A Course in

FUNCTIONAL ANALYSIS FOR CHEMICAL ENGINEERS

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THERE HAVE BEEN A NUMBER of recent books by mathematicians aimed at educating engineers and applied scientists to varying degrees of depth on the subject of functional analysis. For example, we have "Linear Operator Theory in Engineering and Science," by A. W. Naylor and G. R. Sell [1] and "Introductory Functional Analysis with Applications," by E. Kresig [2], to name only a couple. There are at least two main motivating factors for this trend. The first is that mathematical abstraction has accomplished a tremendous unification of apparently diverse classes of problems under a common framework. Consequently, a given problem suitably cast in the foregoing framework derives the benefits of its deductions. The second is that mathematical communications customarily use the language of functional analysis and familiarity with it would greatly facilitate commerce with mathematicians.

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This article reports on a course at Purdue that has evolved over several years since its inception at the Indian Institute of Technology, Kanpur where the author spent his initial years. To Neal Amundson must go the credit for first suggesting the study of modern analysis and for insisting that mathematical abstraction should not be just an instrument for elegant reformulation but must rather be exploited for problem solving. In this regard it is a pleasure to record here the author's continuing collaborative effort with Amundson that has led to numerous papers demonstrating the usefulness of abstract mathematical concepts.

COURSE OBJECTIVES AND CHALLENGES

IN THE DEVELOPMENT OF an engineering graduate course on the subject, one is first faced with the task of laying out the somewhat heavy machinery of functional analysis in terms rudimentary enough to be comprehensible but substantial enough to be useful. Secondly, the utility of this machinery must be established by suitable applications. Functional analysis is an investigation of function spaces in an abstract framework which regards a function as a vector. The course, under discussion, in its present stage of evolution, restricts itself to linear problems, more specifically analysis of linear operators on vector spaces. That functional analysis has much to offer nonlinear

problems in chemical engineering is well established by Gavalas's masterly monograph [3]. The objective of the present course however is to demonstrate that a much wider class (than normally recognized) of linear boundary and initial value problems of interest to chemical engineers can be solved with the same conceptual ease as is inherent in, say, a one dimensional unsteady state heat conduction problem. The prerequisite is the proper formulation of the problem, frequently in an abstract setting, so that the theory of linear operators becomes applicable. The class of what are called selfadjoint operators is of focal interest to the course since they have powerful properties that can be used to solve equations involving them.

Just how one goes about laying out the background is the most difficult part of such a course. The author's approach has varied from "theorem-proof" style to qualitative arguments appealing to geometric intuition. Indeed the entire elimination of either feature would fail to inculcate appreciation for the benefits of abstract thinking, although it must be admitted that the course has gravitated towards more of the qualitative reasoning mainly because of the normal background of engineering graduate students. Since the depths to which background material has been treated have varied considerably, the scope of this article will be limited to a briefing of the preliminary topics while focussing more on the useful applications of the theory of linear operators. It is this latter issue that is particularly crucial and in which many expositions have left something to be desired. An interesting exception is Friedman's "Principles and Techniques of Applied Mathematics" [4].

SCOPE OF COURSE

THE FOLLOWING TOPICS ARE dealt with in a semester's course:

Fields; real and complex numbers. Linear spaces. Metric spaces. Normed linear and inner product spaces. Spectral theory of linear selfadjoint operators in Hilbert Space. Sturm-Liouville theory. Partial differential operators. Applications to chemical engineering problems.

Obviously, the foregoing list is too formidable to permit a detailed treatment of each topic in one semester. Thus, for example, the emphasis on real numbers is limited to demonstrating the structure of the real number system in an elementary way, which carries over to normed linear spaces. As another example, the generalization of a matrix operator in finite dimensional space to a completely continuous operator in infinite dimensional space is an important concept. This is introduced sketchily by analyzing certain properties of closed, bounded sets on the real line and in finite dimensional space. The spectral theorem for selfadjoint completely continuous operators is a central feature of the course on which the applications are built. The background that is required of students includes familiarity with matrices and differential equations at the level of a first course on applied mathematics for entering engineering graduate students.

We return to the main purpose of this article, which is an exposition of key applications in the course demonstrating the utility of abstract formulations. Let us begin by recalling the familiar concept of a physical vector as an entity visualized by components w.r.t. a chosen frame of reference but whose identity is preserved by specified transformation rules for the components when the coordinate frame of reference is changed from one to another. This definition is inspired by the necessity to protect the integrity of a physical quantity regardless of the frame of reference w.r.t. which it is viewed. Mathematically, a vector is an abstract quantity from a vast collection of similar objects characterized by certain properties. These properties include the concepts of multiplying a vector by a scalar to obtain another vector and of summing any two vectors to get a third vector such that certain properties as commutativity, associativity and distributivity are satisfied. Further, a zero vector is defined with which summation of any vector yields the same vector. One is then naturally led to the idea of a linear combination of vectors and the important concept of a basis set. Thus any vector in the collection may be expressed as a linear combination of vectors in a basis set, the coefficients of expansion representing the com-

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ponents of the expanded vector. The components may then be used to identify a vector relative to a basis in much the same manner as the physical vector to which we referred earlier. A vector regarded in the foregoing terms is indeed an abstract quantity. The collection of vectors is called a linear space. The discussion so far has been on algebraic concepts divorced from such notions as magnitude (or norm) of a vector or angle between vectors. These additional notions are introduced as abstract mappings of vectors into numbers. Thus a norm must map a vector into a real number consistent with the following stipulations.

In other problems featuring transient energy or mass transfer, boundaries or interfaces may be encountered with capacitance.

(i) $||\mathbf{x}|| \geq 0$, $||\mathbf{x}|| = 0$ if and only if $\mathbf{x} = \mathbf{0}$
(ii) $||\alpha\mathbf{x}|| = |\alpha|\ ||\mathbf{x}||$
(iii) $||\mathbf{x} + \mathbf{y}|| \leq ||\mathbf{x}|| + ||\mathbf{y}||$

In the above $\mathbf{x}$ and $\mathbf{y}$ are vectors, α is a number with $|\alpha|$ as its absolute value and $||\ ||$ is the symbol for the norm of the vector which it flanks. Property (iii) is the triangular inequality.

The angle between two vectors arises from their inner product (dot product), which is a mapping of pairs of vectors into real (more generally complex) numbers satisfying certain properties. For real spaces the properties are conveniently stated in symbols as follows.

(i) $\langle \mathbf{x},\mathbf{y} \rangle = \langle \mathbf{y},\mathbf{x} \rangle$
(ii) $\langle \mathbf{x},\mathbf{x} \rangle \geq 0$, $\langle \mathbf{x},\mathbf{x} \rangle = 0$ if and only if $\mathbf{x} = \mathbf{0}$
(iii) $\langle \mathbf{x}+\mathbf{y},\mathbf{z} \rangle = \langle \mathbf{x},\mathbf{z} \rangle + \langle \mathbf{y},\mathbf{z} \rangle$
(iv) $\langle \alpha\mathbf{x},\mathbf{y} \rangle = \alpha\langle \mathbf{x},\mathbf{y} \rangle$

In (i) through (iv) $\langle , \rangle$ represents the inner product of the enclosed vectors. Clearly the inner product is a bilinear mapping from properties (iii) and (iv). Another important point is that properties (i)-(iv) help generate a norm from the inner product. Thus we may write $||\mathbf{x}|| \equiv \sqrt{\langle \mathbf{x},\mathbf{x} \rangle}$. Orthogonality between two vectors is described by the vanishing of their inner product.

The importance of the foregoing stipulations (or axioms) for a linear space, norm and inner product is that while one is quickly satisfied that the familiar physical vectors are faithful to the axioms, they are not the only conformists. There are other collections of vectors that produce no geometrical pictures in the mind but are at least as useful. As an example, the collection of functions $f(x)$, $a \leq x \leq b$ such that

$$\int_a^b f^2(x)\,dx < \infty$$

represents a linear space of vectors $\mathbf{f} \equiv [f(x) : a \leq x \leq b]$. The inner product in this space is defined by

$$\langle \mathbf{f},\mathbf{g} \rangle = \int_a^b f(x)\,g(x)\,dx$$

Other choices are available for defining the inner product but the choice to be made depends on the end to be met. It is this end that deserves some discussion here.

Vital to engineering applications is the concept of an operator which is a rule for transforming one vector into another. This mapping is said to be linear, when any linear combination of a pair of vectors are transformed into the same linear combination of the transformed vectors. In symbols, denoting a linear operator by $\mathbf{L}$ we have

$$\mathbf{L}(\alpha\mathbf{x} + \beta\mathbf{y}) = \alpha\mathbf{L}\mathbf{x} + \beta\mathbf{L}\mathbf{y}$$

By continued application of the operator it is easy to see how powers, polynomials, analytic functions etc. of operators may be defined. Thus one may talk about operators such as $\mathbf{L}^n$ or $\exp \mathbf{L}$ and so on. By the same token two operators may be multiplied. Such operations are not necessarily commutative. An operator of particular interest is the projection operator $\mathbf{P}$ which, besides being linear, has the property $\mathbf{P}^2 = \mathbf{P}$.

Let us recall the operator of central importance, the selfadjoint operator. It is defined as the operator for which

$$\langle \mathbf{L}\mathbf{x},\mathbf{y} \rangle = \langle \mathbf{x},\mathbf{L}\mathbf{y} \rangle \qquad (1)$$

for any pair of vectors $\mathbf{x}$ and $\mathbf{y}$. For a completely continuous selfadjoint operator the spectral theorem (see for example [1]) assures us the existence of real eigenvalues $[\lambda_j]$ and associated projection operators $[\mathbf{P}_j]$ with the property that $\mathbf{P}_j\mathbf{P}_k = \mathbf{0}$ when $j \neq k$ such that

$$\mathbf{L} = \sum_{j=1}^{\infty} \lambda_j \mathbf{P}_j \qquad (2)$$

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Where $\mathbf{P}_j$ is defined by its action on any vector $\mathbf{x}$, viz.,

$$\mathbf{P}_j\mathbf{x} = \langle \mathbf{x}, \mathbf{z}_j \rangle \mathbf{z}_j \tag{3}$$

where $\mathbf{z}_j$ is the normalized eigenvector of $\mathbf{L}$ corresponding to the eigenvalue λ_j; i.e.

$$\mathbf{L}\,\mathbf{z}_j = \lambda_j \mathbf{z}_j, \quad ||\mathbf{z}_j|| = 1$$

The equality (2) along with the property $\mathbf{P}_j\mathbf{P}_k = 0$ implies that

$$\mathbf{L}^n = \sum_{j=1}^{\infty} \lambda_j^n \mathbf{P}_j, \quad \exp \mathbf{L} = \sum_{j=1}^{\infty} e^{\lambda_j} \mathbf{P}_j,$$

$$\mathbf{L}^{-1} = \sum_{j=1}^{\infty} \lambda_j^{-1} \mathbf{P}_j \tag{4}$$

whenever it is meaningful to talk about the left-handsides of the above equalities. The foregoing expansions make it possible to solve steady state equations of the form

$$\mathbf{L}\mathbf{x} = \mathbf{y} \tag{5}$$

where $\mathbf{y}$ is a known vector. The solution $\mathbf{x}$ using the last equality in (4) is given by

$$\mathbf{x} = \sum_{j=1}^{\infty} \lambda_j^{-1} \mathbf{P}_j \mathbf{y} \tag{6}$$

where $\mathbf{P}_j\mathbf{y}$ is given by (3). Unsteady state initial value problems of the form

$$\frac{d\mathbf{x}}{dt} = \mathbf{L}\,\mathbf{x}, \; \mathbf{x}(0) = \mathbf{x}_i \tag{7}$$

are solved using the second equality in (4) to obtain

$$\mathbf{x} = \sum_{j=1}^{\infty} e^{\lambda_j t} \mathbf{P}_j \mathbf{x}_i \tag{8}$$

BOUNDARY VALUE PROBLEMS

IN DEALING WITH BOUNDARY value problems differential operators are involved. By a differential operator is meant a differential expression, for example of the Sturm-Liouville type such as

$$\frac{1}{r(x)} \frac{d}{dx} \left[p(x) \frac{d}{dx} \right] + q(x)$$

along with homogeneous boundary conditions representing the domain of the differential expression. The domain of definition (or equivalently along with homogeneous boundary conditions representing the domain of the differential expression. The domain of definition (or equivalent-the homogeneous boundary conditions) is crucial to whether or not the differential operator is self-adjoint. Although a selfadjoint Sturm-Liouville differential operator does not directly satisfy the conditions for the spectral resolution (2), the existence of a Green's function, i.e., a completely continuous inverse operator, makes it possible to apply formula (2).

To summarize, many linear problems in engineering may be cast in the form of an operator equation* (5) or (6) in which the operator has the selfadjointness property (1) and consequently the solution is obtained from either (7) or (8). The essential point is that the scope for abstraction at each of the various stages of the above development offers manipulative flexibility to fit the given problem to the mold of selfadjoint operators. Indeed it is not implied that all problems would yield to such manipulation by becoming selfadjoint problems. Rather the implication is that there is a class of selfadjoint problems not easily recognized without such abstract formulations. We consider some examples below.

Let $\mathbf{A}$ and $\mathbf{B}$ be symmetric matrices (or completely continuous operators selfadjoint under the same inner product). The operator $\mathbf{L} = \mathbf{AB}$ is not necessarily selfadjoint. If however $\mathbf{A}$ is positive-definite, then a new inner product may be defined on the space of vectors by

$$\langle \mathbf{x}, \mathbf{y} \rangle = (\mathbf{A}^{-1}\mathbf{x}, \mathbf{y}) \tag{9}$$

where the inner product (,) is that w.r.t. which $\mathbf{A}$ and $\mathbf{B}$ are selfadjoint. The definition (9) earns its legitimacy by satisfying all the properties of an inner product. Now it is readily shown that $\mathbf{L}$ is selfadjoint w.r.t. the inner product (9).

$$\langle \mathbf{Ax}, \mathbf{y} \rangle - \langle \mathbf{x}, \mathbf{Ay} \rangle = (\mathbf{Bx}, \mathbf{y}) - (\mathbf{x}, \mathbf{By}) = 0$$

Thus $\mathbf{L}$ has real eigenvalues and its eigenvectors from an orthonormal basis w.r.t. the inner product (9). This concept has been applied to problems in heat transfer [5], first order kinetics and multicomponent rectification [6].

With differential operators the domain of definition (homogeneous boundary conditions) is important. Transport of energy or mass in composite (or multiphase) media lead to selfadjoint

*Frequently, inhomogeneous differential equations and inhomogeneous boundary conditions are involved but they pose no special problems.

problems in which the domains of the differential operators include the boundary conditions and interface conditions. Different inner products must be used depending on the interface conditions [7].

In other problems featuring transient energy or mass transfer, boundaries or interfaces may be encountered with capacitance. The selfadjoint nature of these problems can be realized by defining linear spaces in which the vectors would consist of not only the dependent variable (such as temperature or concentration) in the interior but also the values at boundaries and interfaces which have capacitance, "appended" as separate components. The details are available in [8, 9]. These methods are also useful, for example, in dealing with heat (or mass) transfer in composite media in which one or more of the media may possess transport properties considerably higher than those of other media so that gradients of temperature (or concentration) may be neglected therein.

There are also problems in steady state energy or mass transfer in stationary media (solids) in which energy or mass generated in the medium is removed by a peripherally flowing fluid, whose temperature or concentration changes in the direction of flow. The boundary conditions here depart from the normal Dirichlet, Neumann or Robin boundary conditions. Although the original problem is nonself-adjoint, it is shown [10] that by decomposing the second order Poisson equation into a pair of first order equations a selfadjoint problem is obtained.

As another illustration of the above idea consider the classical Graetz problem at low Peclet number which necessitates the axial conduction term in the energy equation. The differential equation is

$$-\frac{k}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)-k\frac{\partial^2 T}{\partial z^2}+\rho C_p v_z(r)\frac{\partial T}{\partial z}=0,$$

$$0<r<R,\ -\infty<z<\infty \qquad (10)$$

Although in what follows the nature of the boundary condition is immaterial we will assume for the sake of specificity the following boundary conditions.

$$r=0,\ \frac{\partial T}{\partial r}=0,\ -\infty<z<\infty\ ;\ r=R,$$

$$T=\begin{cases} T_0 & z<0 \\ T_1 & z>0 \end{cases},\ T<\infty \text{ as } z\to\pm\infty$$

This problem treated in the usual way (as in the literature) is a nonselfadjoint problem. However by defining what one might refer to as the axial energy flow function,

$$S(r,z)=\int_0^r\left[-k\frac{\partial T}{\partial z}+\rho C_p v_z(r)\,T\right]2\pi r\,dr \qquad (11)$$

Eq. (10) is readily found to be equivalent to a pair of partial differential equations written in terms of a matrix differential expression

$$\begin{bmatrix} \dfrac{\rho C_p v_z(r)}{k} & -\dfrac{1}{2r}\dfrac{\partial}{\partial r} \\ 2r\dfrac{\partial}{\partial r} & 0 \end{bmatrix}\begin{bmatrix} T(r,z) \\ S(r,z) \end{bmatrix}$$

$$=\frac{\partial}{\partial z}\begin{bmatrix} T(z,r) \\ S(z,r) \end{bmatrix} \qquad (12)$$

If we denote the matric differential expression in (12) by L then its domain is contained in a vector space in which each vector is an ordered pair of functions of r satisfying some conditions to be discovered presently. Denote a typical vector in this space by $\mathbf{f}\equiv\begin{bmatrix} f_1(r) \\ f_2(r) \end{bmatrix}$. From the boundary conditions it can be shown that we must have $f_2(r)\to 0$ faster than r and $f_1(R)=0$, which then is the domain of L. Thus we have a differential operator **L** which is defined by L and its domain. If we define the inner produce to two vectors **f** and **g** by

$$\langle \mathbf{f},\mathbf{g}\rangle\equiv\int_0^R\left[f_1(r)\,g_1(r)\,2r+f_2(r)\,g_2(r)\,\frac{1}{2r}\right]dr \qquad (13)$$

it implies that our linear space must consist of vectors **f** such that $f_1(r)$ must be square-integrable in [0,R] with weight 2r and $f_2(r)$ must be square-integrable with weight 1/2r. Moreover, it is readily seen that

$$\langle \mathbf{Lf},\mathbf{g}\rangle-\langle \mathbf{f},\mathbf{Lg}\rangle$$

$$=\left[f_1(r)\,g_2(r)-f_2(r)\,g_1(r)\right]_0^R=0 \qquad (14)$$

Thus **L** is found to be selfadjoint and the problem has fitted the mold we were talking about. Hence

analytical solutions can be obtained for this and other problems via the spectral representation of L. This work is as yet unpublished and is presently the subject of a doctoral dissertation by Papoutsakis [11].

There are thus a substantial class of problems of interest to engineers that can be solved using the elegant theory of selfadjoint operators. The need for familiarity with abstract formulations should now be evident. This entire subject has been for some years under preparation into a book by the author in collaboration with Amundson, which it is hoped will some day see the light of print. □

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MIRROR FOG PROBLEM

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PRELIMINARY DISCUSSION

We first remember the steps in model building: define specific objectives, establish physical and chemical principles, make assumptions, derive equations, specify initial and boundary conditions.

OBJECTIVES AND CRITERIA: To find the time t_f when the mirror is completely clear. Part A: since this will be a moving boundary problem, t_f will be the time when the fog line reaches the closed end of the vapor space. Part B: we can calculate the amount of condensate on the mirror, so the time would be the time required to evaporate that much material.

PHYSICAL AND CHEMICAL PRINCIPLES: There are no chemical principles involved. Since heat transfer is taken to be rapid, the system may be taken as isothermal and the problem is simply one of evaporation and diffusion. Given the two closely spaced large parallel plates it may be expected that there will be little concentration difference across (x-direction) the space between the plates. Also because of the fact that there is no flux at any boundary except at the open end (—y direction) and the system is symmetric in z direction, the problem is one dimensional (i.e., at any value of x and y, nothing will vary with z). Mass will be transferred out because of a concentration gradient established between the fogged region (where $C = C_{saturated}$) and the opening $y = 0$ (where $C = C_{room}$). Following the shower, it is assumed that the room returns to house ambient conditions (this is easily achieved overnight with the door open, i.e., rapidly, compared to the defogging process since the outside mirror clears in < 0.5 hr.). However note that the point in the slit where $C = C_s$ retreats farther into the slit as time goes on. Thus the diffusional path increases and we have a moving boundary problem.

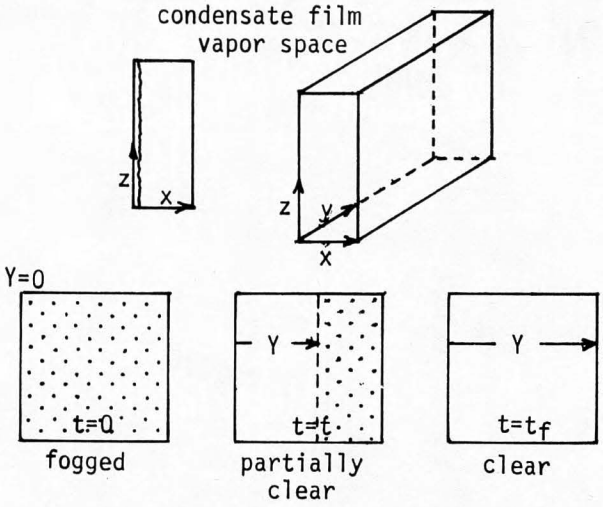

FIGURE 3. All surfaces impermeable except front opening.

ASSUMPTIONS: Several assumptions have been indicated already.

- **$C_A \neq f(x,z)$.**
- **The system is isothermal.**
- **All boundaries except the open end are impervious to mass transfer (doubtful in the actual experiment).**
- **The room air returns quickly to constant composition.**
- **The initial amount of condensate is known.**
- **Bulk flow in the system is negligible (air flows in to balance H_2O flow out). The error due to this assumption was shown to be about 5.5%.**
- **The volume of condensate film is negligible.**

You are now ready for Part A and B. □