the final position of the Beetle depends upon both.

"Solving" the above two problems means that we seek the probable distribution of possible outcomes.

The corresponding equations are called "stochastic" equations.* We can then roughly define stochastic equations as equations that describe a quantity (the position of the Beetle) whose evolution (in time) is determined by both deterministic (the motor, the grade, etc.) and random (wind) influences.

WHY SHOULD CHEMICAL ENGINEERS LEARN STOCHASTICS?

The engineer can quickly think up other, more relevant examples of when outside random influences can have a result on a final answer than the two given above: outside random influence on laboratory experiment measurements or plant processes; randomly fluctuating temperatures or pressures; random changes in feed stream compositions. But there are many other examples which are less than obvious. For example, concentration is the *average* number of molecules per volume in a region of space, and each molecule is acted upon randomly by other molecules. The actual number of molecules in a region of space is stochastic. The pore structure in a catalyst, or in an oil reservoir, is random. The transport of substances through these structures depends upon the random pore network. Cells *in vitro* undergo Brownian motion as they are bombarded by surrounding fluid molecules. Populations of cells may be described by stochastic birth-death equations. Polymer chains may take random conformations and be bombarded by Brownian forces.

We can make a general observation here. When working with a large, complex system (and chemical engineers are certainly interested in large, complex systems) in which it is effectively impossible to include all degrees of freedom in the system, the number of variables being considered must be curtailed. Nonetheless, in any real system, the other degrees of freedom not accounted for explicitly still have an influence, and if this influence is not considered deterministically, it must be considered statistically. At that point, the mathematical equations corresponding to the physical process are stochastic.

We can safely say that chemical engineers need to learn stochastics in order to tackle many of the new problems entering the field. Why? Because chemical engineering is moving toward smaller and smaller length scales as processes become more efficient and less consumptive of material resources. Bugs performing bioremediation are being jostled by water molecules; electrons in plasmas are colliding and reacting with large neutral species; molecules in low-pressure reactors are bouncing off of walls, diffusing on surfaces, and jumping between activation sites. At these length scales, the influence of individual molecules becomes important. But there are still too many molecules to handle explicitly for any timescale of interest, and Brownian forces will be important. On the other hand, many degrees of freedom acting on wildly different length scales appear to be ideally suited for stochastic models.

Understanding stochastics allows us to write down well-posed mathematical equations corresponding to intuitive probabilistic pictures. Equally important, that understanding helps us to design simple computer codes to solve the resulting complex partial differential equations numerically.

COURSE STRUCTURE

The course structure is outlined in Table 1. No textbooks are required for the course, but two are highly recommended. The first, by C.W. Gardner, is called *Handbook of Stochastic Methods for Physics, Chemistry and the Natural Sciences.*[2] It is an excellent handbook for mathematical solutions, is well organized conceptually, and has a good mix of theorem and description. But its background in probability is too thin for most engineers, the connection to physical problems is often minimal, and it contains no problems.

TABLE 1
Outline of Material in the Applied Stochastics Course
(Although not explicitly shown, examples are scattered throughout the course.)

1. Background ideas and definitions
- Averages, variance, moments
- Probability density function, cumulative probability
- Conditional probabilities, Bayes' Rule, joint probabilities
- Contraction or marginal probabilities
- Characteristic functions, moment generating functions
- Sample distribution functions: Gaussian, Poisson

2. Probability transformations
- General formula
- Generating random numbers
- Deterministic processes with random initial conditions
- Central limit theorem

3. Markovian concept
- Definition
- Chapman-Kolmogorov equation

4. Equations characterizing Markovian stochastic processes
- Differential Chapman-Kolmogorov equation
- Liouville equations
- Master equations
- Fokker-Planck equations
- Stochastic differential equations

5. Examples of Markovian processes
- Problems with analytic solutions
- Brownian dynamics simulations
- Dynamic Monte Carlo simulations

** We are using a broader definition of the term "stochastics" than that used by some mathematicians.*

On the other hand, the second recommended text, by N.G. van Kampen, *Stochastic Processes in Physics and Chemistry,*[3] is organized more like a physics book and contains many problems. In general, we followed more closely the overall organization of Gardiner, but used van Kampen for all developments involving master equations. Unfortunately, neither text contains information of numerical methods; a few texts do exist with some discussion of numerical techniques.[4,5]

Typically, most engineers have no formal background in probability or statistics, so a significant amount of time must be spent in the beginning with the basic definitions and concepts shown under the first heading in Table 1. For example, while most engineers know what an average and a variance are, less familiar are probability density and autocorrelation functions, or a conditional probability. We begin by playing with typically simple probabilistic (gambling) problems, incorporating these ideas so that the student gets a good feel for what information the quantities contain. This section of the course takes about three weeks. Some of the important definitions introduced here are shown in Table 2.

This is a also good time to introduce an essential concept used to great extent throughout the course: the dual descriptive character of stochastic processes. We can characterize a Markovian stochastic process either through the (deterministic) time evolution of the probability density function or through the statistical properties of an equation describing the evolution of a single trajectory. These two viewpoints are roughly analogous to Hamilton's versus Liouville's description of classical mechanics.

When we reach the second section, *probability transformations,* we are ready to begin solving physical problems. This section deals with the general problem of transforming some random variable, X, to some new random variable, Y := f(X), when the statistics of X are known and we wish to know the statistics of Y. A physical example is the orientation of network strands in a deformed rubber. Before deformation, the strands have random orientations whose distribution is isotropic, but when the rubber is deformed affinely, each strand moves deterministically to a new orientation. We are interested in finding the new orientation distribution of strands after the deformation.

Probability transformation also plays a role in generating random numbers with given distributions from random numbers drawn from a uniform distribution. The mathematician John von Neumann has been quoted as saying, "Anyone who considers arithmetical methods of producing random digits is in a state of sin." We largely avoid these problems, however, and assume that we have a suitable pseudo-random number generator available. Knuth[6] discusses statistical tests of pseudo-random number generators, and Press, *et al.,*[7] provide some concrete examples. A recent article by Hayes[8] (who cites the above quote) discusses more recent ideas and obstacles of such generators. The ideas contained therein are discussed briefly in class.

This is a good time to introduce the central limit theorem for three reasons: it contains all of the probability concepts introduced before; it plays an important role in many physical systems; and a concrete example, namely random walks on a one-dimensional lattice, provides a good segue into the next topic.

All of the concepts introduced so far are for general stochastic processes. However, the vast bulk of the mathematical literature, most physical models, and nearly all of the numerical work utilizes Markovian processes. Thus, we introduce the mathematical definition and physical interpretation of a Markov process. Intuitively speaking, these are processes where we need to know *only* the current state of the system in order to know future probabilities; knowing all of the past states of the system gives us no additional

TABLE 2

NOTE: The symbol Prob{...} reads as "the probability that" and := means "is defined as." The integrals must be taken over all possible values of the integration variables. <...> represents taking an ensemble average.

- **Probability density function**

$P(x;t)dx$:= Prob{The random variable X takes values between x and x+dx at time t} (1)

- **Joint probability function**

$P(x,t;y,t')dxdy$:= Prob{The random variable X takes values between x and x+dx at time t and values between y and y+dy at time t'.} (2)

- **Conditional probability function**

$P(x;t|y;t')dx$:= Prob{The random variable X takes values between x and x+dx at time t *given that* it had value y at time t'.} (3)

- **Averages may be found from these by**

$$\langle f(X)\rangle_t = \int xP(x,t)dx \quad (4)$$

- **Autocorrelation functions are found by**

$$\left\langle X(t)X\left(t'\right)\right\rangle = \iint xyP\left(x,t;y,t'\right)dxdy \quad (5)$$

insight into future probabilities if we know the current state.

Using the definition of Markov and Bayes' rule, we can derive the Chapman-Kolmogorov equation, a nonlinear, integral equation for the conditional probabilities of Markovian processes. This form of the equation has only limited practical use, so we can derive from that the so-called differential Chapman-Kolmogorov equation which has greater utility for our purposes: namely, the solution and description of stochastic processes. Most of the equations for the rest of the course are specific cases of the differential Chapman-Kolmogorov equation.

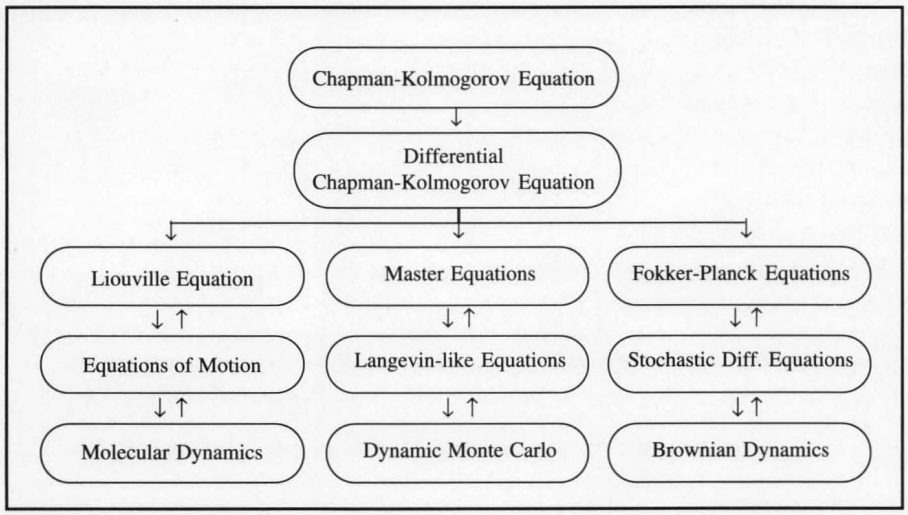

Figure 1. *Interrelation between important equations for Markovian processes.*

The differential Chapman-Kolmogorov equation can also be split into three rough catagories: 1) master equations for discrete or discontinuous jump processes; 2) Fokker-Planck equations for continuous (but nondifferentiable) diffusion processes; and 3) the Liouville equation for deterministic processes which may or may not have random initial conditions. The general forms for these equations are shown in Table 3, and the interconnection between them are shown in Figure 1.

Before deriving the differential Chapman-Kolmogorov equation from the Chapman-Kolmogorov equation, we go through derivations of simple examples of each type of equation. In addition, we repeat Langevin's derivation[9] of the first stochastic differential equation.

An entire week is spent deriving the differential Chapman-Kolmogorov equation and analyzing its different subclasses as combinations of deterministic motion, diffusive motion, and jump processes. Emphasis is placed on interconversion between the evolution equation of the probability density function and sample trajectories of the equivalent process. In this way the students get a feel for how to translate physical pictures into, say, master equations, or how to interpret the physical process represented by, for example, a Fokker-Planck equation. Many simple examples are useful here.

Finally, in this section we cover stochastic differential equations, which are intuitively very appealing—but mathematically they are usually intimidating for students on their first exposure. The primary

TABLE 3

The vector **A** describes the deterministic forces on the random vector, and **B** (or **b**) describes the random forces. The transition probability **W**(**x**|**z**,t) describes the probability per unit time that the random vector makes a discontinuous and instantaneous jump from **z** to **x** at time t. The Wiener process, $d\mathbf{W}_t$, is a delta-correlated, Gaussian white noise.

• Chapman-Kolmogorov equation:

$$P(x_3;t_3|x_1;t_1)=\int P(x_3;t_3|x_2;t_2)P(x_2;t_2|x_1;t_1)dx_2 \tag{6}$$

• Differential Chapman-Kolmogorov equation

$$\frac{\partial}{\partial t}P(\mathbf{z};t|\mathbf{y};t') = -\sum_i \frac{\partial}{\partial z_i}\left[A_i(\mathbf{z},t)P(\mathbf{z};t|\mathbf{y};t')\right] + \frac{1}{2}\sum_{i,j}\frac{\partial^2}{\partial z_i \partial z_j}\left[B_{ij}(\mathbf{z},t)P(\mathbf{z};t|\mathbf{y};t')\right]$$
$$+\int\left[W(\mathbf{z}|\mathbf{x};t)P(\mathbf{x};t|\mathbf{y};t') - W(\mathbf{x}|\mathbf{z};t)P(\mathbf{z};t|\mathbf{y};t')\right]d\mathbf{x} \tag{7}$$

• Master equation

$$\frac{\partial}{\partial t}P(\mathbf{z};t|\mathbf{y};t') = \int\left[W(\mathbf{z}|\mathbf{x};t)P(\mathbf{x};t|\mathbf{y};t') - W(\mathbf{x}|\mathbf{z};t)P(\mathbf{z};t|\mathbf{y};t')\right]d\mathbf{x} \tag{8}$$

•Fokker-Planck equation

$$\frac{\partial}{\partial t}P(\mathbf{z};t|\mathbf{y};t) = -\sum_i \frac{\partial}{\partial z_i}\left[A_i(\mathbf{z},t)P(\mathbf{z};t|\mathbf{y};t')\right] + \frac{1}{2}\sum_{i,j}\frac{\partial^2}{\partial z_i \partial z_j}\left[B_{ij}(b\mathbf{z},t)P(\mathbf{z};t|\mathbf{y};t')\right] \tag{9}$$

•Liouville equation

$$\frac{\partial}{\partial t}P(\mathbf{z};t_3|\mathbf{y};t_2) = -\sum_i \frac{\partial}{\partial z_i}\left[A_i(\mathbf{z},t_3)P(\mathbf{z};t_3|\mathbf{y};t_2)\right] \tag{10}$$

• Langevin equation

$$d\mathbf{X}_t = \mathbf{A}(\mathbf{X},t)dt + \mathbf{b}(\mathbf{X},t)\cdot d\mathbf{W}_t \tag{11}$$

impediment for students is that this is often the first time they need non-Riemannian calculus to integrate equations. But we have borrowed an introduction strategy from Gardiner that seems to be successful in getting across the importance of attaching an interpretation to any stochastic differential equation with multiplicative noise.

By the end of the section most students have little problem working with either Itô, Stratonovich, or the more recent kinetic interpretations.[10] This section requires two weeks of coverage to make the students comfortable, but the payoff for the hard work is unquestionably great since Brownian dynamics simulations are straightforward once the interpretation questions have been tackled.

I find discussion of numerical techniques to be a natural extension to the analytical solutions found for these equations. It is also at this point in the course that the students begin to see the power of stochastics. They see that complicated master equations have straightforward interpretations and may be solved easily by dynamic Monte Carlo techniques. Likewise, a complicated Fokker-Planck equation in thirty dimensions may be solved by a straightforward Brownian dynamics simulation without resorting to finite element methods.

The numerical techniques of stochastic dynamic simulations exploit the equivalence between equations of the third and fourth rows shown in Figure 1. Just as molecular dynamics techniques solve possible trajectories of interacting particles rather than the distributions function in Liouville's equation, Brownian dynamics simulations track the trajectories of realizations to estimate the probability density function in the Fokker-Planck equation. In the course, examples of Brownian dynamics simulations are given for simple polymer and cell motility models.

Likewise, the trajectories of realizations of stochastic processes described by master equations can be described by Langevin-like equations, which suggest dynamic stochastic algorithms. We show detailed examples of nonlinear reaction models that can be solved by such dynamic Monte Carlo techniques.

We spend most of the rest of the semester going through examples of how to model chemical reactions,[11] cell migration,[12] population balances, polymer dynamics,[13] transport equations,[14] lattice gas dynamics[15] for thermodynamic predictions, etc., as stochastic equations, solve them analytically or numerically, and interpret the results. These examples pull together all of the ideas introduced in the course, provide concrete examples of their utilization, and show how powerful and simple the techniques are.

TABLE 4
Term Project Topics Chosen by Students

Critical Review of Single Technical Paper
- Modeling of mechanical degradation of dilute polymer solutions
- A stochastic model of persistent currents in mesoscopic rings

General Review of Research Area
- Application of dynamic Monte Carlo simulation method in study of surface kinetics
- Stochastic models for turbulent diffusion
- Diffusion models for characterizing the firing sequences of neurons
- Stochastic two-phase flow in porous media
- Stochastic representation of reservoir heterogeneity
- Markov models for behavior
- Stochastic modeling of air pollution

Original Research
- Stochastic dynamic simulation of cubic autocatalytic reactions to study bifurcations in chemical reactions
- Stochastic modeling of coalescence of viscous drops in liquid-liquid dispersion
- Stochastic simulation of combined molecular diffusion and chemical reaction
- Solution of the Boltzmann equation by using dynamic Monte Carlo simulation
- Brownian dynamics simulation of a Hookean dumbbell with internal viscosity in steady shearing flow

TERM PROJECTS

Many of the examples in engineering are quite new. Nonetheless, I require that the students do a term project that fits into one of three categories:

1. *A critical review of a single technical manuscript that utilizes stochastic modeling.*
2. *A general review of stochastic modeling in a chosen field critiquing several manuscripts.*
3. *Original work using stochastic modeling for a research project.*

I recommended the third category primarily for those students who may have had an original idea for a simple project while working on a project in the first category. After discussion, I made specific recommendations to a few students for original projects which they followed up on.

CONCLUSIONS

Table 4 shows a list of the projects chosen by the students in each category. Surprisingly, one-third of the class chose projects which were strictly original, whereas the projects in the first category included some original work and research suggestions.

The quality of the original work was quite good,

suggesting that problems of interest to chemical engineers are fertile ground for the use of stochastics. Also, the students doing critiques of manuscripts for projects often found that much well-respected work can be greatly improved by someone with a working knowledge of stochastics.

In summary, I can write with a high probability of certainty that any chemical engineering faculty using stochastic modeling in research will find that introducing colleagues and graduate students to these techniques can be very fruitful.

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ROLE OF ACADEMIA

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on this historical record, the *Scholarship Reconsidered* report argues, however, that there are at least three other types of scholarship: Scholarship of Teaching, Scholarship of Integration, and Scholarship of Application—and that our current thinking might be too narrow to value all of them.

Scholarship of Teaching entails not only transmitting knowledge, but also transforming it and extending it as well; Scholarship of Integration is to "give meaning to isolated facts, putting them in perspective...making connections across disciplines, placing issues in a larger context, illuminating data in a revealing way, often educating nonspecialists too." This clearly points toward interdisciplinary work and drawing unexpected connections between dissimilar areas (without which some disciplines might wane and die). An acceptance of Scholarship of Application demands that we broaden our horizons as well. The usual mode is that pure is better than applied, and that things are discovered and then applied. This need not be so: new intellectual understandings can arise out of the very act of application.

The best use of the human potential already in place calls for recognition of diversity. Faculty diversity should be celebrated, not restricted, and faculty evaluation should be flexible as well as systematic—it will be increasingly more difficult to impose uniform standards on something that by its very mission should be diverse. A professor's job description is often unchanged over an entire lifetime; institutions should explore alternatives on how to sustain productivity. Creativity contracts—an arrangement where faculty define their professional goals for a three-to-five year period, possibly shifting from one principal scholarly focus to another—might offer an alternative.

It is imperative that universities become more structurally robust. Only in this way are they going to be able to deal with the pressures imposed by an ever-broadening mission. The dual mission of disseminating and transforming old knowledge while at the same time pushing the boundaries of what is known can only be fulfilled by a combination of talents and an acceptance of peaceful and profitable coexistence of various modes of scholarship. Yet, at the same time, universities cannot be all things to all people. A broader viewpoint including different models of success seems to be called for if the institutions that have served so well in the past are to withstand the pressures of the future.

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