NUMERICAL METHODS FOR CHEMICAL ENGINEERING PROBLEMS

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Over the past decade, we have developed a course that has taught numerical methods to seniors and graduate students; emphasis has been placed on the computer application of these methods to the solution of chemical engineering problems.

The course (now ChE 508) had its origins in the summer of 1962, during the last days of the Ford Foundation Project on the Use of Computers in Engineering Education. The project director, Professor D. L. Katz, then suggested to us and Professor H. A. Luther, visiting from the department of mathematics at Texas A&M University, that we might prepare a manual that outlined typical implementations of numerical methods on the digital computer. Within 18 months, we had prepared a 781-page preliminary edition of *Applied Numerical Methods*, and its publication was appropriately celebrated on February 29, 1964. This preliminary edition contained many illustrative computer examples written in the MAD (Michigan Algorithm Decoder) language. After we had rewritten these in FORTRAN IV, added many end-of-chapter problems, and made further revisions based on classroom experience, *Applied Numerical Methods* was finally published by John Wiley & Sons, Inc., in 1969.

Meanwhile, in spite of a ready student demand in 1962, the introduction of ChE 508 as a legitimate engineering course was vetoed by a majority of the engineering faculty, who then thought that numerical methods *and* their *applications* to engineering problems could better be handled in the mathematics department. Fortunately, this view did not prevail for any length of time, and we have long since been "respectable" in that regard. The course has been given annually for ten years with enrollments typically in the range of 12-30, the majority of whom are graduate students.

COURSE ORGANIZATION

ChE 508 is a 3-credit hour course, lasting for one trimester of 13 or 14 weeks. The only formal prerequisite is a course in computer programming. The course level automatically ensures a reasonable background of mathematics, together with a wide exposure of typical chemical engineering problems. Our own book[1] is now required, although earlier we had used the text by Lapidus,[3] supplemented by our notes, particularly in the area of computer applications. There are three lecture/recitations per week. Four or five computer problems constitute the major part of the homework. There is a 1-hour midterm and a 2-hour final examination, both closed book.

Our current budget allows us to allocate an upper limit of $100 for computing charges per student. On our IBM 360/67 system, a typical ChE 508 FORTRAN batch job costs in the range $0.80-$2.00. Experience shows that the total computing charges average about $75 per student. Although teletypewriter facilities are available, the great majority of ChE 508 jobs are run in batch mode. A typical breakdown of topics covered is shown in Table 1. The order depends on the particular computer problems assigned, although whenever possible it is desirable to preserve the particular sequence of: (1) numerical approximation, (2) numerical integration, and (3) ordinary differential equations. Three weeks are usually allowed for the solution of each computer problem.

REPRESENTATIVE PROBLEMS—THE 1972 ASEE BOULDER WORKSHOP

Workshop No. 4 at the ASEE Chemical Engineering Division meeting in Boulder gave us an opportunity to discuss some of the approaches used in teaching numerical methods and their applications. The major topics covered were the solution of ordinary differential equations, partial differential equations, and simultaneous nonlinear equations; to a lesser extent, poly-

Workshop No. 4 at the ASEE Chemical Engineering Division meeting in Boulder gave the authors an opportunity to discuss some of the approaches used in teaching numerical methods and their applications. The 18 workshop participants had the opportunity to solve a wide variety of problems typical of those assigned in one of the senior/graduate courses at Michigan. Three of the problems are discussed in this paper.

nomial approximation, numerical integration, and simultaneous linear equations were also discussed. The 18 participants had the opportunity to solve a wide variety of problems, but the majority chose to modify and supply data for three existing programs, which were then run on the computer at the University of Colorado. Since these three programs are typical of material discussed in ChE 508, we shall summarize them here.

Program 1: Cubic spline-polynomial approximation

Consider a function $f(x)$ of which n accurately known sample points $(x_i, f(x_i))$, $i = 1,2, \ldots, n$ are available. The function may be approximated by a series of cubic polynomials $p_{3,i}(x) = a_i + b_i x + c_i x^2 + d_i x^3$ on each of the $n - 1$ intervals between successive base points. The $4(n - 1)$ coefficients may be determined by requiring that: (a) the succession of polynomials pass through each of the functional values, (b) there be continuity of first and second derivatives at each of the points $i = 2,3, \ldots, n - 1$ and (c) there be zero curvature at the end points. The subsequent algebraic development (see e.g., Problem 1.24 of [1], or Section 6.7 of [2]) leads to a tridiagonal system of equations in the second derivatives of $p_{3,i}(x)$ at each base point; from these, the individual cubic polynomials can be determined.

If the base points are regarded as supports in the x direction, this piecewise cubic spline polynomial also represents the shape of a simply supported beam. This is readily apparent by noting that (for small deflections) the deflection $y = y(x)$ is governed by $EId^2y/dx^2 = M$, where E is Young's modulus of elasticity and I is the cross-sectional moment of inertia. Since the bending moment M is linear in x between supports—and is zero at the two end supports—integration immediately leads to the piecewise cubic polynomial. Note in passing that the shape of the cubic spline polynomial is not invariant under rotation of axes. This problem is discussed in

TABLE 1. Typical Content of ChE 508

Topic	Class Periods
Introduction	1
Solution of equations: Graeffe's method, successive substitutions, Newton's method, **regula falsi** and half-interval methods.	2
Matrix algebra and solution of simultaneous linear and nonlinear equations: Gauss-Jordan method, matrix inversion, maximum-pivot criterion, successive substitution and Newton-Raphson methods.	5
Numerical approximation: one-and two-dimensional interpolation, Taylor's expansion, spline approximation, Chebyshev polynomials.	6
Numerical integration: Newton-Cotes formulas, Romberg and composite rules, Gauss-Legendre quadrature, multidimensional forms. Numerical differentiation.	4
Midterm examination.	1
Ordinary differential equations: Euler, Runge-Kutta, and multistep methods; stability; boundary-value problems.	8
Partial differential equations: finite-difference methods for parabolic and elliptic type equations; stability; multidimensional problems; boundary conditions.	8
Eigenvalue and characteristic-value problems.	3
Statistical methods: polynomial and multiple regression; random-number generators.	2
Total:	40

greater detail by Lee and Forsythe,[4] who also present the criterion of the minimization of total strain energy for the determination of closed (i.e., continuous) spline curves. Spline-function approximation is also fully discussed by Ahlberg, Nilson, and Walsh[5]; a related technique is described by Akima.[6]

Two representative cubic splines are shown in Figures 1 and 2. The first of these passes through the five points $(x, \sin x)$, for $x = 0, \pi/4, \pi/2, 3\pi/4$, and π. Representative predicted values are $p_3(\pi/6) = 0.4997$ and $p_3(\pi/3) = 0.8651$ (cf. $\sin 30^\circ = 0.5$ and $\sin 60^\circ = 0.8660$).

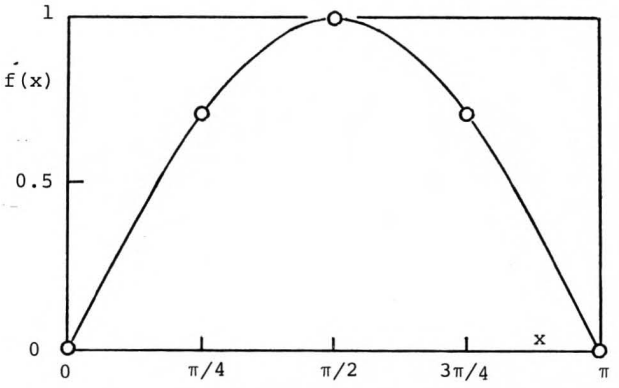

Fig. 1.—Spline approximation for five points conforming to sin x.

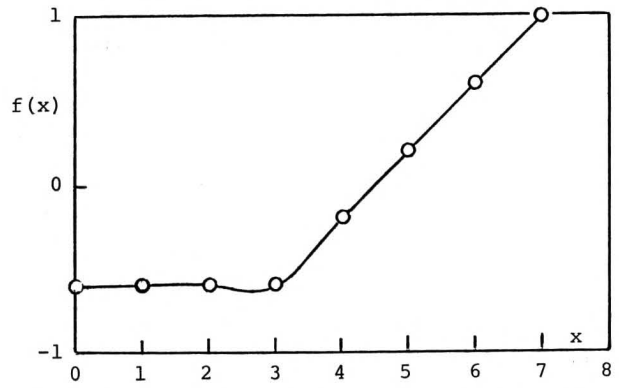

Fig. 2.—Spline approximation for points conforming to ramp function.

Program 2: Ethane Pyrolysis in a Tubular Reactor

In the temperature range 1200°F to 1700°F, ethane decomposes essentially into ethylene and hydrogen, with first-order irreversible kinetics. If the reaction occurs in a heated tubular reactor, and the development in Example 6.2 and Problem 6.20 of [1] is followed, the variations with reactor length L (ft) of conversion z, temperature T (°R), and pressure p (psia) are given by:

$$\frac{dz}{dL} = \left(\frac{2.075\times10^{20} A p\, e^{-74,358/T}}{n_0 RT} \right) \left(\frac{1 - z}{1 + z} \right) ,$$

$$\frac{dT}{dL} = \frac{q/n_0 - \Delta H_R dz/dL}{(1-z)C_{p,C_2H_6} + z(C_{p,C_2H_4} + C_{p,H_2})} ,$$

$$\frac{dp}{dL} = -\frac{f_M m^2 RT(1 + z)}{28125\times32.2\times\pi^2 pD^5} .$$

Here, A (ft²) is the cross-sectional area of the tube, D (in.) is its internal diameter, R = 10.73 ft³ psia/lb mole — °R, n_0 (lb moles/hr) is the inlet molal feed rate of ethane, q (BTU/hr-ft) is the heat input per unit length of tube, f_M is the Moody friction factor, and m (lb/hr) is the mass flow rate. The heat of reaction ΔH_R (BTU/lb mole) and the specific heats C_p (BTU/lb mole-°R) are functions of temperature.

Starting from known inlet conditions (z = 0, T = 1660°R, p = 30 psia), the above three simultaneous ordinary differential equation may be solved by a variety of conventional techniques. In the present case, Euler's method with a step size of $\Delta L = 5$ ft proves satisfactory. For m = 1800 lb/hr and q = 5000 BTU/hr-ft, variations of z, p, and T with L are shown as the continuous lines in Figures 3 and 4 for internal diameters D = 4.026 and 3.068 in. Since the reaction is endothermic, its rate is largely controlled by the available external heat input. Therefore, once the temperature is high enough for the reaction to occur, the conversion is approximately linear with respect to distance. The pressure drop is severe for the smallest tube diameter. Since the reaction is first order, there tends to be a lower conversion at these lower pressures, and the temperature level rises accordingly. The broken lines on Figure 4 show the computed results when an excessively large step size of $\Delta L = 50$ ft

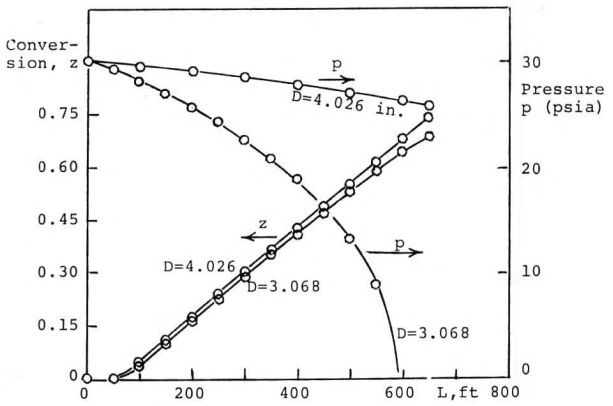

Fig. 3.—Variations of conversion and pressure along reactor.

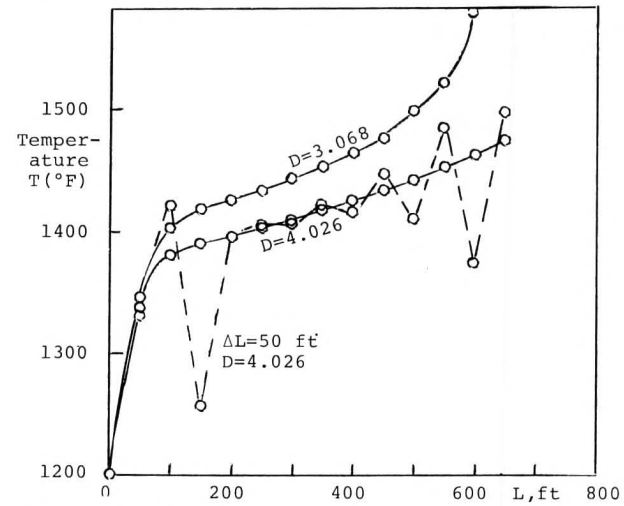

Fig. 4.—Variation of temperature along reactor.

is taken. The oscillations (which are particularly evident in T) have a simple explanation. In Euler's method, the reaction rate prevailing at the beginning of a step is assumed to be a suitable average value for use over the entire step. However, should it be too low, T will rise unduly because of the external heat input. Conversely, if it is too high, the correspondingly large reaction rate will consume some of the sensible heat of the stream, causing T to fall unduly. The effect is clearly propagated from one step to the next.

Program 3: Simulation of a General Piping Network

The last program to be discussed accepts as data the following parameters concerning a piping network:

1. The number of nodes, n.

2. A vector $\vec{t}$ of node types. For the ith node, the corresponding element t_i will be either 0 (free node, with the pressure p_i, psig, to be computed), 1 (p_i specified) or 2 (volumetric injection rate v_i, gpm, specified).

3. The connection matrix, C. Each element c_{ij} will be either 0 (nodes i and j not joined directly), 1 (a pipe joining nodes i and j), or 2 (a centrifugal pump that pumps *from* node i *to* node j).

4. A pressure vector, $\vec{p}$, in which the p_i are either specified values (for $t_i = 1$) or initial approximations.

5. An injection vector, $\vec{v}$, in which v_i is specified for each node i for which $t_i = 2$.

6. Symmetric matrices D, L, and E whose elements D_{ij}, L_{ij} and e_{ij} contain the diameter (in.), length (ft), and roughness (in.) of the pipe joining nodes i and j (if $c_{ij} = 1$). For flow with mean velocity u_{ij} from node i to node j, the pressure change is given by

$$p_i - p_j = \frac{1}{2} f_M \rho u^2_{ij} \frac{L_{ij}}{D_{ij}} + \rho g(z_j - z_i),$$

in which f_M is the Moody friction factor. For laminar flow, $f_M = 64/Re$; for turbulent flow, f_M is given approximately by the Colebrook equation.

7. An elevation vector, $\vec{z}$, whose elements contain the elevations (feet above datum) of the nodes.

8. Matrices A and B whose elements a_{ij} and b_{ij}—specified only if $c_{ij} = 2$—contain the characteristics of the centrifugal pump between nodes i and j. For normal operation, the increase in pressure is approximated by the falling head/discharge characteristic curve

$$p_j - p_i = a_{ij} - b_{ij} Q^2_{ij}$$

However, the pump is also equipped with: (a) a check valve, so that the flow rate Q_{ij} cannot be negative, and (b) a regulator, so that Q_{ij} cannot exceed $(a_{ij}/b_{ij})^{1/2}$, even if $p_i > p_j$.

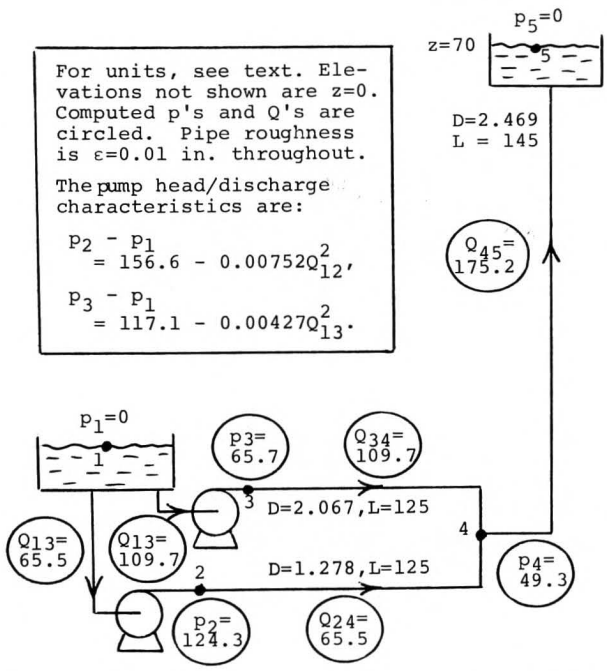

Fig. 5.—Computed pressures and flowrates for pumping system.

9. The density ρ and viscosity μ of the fluid, assumed constant.

Assuming steady conditions, a material balance at each node leads to a set of nonlinear simultaneous equations in the unknown pressures at each node, which are then found by the Newton-Raphson method[1]. The flowrates Q_{ij} (gpm) through each pipe and pump are then readily calculated. Full details of the program are given in[7].

A simple representative network is shown in Figure 5. The pressures and flowrates computed by the program are circled. The liquid is water ($\rho = 62.4$ lb/ft^3, $\mu = 1$ centipoise). □

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