A COURSE IN SPECIAL FUNCTIONS AND APPLICATIONS

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At Waterloo, applied mathematics-oriented courses are an important constituent of the undergraduate programme in chemical engineering. Since the compulsory (called core) courses cannot possibly cover all subject matters of interest, a number of electives are open for students with a particular penchant for applied mathematics. It is a genuine pleasure to prepare and teach these elective courses; students who enroll in them are usually very well motivated, possess a good command of background mathematics and are willing to learn more than the absolute minimum required to pass.

The course described in this article deals with special functions and their applications to (mostly chemical) engineering problems. It is taught currently at the third year/second semester (3B) level, although some fourth-year and beginning graduate students would be found in a typical class. All students would have taken by this time a certain sequence of *core* courses on calculus, differential equations and linear algebra, and would be somewhat familiar with some Bessel functions such as $J_0(x)$, $J_1(x)$ and perhaps $J_{1/2}(x)$. They would also have a reasonably good understanding of certain key relationships in physical chemistry, fluid flow, and transport processes, which can be obtained via special functions, although they would not have been exposed to detailed derivations and to all important properties of these special functions. Such a background is considered adequate for the pursuit of advanced studies.

Table 1 shows the course structure and relative lengths of time spent on major topics. The one-semester course consists of about twenty four one-hour lectures with periodic tutorials of about two hours length. There are two one-hour mid-term tests and a three-hour final examination; all three examinations are open-book-and-notes type and the use of numerical tables and small computing devices is required. Orthogonal polynomials and Bessel functions make up approximately one half of the course inasmuch as these quantities are particularly important in many applications. The major objective here is to provide students with at least an adequate understanding and appreciation of the usefulness of special functions in the modelling of problems taken from various areas of engineering and applied physics. The course emphasizes that special function-oriented techniques can often be superior time savers with respect to numerical solutions of certain types of differential equations, based on the calculus of finite differences. Apart from instilling factual

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knowledge, the course reminds students that (classical) analytical techniques invariably hold their place in the sun and that excessive emphasis on purely numerical methods is often detrimental to analytical judgment. The course illustrates that the knowledge of special functions often allows the solution of a problem literally on the back of an envelope.

One of the didactic problems facing the instructor is the proper blend of background theory and applications. My experience indicates that building the course material around "model-nuclei" was very useful in trying to strike the right balance between theory and applications. To illustrate this concept, consider, for instance the Legendre polynomials, $P_n(x)$; $x = \cos\theta$. The expansion

TABLE 1
Structure of the Course in Special Functions*

Topic	Major Headings and Illustrative Examples	Appx. Fraction of time spent on topic, per cent
Gamma and Beta Functions	General theory; motion in force fields; convective diffusion in a rotating disk electrode cell; perimeter- and area- calculations	15
Error- and related Functions	General theory: quality control problems; diffusion and heat conduction	15
Exponential and related integrals	General theory; evaluation of specific integrals; exploitation of a shallow oil field; reactor performance problems	10
Orthogonal polynomials	General theory of Legendre and Chebyschev polynomials; steady state potential distribution problems; numerical integration (Gaussian quadratures)	20
Bessel functions and Kelvin functions	General theory of the J, Y, I and K functions. Diffusion in cylindrical porous media; heat dissipation problems; variable mass dynamics; heat transfer in fins; skin effect in transmitting AC power	25
Elliptic integrals and elementary Jacobi elliptic functions	General theory; pendulum, mechanical braking, capillary, magnetic field generated by circular current paths. Problems in elliptical geometry	15

*One semester course; total number of one-hour lectures is about twenty-four.

The major objective is to provide . . . an adequate understanding and appreciation of the usefulness of special functions in the modeling of problems taken from various areas of engineering and applied physics.

$$\psi(r, \theta) = \sum_{n=0}^{\infty} \left(A_n r^n + \frac{B_n}{r^{n+1}}\right) P_n(\cos\theta) \quad (1)$$

describes steady state potential distributions in spherical geometry; the set of indeterminate constants A_n and B_n depends on the specific auxiliary conditions of a given physical problem. Eq. 1 would be typically introduced by discussing in a class lecture the steady state temperature distribution in a homogeneous hemisphere whose surface is maintained at a constant temperature and whose base (equatorial plane) is insulated. Starting from the appropriate heat balance written for the fractional temperature u:

$$r^2 u_{rr} + 2ru_r + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}[\sin\theta \cdot u_\theta] \quad (2)$$

(the subscripts denote partial derivatives), Eq. 1 is derived by the classical separation of variables approach and then it is shown by means of the auxiliary conditions $u(R, \theta) = 1$; $u_\theta\ (\theta = \pi/2) = 0$ that the *specific* solution of this problem may be expressed as

$$u\ (r,\theta) = \sum_{n=0}^{\infty} A_n\, r^{2(n+1)} P_{2(n+1)}(\cos\theta) \quad (3)$$

where

$$A_n = \frac{2n+3}{R^{2(n+1)}} \int_0^{\pi/2} P_{2(n+1)}(\cos\theta)\, \sin\theta d\theta \quad (4)$$

A subsequent homework assignment contains several problems where the physical systems are quite different, nevertheless Eq. 1 plays a pivoting role; one such problem would be e.g. the electrostatic potential distribution around a conducting sphere placed suddenly into an electric field of uniform strength of E_o. Since from the theory of electrostatics, $V(r \rightarrow \infty) = -E_o r P_1(\cos\theta)$, the solution is obtained as $V(r,\theta) = -E_o r \left(1 - \frac{R^3}{r^3}\right)\cos\theta$, if R is the radius of the

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An important aspect of problem selection is what I would call general scientific education; i.e. the presentation of material of historical interest or imaginativeness. One of my favourites is Lord Kelvin's estimation of the age of the Earth in the last century, well before the advent of big-bang theory (I owe this problem with thanks to Professor Jim Westwater's graduate course in heat transfer at the University of Illinois). In 1897 Kelvin used the following model for the stated computation. The Earth was a liquid sphere until time zero when solidification of the crust began. The temperature in the centre of the Earth is T_o = 7000°F, the average temperature on its surface is T_s = 50°F; the geothermic gradient at the surface is -1°F per 50 ft. Finally, the average thermal diffusivity of the crust is $\alpha = 0.0456$ ft²/h. The model is related to the error function, and if T is the temperature at radial position r, then if x = R-r,

$$\frac{T - T_s}{T_o - T_s} = \operatorname{erf} \frac{x}{2\sqrt{\alpha t}} \qquad (5)$$

and it follows that

$$\left.\frac{dT}{dx}\right|_{x=0} = \frac{T_o - T_s}{\sqrt{\pi \alpha t}} \qquad (6)$$

Thus we calculate $t \cong 10^7$ years; accepting the much more probable value of about 4.6 x 10^9 years from the study of fragments of moon rocks, we cannot help marvelling at the relative closeness of Kelvin's result in spite of the gross simplifications carried with it; after all, two orders of magnitude in astronomy is "peanuts", and Lord Kelvin did not even possess an LCD programmable calculator, to boot! It is even more intriguing to estimate the temperature of the Earth 100 miles below the surface: from Eq. 5, and neglecting the slight difference between 1979 and 1897 we obtain about 6,600°F. This is only about 6% off the core temperature.

Problems of closer chemical engineering interest, whose solution may be obtained in terms of special functions, include unsteady-state diffusion of pollutants (error function), heat loss through metal fastenings of insulators (error function), chemical reactor performance (exponential integral), concentration distribution near the surface of a rotating disk electrode (gamma functions and incomplete gamma functions), heat transfer in a non-homogeneous bar (Legendre polynomials), heat transfer from fins (Bessel functions), capillary between parallel plates (elliptic integrals) and a number of others. To illustrate one such problem, consider the consecutive reaction scheme $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ where the first decomposition is second order and the second decomposition is first order. If we set the initial concentration of species A to A_o, and if there are no B and C moles present at zero time, the mass balance equations

$$\frac{dB}{dt} = k_1 A^2 - k_2 B \qquad (7)$$

$$\frac{dA}{dt} = -k_1 A^2 \qquad (8)$$

with initial conditions $A(o) = A_o$, $B(o) = C(o) = 0$ fully define the reaction system. Eq. 8 is solved immediately as

$$A = \frac{A_o}{1 + A_o k_1 t} \qquad (9)$$

and upon substitution into Eq. 7 and applying Laplace transformation we obtain

$$\bar{B}(s) = \frac{1/k_1}{s + k_2} [A_o + R_1 + s e^{\frac{s}{A_o k_1}} \operatorname{Ei}(-\frac{s}{A_o k_1})] \qquad (10)$$

where

$$\operatorname{Ei}(x) \equiv \int_{-\infty}^{x} \frac{e^t}{t}\, dt \qquad (11)$$

is the exponential integral. Eq. 10 may be inverted by means of the convolution theorem, which yields

$$B(t) = \frac{1}{k_1} \int_0^t \frac{e^{-k_2(t-u)}du}{\left(\frac{1}{A_o k_1} + u\right)^2} \qquad (12)$$

Upon integration and some algebraic manipulation, this gives

$$B(t) = A_o e^{k_2 t} - \frac{A_o}{A_o k_1 t + 1} - \frac{k_2}{k_1} e^{-k_2 (t + \frac{1}{A_o k_1})} [\operatorname{Ei}(k_2 t + \frac{k_2}{A_o k_1}) - \operatorname{Ei}(\frac{k_2}{A_o k_1})] \qquad (13)$$

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The existence of a maximum concentration of the intermediate in the reaction scheme may be quickly demonstrated, by looking at limiting values:

$$\lim_{t\to 0} B(t) = 0 \quad ; \quad \lim_{t\to\infty} B(t) = 0$$

If, for instance, $A_o = 1$ mol/L; $k_1 = 0.5$ L/mol·min, $k_2 = 1.0\ \text{min}^{-1}$, then $B_{max} \cong 0.199$ mol/L and the corresponding $t_{max} \cong 1.2$ min.

The wealth of Bessel-function oriented problems is given a somewhat condensed yet representative treatment, as seen in Table 1; about one fourth of the course is devoted to Bessel functions. Here one typical problem discussed is the cooling of a cast metal tube in still air, when axial conduction may be neglected. The unsteady state heat balance

$$\frac{\partial T}{\partial t} = \alpha\left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r}\right) \quad (14)$$

with auxiliary conditions $T(o,r) = T_o$ and $-k \left.\frac{\partial T}{\partial r}\right|_R = h(T - T_a)$, ($T_a$ is the constant ambient temperature), is solved to

$$\frac{T - T_a}{T_o - T_a} = 2 \sum_{n=1}^{\infty} e^{-\frac{x_n^2}{R^2}\alpha t} \frac{J_1(x_n)}{x_n[J_o^2(x_n) + J_1^2(x_n)]} J_o\left(x_n \frac{r}{R}\right) \quad (15)$$

where the eigenvalue set (x_n) is obtained via Eq. 16:

$$\frac{J_o(x_n)}{J_1(x_n)} = \frac{kx_n}{hR} \quad (16)$$

In the case of metals of good conduction properties, a useful short-cut reduces numerical work drastically, if R is relatively small: because of the relative largeness of the k/hR group, x_1 will be substantially less than unity, hence $J_o(x_1)/J_1(x_1)$ will tend to $2/x_1$ and a very close approximation to the first eigenvalue is $x_1 \cong \sqrt{\frac{2hR}{k}}$. Moreover, since $x_2 >> x_1$, Eq. 15 may be safely truncated after the first term. Taking e.g. a 5 cm diameter zirconium tube and $T_o = 900°C$, $T_a = 30°C$, then with the physical data: $c_p = 320$ J/kg·K, $\rho = 6500\ \text{kg/m}^3$, $h = 26\ \text{W/m}^2\cdot\text{K}$, $k = 24$W/m·K, a good approximation is obtained by using the short-cut estimate of $x_1 \cong 0.233$ in Eq. 17 (t is in hours, r in metres):

$$T \cong 30 + 1176.15\, e^{-3.608t} J_o(9.32r)\ °C \quad (17)$$

By trial and error, the first root of Eq. 16 is found to be slightly larger than 0.24, thus the short-cut approach is quite acceptable. Note that $x_2 \cong 3.84$ and, in consequence, the corresponding exponential term in Eq. 15 will be small enough at times not too close to zero to justify the omission of the second and higher order terms in the expansion. This problem is a good illustration of the superiority of the analytical approach employed to a finite-difference based numerical solution of Eq. 14, as far as time and effort is concerned.

A somewhat vexing problem associated with the course is the selection of a particular textbook. The text of Lebedev [1], while well written and comprehensive in orthogonal polynomials, spherical harmonics and hypergeometric functions, is light on gamma—and related functions, and on the application of exponential—and related integrals; elliptic integrals are not treated at all. Moreover, the somewhat restricted number of examples do not reach into the depth of the variety of engineering-oriented problems and students find this aspect rather frustrating. Nevertheless the text can be used with caution as background material for the theoretical framework of the course and a large proportion of the lectures can thus be devoted to solving practical problems. In this respect the excellent book by Reddick and Miller [2], now unfortunately out of print, served as references for the lecture notes and for numerous homework problems; to a lesser extent, Arfken's [5] sections on gamma functions, Legendre functions and Chebyschev polynomials were found useful. The chapter in Mickley et al. [6] on Bessel functions is one of the best of its kind. In treating computational aspects, the handbook of Abramowitz and Stegun [3] and the algorithmic tabulations of Smith [4] are more than adequate. By contrast, texts under the generic title of "advanced engineering mathematics" are in my view rather disappointing, with the possible exception of Kreyszig [6]. Some Dover paperbacks serve as excellent references for certain topics e.g. Bowman [8], Relton [9], Farrel and Ross [10] and Sneddon [11] in the area of applied Bessel functions.

The students' response to the course has been quite positive. They appreciate the relevance of the topics covered to other chemical engineering courses, especially in solving homework problems which facilitate a deeper understanding of the mathematics pertaining to heat- and mass transfer, chemical reaction engineering and other components of our discipline. In courses where these subject matters are taught, there is usually insufficient time for an instructor to go into the depth of the mathematical treatment (even if he is inclined to do that at all) and mathematical background receives superficial attention. The course on special functions reduces this gap at least for those students who are interested in obtaining a better mathematical education than what is normally available in core courses.

Finally as a developer and instructor of this course, I enjoy it immensely not only for the pleasure of a mature and motivated audience but also for having learned a great deal about the impressive richness of XVIIIth and XIXth century mathematics, whose full potential, I believe, has not yet been fully discovered. Apart from its usefulness, it offers much intellectual beauty for chemical engineering educators who see more in mathematics than a mere tool for solving problems. □

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ChE division activities

SUMMER SCHOOL '82

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The next Summer School for Chemical Engineering Faculty, sponsored and organized by the Chemical Engineering Division of the ASEE, will be held August 1-6, 1982, at the University of California at Santa Barbara. Prof. Dale E. Seborg, Chairman of Chemical & Nuclear Engineering, will be handling the local arrangements.

The 1982 Summer School will expand upon the theme that chemical engineers need to have an impact on society in a broader sense. Sessions are planned to discuss means of making students aware of their potential role in issues such as public policy, the environment, and energy policy. A poster session devoted to new course and curricula development is planned, as well as a set of sessions devoted to those technical subjects which will become of key importance in the next decade. The subjects of the workshops are not yet fixed. We are still receiving input from chemical engineering faculty regarding subjects which would match well with the evolving needs of industry and our society.

In August 1980 proposals requesting donations to support the 1982 Summer School were mailed

TABLE A
Donations Received or Pledged
(as of March 1, 1981)

BASF Wyandotte Corporation
Celanese Corporation
Dow Chemical U.S.A.
E. I. du Pont de Nemours & Company, Inc.
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