A Course in Applied Mathematics

WHY MATHEMATICS?

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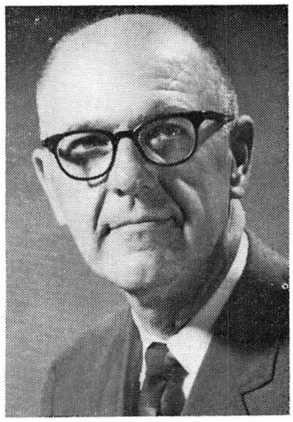

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COURSES IN APPLIED MATHEMATICS for chemical engineers are relatively recent additions to graduate programs, although some go back about twenty-five years. Often such courses were initiated because of a certain dissatisfaction with pure mathematics offerings and the reluctance of mathematicians to teach topics in applied mathematics. Courses with purely mathematical content should be taught in mathematics departments, while those offered in chemical engineering departments should contain something else. That something else is usually associated with the name "model building," although if the course is primarily that, it should probably be given as a part of one of the regular engineering science courses. In short, we seem to be speaking here of an offering which neither fits into the regular framework of a mathematics department nor into the regular kinetics, reactor, transport, control, and thermodynamics scheme of the conventional department. In addition to model building, the course must provide instruction in a number of techniques and actually show the student how to solve problems, a feature that is often anathema to the pure mathematician. In this seems to lie the reason for its being. Early courses were primarily exercises in elementary ordinary differential equations with applications to chemical kinetics and oversimplified models of the unit operations. The emphasis is still on differential equations but other topics with a more recent origin are now included.

Our own course has gone through almost a continuous change in the last twenty years and is taken by almost all graduate students throughout their first year in residence. **The purpose of such a course is not to make mathematicians of engineers but rather to give the student enough experience that he can better cope with the other graduate courses in the department.** Such a course is valuable for the MS student since he may take little other physically motivated mathematics during his one year of course work. For the PhD student it can serve as the first course where significant and complex problems may be solved by advanced techniques and if he has theoretical inclinations frequently urges him on to take more abstruse and rigorous courses from a proper mathematician. As mentioned earlier, our own course has changed considerably through the years and this was forced on us by the fact that new graduate students now enter with a considerably better background than formerly. The average entering student has now had about three years of undergraduate mathematics, some have had four years, and only a few the minimum required for the BS degree. This creates a problem for the instructor, for the class is very heterogeneous not only in terms of quantity of mathematical experience but also because of the fact that in terms of coverage junior and senior mathematics courses can be much more variable than those of the first two undergraduate years. Because of the former I have attempted to give material which will overlap as little as possible with what I think they may have been exposed to. There is an additional problem since many of them are taking advanced mathematics courses concurrently. A number of theoretical and numerical problems are assigned and these seem to be a

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departure from mathematical experience of most of the students, and I believe may be the most valuable part of the course. These are graded and returned to the student. For the most part the problems are long and an attempt is made to complement the lectures, bring out points not covered, and to illustrate the numerical procedures and difficulties. Over half of the students do the numerical problems on the University Computer (CDC 6600) although no time in the course is spent on programming. Usually a student will do between 25 and 40 problems in each ten-week quarter. The course is run from 8:00 to 10:00 on Tuesdays and Thursdays (with a five-minute break) and largely as a lecture, although because of the small class size (15-25 students) there are frequent interruptions for questions.

The fall quarter for some years has covered essentially the content of my book on matrices[1], although not all of the book is covered in any single offering. Sections of the book may be skipped and assigned as reading. Other sections are omitted entirely and this varies from year to year. Chapters 1, 2, and 3 are covered almost entirely along with Chapter 4, through section 4.8; occasionally section 4.12 is presented. Chapter 5 through section 5.14 is in many respects the most important part of the course. A choice is usually made among the sections in Chapter 6, not all of it being given. Chapter 7 through section 7.13 is almost always presented. On rare occasions a shortened version of sections 8.1-8.12 is included. The two volumes of Gantmacher[2] serve as a reference for the course.

All of the material presented in this quarter has a sort of nineteenth-centuryish ring about it and I have thought for some time that it should be modernized, probably in the direction of Shilov[3] "Theory of Linear Spaces" and with introduction of material on tensor analysis (covered at Minnesota in the first graduate course in fluid mechanics). This has not come to pass yet, but probably will since the transition to functional analysis would be much easier.

The winter and spring quarters are devoted to an organized exposition of ordinary and partial differential equations with related topics. It is assumed that the student understands the generation of solutions of simple differential equations. Some time is spent on the theory of differential equations covering linear dependence of solutions, existence and uniqueness, and continuous dependence of the solutions on the data. **It is important that a student understand the engineering significance of these concepts and what they tell him about a mathematical model, for in the qualitative theory of differential equations these ideas play a central role.** A good bit of time is spent on seeking to extract as much information as possible about the solution from the model without recourse to numbers. It is surprising how much information one can obtain for stirred reactors, tubular reactors[4], simple distillation schemes, heat conduction, diffusion, etc., from the equations by using qualitative but rigorous arguments such as existence and uniqueness and the various maximum principles for both ordinary and partial differential equations. Often all of the intuitively obvious qualitative physical properties of the system can be drawn from the equations and this is the ultimate test of a model. For example, it should not be necessary to compute a solution to prove that a mol-fraction lies between zero and one in a distillation calculation, that in an adiabatic tubular reactor there can be no temperature maximum, or that in an absorption column the transient cannot oscillate.

After this qualitative theory a brief discussion of numerical methods for ordinary differential equations is given covering predictor-corrector schemes and Runge-Kutta methods with applications. The question of numerical stability is briefly discussed since anyone who does a significant amount of computer work eventually runs into stability problems.

At this time a general discussion of the nth order linear differential operator is begun. Most of the interesting problems in ordinary and partial differential equations are boundary value problems. The concept of the adjoint operator and adjoint boundary conditions is introduced and the general idea of a self-adjoint boundary value problem is presented. For example, given the nth order operator L

$$Ly=a_0\frac{d^ny}{dx^n}+a_1\frac{d^{n-1}y}{dx^{n-1}}+a_2\frac{d^{n-2}y}{dx^{n-2}}+\ldots+a_ny$$

the adjoint operator L* operating on z is

Nature operates on inputs to give outputs while mathematical operators, couched in the language of differential equations, operate on outputs to give inputs.

$$L^*z = (-1)^n \frac{d^n}{dx^n}(a_0 z) + (-1)^{n-1}\frac{d^{n-1}}{dx^{n-1}}(a_1 z) + \dots + - \frac{d}{dx}(a_{n-1}z) + a_n z$$

and it may then be shown if the region of interest of x is (a,b) that

$$\int_b^a (zLy - yL^*z)\,dx = \pi(z,y)$$

where $\pi(z,y)$ is called the bilinear concomitant and contains the functions z and y and their first (n-1) derivatives evaluated at a and b. In most physical problems we are given n boundary conditions on y, n is even, and we have n/2 boundary at x=a and n/2 at x=b which we assume are homogeneous. Suppose these boundary conditions are denoted collectively by

$$Y(y)=0$$

A fundamental theorem says that there exists a set of boundary conditions on z, called adjoint, unique except for linear combinations such that

$$Z(z)=0$$

so that

$$\Pi\ (z, y)=0$$

The system made up of the operator L and the boundary condition Y is said to be self-adjoint if

$$L=L^*$$

and

$$Y=Z$$

$$\int_b^a (zLy - y^*z)\,dx=0$$

L can only be self-adjoint if its order is even. This equation is a form of Green's Theorem and is the key formula in much of that which follows.

Our aim is to study linear differential equations on finite domains. In most applications these are second or fourth order operators, the former arising in heat conduction and diffusion problems and the latter in elasticity and fluid mechanics. We assume that the students know how to find solutions of ordinary differential equations either by inspection, expansion in series, or numerically. (A pamphlet on series solutions is handed out to the students but is not discussed.)

We consider a self-adjoint eigenvalue problem

$$Lw = -\lambda\rho w;\ a<x<b$$
$$W(w) = 0;\ x=a \text{ and/or } x=b$$

where ρ is a function of x and $\rho(x)>0$. W(w) stands collectively for the n boundary conditions. There are a number of theorems on the existence and character of the eigenvalues and eigenfunctions of such a system. To be brief, however, there exists a discrete sequence of real eigenvalues λ_1, λ_2, λ_3, ... and a corresponding set of eigenfunctions $w_1(x)$, $w_2(x)$, $w_3(x)$,... with an orthogonality property

$$\int_a^b \rho\, w_j w_i\, dx=0\ ;\ i\neq j$$

Provided the set of functions $[w_n(x)]$ is complete with respect to a certain class of functions f(x) we can expand f(x) into a series

$$f(x) = \sum_{j=1}^{\infty} c_j w_j(x)$$

with

$$c(j) = \int_a^b \rho(x) f(x) w_j(x)\,dx$$

provided the eigenfunctions have been normalized. These two relations play an important role, for if we write

$$c(j) = \int_a^b \rho f w_j\,dx$$

$$f(x) = \sum_{j=1}^{\infty} c_j\, w_j(x)$$

then c(j) is called the finite Fourier transform of f(x) and f(x) is the inverse Fourier transform of c(j). Without laboring the point here this pair of formulae may be used to solve a number of partial differential equations in an almost automatic way once one recognizes the operator L and its associated boundary conditions. If a partial differential equation has the form

$$Ly = \rho(x)\ M(y)$$

with boundary conditions

All of our problems are physically motivated and the translation of the problem into mathematical terms is not mathematics.

$$Y(y) = 0$$

where M is an operator not containing x explicitly and having its own boundary or initial conditions. We can write

$$w_n Ly = \rho w_n M(y)$$

and integrate with respect to x

$$\int_a^b w_n Ly\, dx = \int_a^b \rho w_n \, M(y)\, dx$$

Using the Green's formula we obtain

$$-\lambda_n \int_a^b \rho(x)\, w_n(x)\, y(x)\, dx = M \int_a^b \rho\, w_n\, y\, dx$$

or

$$-\lambda_n c_n = M c_n$$

This is a system which is simpler since all reference to x has been removed and may be solved (hopefully) to give c_n and hence y(x) by using the inverse transform. In the course this idea is exploited to obtain solutions of a wide variety of diffusion, heat transfer, and reactor problems, and, while, in principle, it is no different than separation of variables, it possesses an automatic quality which appeals to the students.

At this point we also discuss Duhamel's Theorem and the relationship among solutions for impulse, step function, periodic, random, and general inputs, thereby solving the nonhomogeneous problems which have been avoided up to this time. A qualitative discussion ensues showing the difference between mathematical operators and natural operators. **Nature operates on inputs to give outputs while mathematical operators, couched in the language of differential equations, operate on outputs to give inputs.** For example, a distillation column operates on inputs (feeds) to give outputs (products). The model for a distillation column in the steady state is a system of algebraic relations (which must be inverted) among the outputs. Some mention of non-self adjoint problems is also made showing how the biorthogonal set of eigenfunctions can be used to generate finite Fourier transforms for these problems. However, because of the extreme difficulty of numerical work the problem is not pursued in detail.

Using solutions to problems on finite domains standard limiting procedures may now be used to find Fourier transforms for a variety of boundary conditions on semi-infinite domains (infinite hollow cylinders, etc.). The bag of the student has thus been equipped with a technique which will produce solutions with ease and his confidence is increased. A discussion of the Laplace transform is also included with applications to partial differential equations. This discussion usually takes until about the sixth week of the spring quarter (a total of approximately fifteen weeks).

One of the difficult things about differential equations is that there are no textbooks available intermediate in level between the elementary undergraduate books and books such as Coddington and Levinson[5], Ince[6], Hartman[7],, etc. The book by Weinberger[8] is an excellent intermediate book on partial differential equations but there is no corresponding treatment for ordinary differential equations. I have used some parts of Kaplan[9] and Ross[10] but it is surprising that with the number of books on differential equations and the age of the topic there are none that are really suitable.

The remainder of the quarter (5 weeks) is spent in a variety of ways, but for the past two years first order partial differential equations have been presented with applications to chromatography. This is a topic not well-presented in the literature (a lacuna which Professor Aris and I hope to fill). At other times topics such as dynamic programming and calculus of variations, stochastic processes, numerical solution of partial differential equations with stability considerations, continuous models for discrete processes and many others have been presented.

The question arises as to how much rigor should be presented in such a course. The writer has a simple answer to this. Rigor is presented whenever the student feels the need for it. The solution of a partial differential equation involves a series of arbitrary operations and the bright student should ask whether what one obtains really is a solution to the problem. Such a proof requires the introduction of some rigor and it is not avoided. Different representations of a solution frequently arise and the student should wonder whether they are the same; a uniqueness proof is in order here and it is given. Expansions of functions into series require completeness of the set of functions

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now be used advantageously to analyze the control of distributed parameter systems. Here we treat the control problem in its normal form or carry out a partial type of lumping (finite differencing) to convert the system to sets of ordinary differential equations. In both cases a variety of possible control algorithms following from the minimum principle and dynamic programming are developed.

Finally we consider the identification problem either in its full complexity where no apriori information about the reaction system is known or where a model is available but the parameters must be adjusted to fit experimental data (parameter estimation). Here we turn to the linear-quadratic case treated as a filtering problem, carry out nonlinear last-square regression and fit the system data with generalized orthogonal polynomials. Questions such as the noise involved in the inputs and on the measurement are of importance.

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and some comments must be made and analogies are drawn with finite vector systems.

The object of such a course should be to present methods for new problems. If a problem has been solved once then the engineer should use it. But with a new problem there is no one to tell him when the problem is properly posed. Has the model been drawn so it makes mathematical sense and how does one test whether it does? Whether a solution fits certain physical and chemical requirements will be determined by comparison with experiment, but this comparison is meaningless if the model is not self-consistent.

There is frequent confusion in the minds of beginning graduate students on what is mathematics and what is not mathematics, and, if such a course serves no other function, this question should be answered for him. All of our problems as engineers are physically motivated and the translation of a problem into mathematical terms is **not** mathematics. The generation of the appropriate mathematical model is the job of a good engineer and whether conclusions drawn from the model agree with experiment is the test of how good an engineer he is. If the model does not agree with the experiments, one of two things may be at fault. Either the model was poorly drawn in that it does not describe the physical situation or the model is incomplete or inconsistent. Once the model is put to paper a mathematical problem must be solved. The engineer must somehow convince himself either by intuition or rigorous mathematical argument that the mathematical problem is properly posed. The old argument that the problem is a physical one and therefore possesses a unique solution is a useful argument but not infallible, since only nature solves physical problems and she is quite capable of giving a non-unique solution. The argument also betrays an unrealistic confidence in the engineer for it assumes that he has translated the physical problem into mathematical language **exactly**, a most unlikely event. This is really a very complicated problem, for in the course of the solution certain changes or approximations in the model, both physical and mathematical, are made and these should be examined in some detail to insure that the structure has not been destroyed.

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In conclusion, such a graduate course should not only teach techniques but it should also give the student a feel for what he is doing and what is involved. It has been frequently asserted that we teach only mathematics and neglect engineering. On the contrary, we are trying to teach the student the proper place and function of mathematics, showing not only its strengths but also the pitfalls which may befall the unwary and the uninstructed.

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