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NUMERICAL SOLUTION of NONLINEAR BOUNDARY VALUE PROBLEMS with APPLICATIONS

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Details the development, analysis, and practical application of various numerical techniques in solving nonlinear boundary value problems

Numerical Solution of Nonlinear Boundary Value Problems with Applications

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Preface

During the past decade there has been a remarkable growth of interest in problems associated with systems of linear and nonlinear ordinary differential equations with split boundary conditions. Throughout engineering and applied science, we are confronted with nonlinear two-point boundary value problems that cannot be solved by analytical methods. With this interest in finding solutions to particular nonlinear boundary value problems has come an increasing need for techniques capable of rendering relevant profiles. Although considerable progress has been made in developing new and powerful procedures, notably in the fields of fluid and celestial mechanics, and chemical and control engineering, much remains to be done. It is apparent that although physical models of boundary value type are evident in many branches of modern engineering and applied science, the application of methods has remained largely within the sphere of chemical engineering. On the other hand, in this text we do not overlook the importance of physical systems that lie outside the realm of chemical engineering: for example, orbital mechanics, theory of elasticity, and mathematical biology.

This book is concerned with the development, analysis, and practical application of various numerical techniques that can be adapted successfully for the solution of nonlinear boundary value problems. One cannot expect a particular technique to be superior to others for all problems. We have tried to present an account of what has been accomplished in the field. Accordingly, it seemed appropriate to shape this text to those interested in numerical analysis as a working tool for physicists and engineers. Our emphasis is on description and straightforward application of numerical techniques without presenting in detail the underlying theory. The theory selected reflects our own interest and experience with the application of diverse numerical algorithms. We believe that the techniques described in this book will provide investigators with tools that will permit them to solve difficult problems in modern engineering, applied science, and other fields.

It is assumed that readers are acquainted with numerical analysis to the extent that it is taught in the usual engineering courses. They also must have some experience with applied analysis and programming.

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Contents

Occurrence and Solution of Nonlinear Boundary Value Problems in Engineering and Physics 1

1.1 Occurrence of Nonlinear Problems for Ordinary Differential Equations

There are a large number of problems in engineering and physics that can be described through the use of nonlinear ordinary differential equations. When the (boundary) conditions, which together with the differential equations describe the behavior of a particular physical system, are determined at various points, the resulting problem is referred to as a boundary value problem.

The boundary conditions may be classified according to various criteria: (1) linear–nonlinear boundary conditions, (2) separated conditions–mixed conditions, (3) two-point–multipoint problems, and so on.

A great number of nonlinear boundary value problems are represented by equations of diffusional type. Here the boundary conditions result after specification of dependent variables (or fluxes) at the boundary of the system. These conditions are usually of the separated type; that is, at a given value of the independent variable, the values of the dependent variables, derivatives, or a combination of both are prescribed. The boundary conditions for diffusion problems may be of nonlinear type, especially for radiation problems. If there is an external relation between boundary conditions (e.g., recycle problems in chemical engineering), the boundary conditions are of the mixed type; that is, for a given value of the independent variable, a combination of dependent variables (or derivatives) with different arguments results. Sometimes the boundary conditions may be given in integral form; for example, if the total amount of heat transferred is specified.

In problems of mechanics, multipoint boundary value problems occur; for example, for a multibody system, the velocity at different points may be specified.

A number of nonlinear boundary value problems result after the formulation of a model for a particular physical situation. Examples include diffusion occurring in the presence of an exothermic chemical reaction [1], heat conduction associated with radiation effects [2], deformation of shells [3], and so on†. For these examples, the nonlinear equations represent the true physical situation. However, there are a number of nonlinear boundary value problems which result after certain mathematical transformations. To illustrate this family of equations, boundary layer problems will be presented [4]. Although the flow of a viscous fluid is described by rather complicated nonlinear partial differential equations (Navier–Stokes equations), certain transformations make it possible to convert them to nonlinear ordinary differential equations (boundary value problems). The new dependent variables include some dependent and independent variables occurring in the original problem. Whereas solution of the original Navier–Stokes equations represents a difficult numerical problem, the transformed equations (i.e., the boundary layer equations) are more conducive to numerical treatment. Similar transformations may be used to convert the nonlinear parabolic equations to a nonlinear boundary value problem. Sometimes this transformation is referred to in the literature as the Boltzmann transformation [5]. Finally, the nonlinear boundary value problem for ordinary differential equations results after proper discretization of nonlinear elliptic partial differential equations with two independent variables [6, 7]. A specific group of problems is created by the family of optimization problems which are required to establish the "optimum profiles." The equations formulated by use of the Euler–Jacobi variational equations, as well as by the Pontrjagin's maximum principle, belong to this family [8].

1.2 Existence of a Solution

Generally speaking, for a nonlinear boundary value problem it is difficult to prove rigorously the existence of a solution. However, engineers and physicists are more interested in finding in a numerical way a region of parameters where the given nonlinear boundary value problem does not exhibit a solution. Fortunately, for a great number of correctly formulated nonlinear boundary value problems there exists at least one solution. Nevertheless, there are physical problems which for particular values of governing parameters do not possess a solution. For instance, the diffusion equation incorporating a strongly exothermic reaction of zero order need not always exhibit a solution [1]. Another example is represented by the boundary layer equations describing spiral flow in a porous pipe [9].

†Bracketed arabic numbers throughout refer to references at chapter end.

1.3 Problems of a Multiplicity of Solutions

There are a number of nonlinear boundary value problems that may exhibit more than one solution. It is a difficult mathematical problem to investigate the domain in which multiple solutions may occur. From the physical point of view, a strong exothermic or autocatalytic reaction, radiation effect, or other feedback mechanism is responsible for multiple steady states of a particular physical model. Table 1-1 surveys some physical models represented by nonlinear boundary value problems for ordinary differential equations that may exhibit multiple solutions.

1.4 Nonlinear Phenomena

Nonlinearities occurring in boundary value problems are caused by a number of different physical effects. In chemical engineering problems, the following nonlinear phenomena are frequently encountered:

1. Chemical reactions
2. Adsorption phenomena
3. Volume change resulting from the mole change accompanying a chemical reaction
4. Radiation effects and problems connected with nonlinear heat transfer
5. Dependence of the rate, equilibrium, and transport coefficients on concentration and temperature
6. Dissipation of energy
7. Flow of non-Newtonian fluids
8. Gravitation and Coulomb forces

Nonlinearities caused by a chemical reaction may be divided into two major groups: (1) concentration dependences and (2) temperature dependences. The first- and zero-order reaction-rate expressions are the linear relations that occur in transport equations; all other reaction-rate expressions are of the nonlinear type. For instance, an esterification reaction occurring in a liquid phase is represented by a second-order reversible reaction (i.e., the nonlinearity is of quadratic type). For catalytic reactions the reaction-rate expression is of the Langmuir-Hinshelwood type [17] (rational function) or of integer power form. In the realm of bioengineering the reaction-rate expressions for an enzymatic reaction, which are formally equivalent to the Langmuir–Hinshelwood expressions, are referred to as Michaelis–Menten kinetics [18]. The temperature dependences are always nonlinear; for example, the reaction-rate or adsorption constants are exponentials:

$$k = k_0 \exp\left(\pm\frac{E}{RT}\right)$$

Here minus is for the reaction-rate expression, while plus must be used for

Table 1-1
Nonlinear Boundary Value Problems Having Multiple Solutions

Problem	Equations	Number of Solutions
Diffusion and exothermic zero-order reaction in a slab [1]	$y'' = -\delta e^y$ $y'(0) = 0, \quad y(1) = 0$	$0 = \delta_0 < \delta < \delta^*$: two solutions $\delta > \delta^*$: no solution
Diffusion and exothermic first-order reaction in a slab [10]	$y'' = \phi^2 y \exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right]$ $y'(0) = 0, \quad y(1) = 1$	$\gamma\beta > \frac{4\gamma}{\gamma - 4}$, $\phi_1 < \phi < \phi_2$: three solutions Outside this region: one solution
Diffusion and exothermic first-order reaction in a sphere [11, 12]	$y'' + \frac{2}{x}y' = \phi^2 y \times \exp\left[\frac{\gamma\beta(1-y)}{1+\beta(1-y)}\right]$ $y'(0) = 0, \quad y(1) = 1$	Up to 15 solutions have been established
Diffusion, convection, and isothermic reaction with an adsorption kinetic term [13]	$\frac{1}{\mathrm{Pe}}y'' - y' - \mathrm{Da}\left(\frac{1+B}{1+By}\right)^2 y \times \frac{y+C}{1+C} = 0$ $y'(0) = \mathrm{Pe}[y(0) - 1],$ $y'(1) = 0$	For certain values of the governing parameters, three solutions exist for $\mathrm{Da}_1 < \mathrm{Da} < \mathrm{Da}_2$ Outside this region: one solution
Diffusion, convection, and exothermic reaction occurring in a tubular reactor [14]	$\frac{1}{\mathrm{Pe}}y'' - y' + \mathrm{Da}(1-y) \times \exp\left(\frac{\theta}{1+\theta/\gamma}\right) = 0$ $\frac{1}{\mathrm{Pe}}\theta'' - \theta' - \beta(\theta - \theta_c) + B\,\mathrm{Da}(1-y) \times \exp\left(\frac{\theta}{1+\theta/\gamma}\right) = 0$ $y'(1) = \theta'(1) = 0$ $y(0) = \frac{1}{\mathrm{Pe}}y'(0),$ $\theta(0) = \frac{1}{\mathrm{Pe}}\theta'(0)$	Up to five solutions have been established
Equilibrium of suspended charged drops [15]	$y'' + \frac{1}{x}y' = \frac{\beta}{y^2}$ $y'(0) = 0, \quad y(1) = 1$	For $\beta < 0.42$: one solution For $0.42 < \beta < 0.78$: two or three solutions
Flow between two rotating disks [16]	$F'' = \sqrt{\mathrm{Re}}\,HF + \mathrm{Re}(F^2 - G^2 + k)$ $G'' = 2\,\mathrm{Re}\,FG + \sqrt{\mathrm{Re}}\,G'H$ $H' = -2\sqrt{\mathrm{Re}}\,F$ $F(0) = F(1) = H(0) = H(1) = 0$ $G(0) = 1, \quad G(1) = s$	For greater values of Re, more than ten solutions have been found

adsorption effects [17]. Of course, this exponential dependence is the main source of numerical difficulties accompanying the particular physical problem.

Another source of nonlinearities are the adsorption processes since the majority of adsorption isotherms are represented by rational functions. Evidently, as a result, diffusion problems in which adsorption phenomena must be considered represent a nonlinear boundary value problem. One should notice that the expression describing the rate of growth of microorganisms (Monod expression) is formally identical to the Langmuir adsorption isotherm [18].

A chemical reaction may be accompanied by expansion or contraction phenomena. For instance, diffusion, convection, and second-order reactions are described by a simple differential equation,

$$\frac{dy}{dx} = L\frac{d^2y}{dx^2} + ky^2$$

while for the volume-change case the equation is more complicated:

$$\frac{dy}{dx} = L\left[\frac{1}{1 + E(1-y)}\frac{d^2y}{dx^2} + \frac{E}{[1 + E(1-y)]^2}\left(\frac{dy}{dx}\right)^2\right] + ky^2$$

Here L and E are the parameters describing dispersion and volume change, respectively [19]. We may note that both reaction and adsorption give rise to a nonlinear "source term," while the volume-change effect results in nonlinear derivatives or nonlinear coefficients.

Among the most complicated nonlinear problems are those connected with radiation. The heat flux caused by radiation may be written

$$q = \sigma(T^4 - T_0^4)$$

This relation can be incorporated into transport equations in different ways. For instance, for tube radiation through a jacket, the nonlinear radiation term is a part of the differential equation [20], while for radiation by means of the inlet or outlet surface of the tube, the radiation effect is a part of the boundary conditions. There are very complicated physical situations in which the radiation effect is accompanied by a chemical reaction or by a velocity distribution (radiation boundary layer) [21]. For some extreme situations Newton's law for convective transfer does not describe properly the typical features of the process: for instance, convective heat transfer to boiling helium is described by a cubic law [22]:

$$q = \alpha(T - T_0)^3$$

If the concentration or temperature dependences of rate, equilibrium, or transport coefficients are considered in the physical model, nonlinearities in derivatives and coefficients result (see, e.g., [23]). For small variations of concentration or temperature for a particular physical process, average values of coefficients may be used; however, for problems with extreme variations of the order of 1000°C (e.g., supersonic flow of real gases around blunt objects), the temperature dependences of coefficients must be considered [24]. The average values of coefficients cannot be used if jump variations can be expected; for example, as a result of higher temperatures, recrystallization may occur, which can cause an essential change in thermal conductivity. However, the most practical problem is the temperature and concentration dependence of viscosity [25].

Fluids in which the vector of the shear stress τ and the gradient of velocity dy/dx is not linearly proportional are usually referred to as non-Newtonian fluids. A number of semiempirical nonlinear relations used in the literature are presented in Table 1-2 [26, 27]. Problems that are linear for Newtonian fluids may be strongly nonlinear for non-Newtonian fluids.

If energy dissipation is considered in hydrodynamic problems, then in Fourier–Kirchhoff convective heat-transfer equations, a new term occurs which is proportional to the second power of the gradient of velocity. Of course, this term must be considered for those problems in which extreme gradients result, which, however, can also be the case for relatively slow flow conditions.

Finally, the gravitational or Coulomb forces should be mentioned.

TABLE 1-2
SOME SEMIEMPIRICAL RELATIONS BETWEEN VECTOR OF SHEAR STRESS τ AND GRADIENT OF VELOCITY

τ	Model
$-m\left\lvert\frac{dv}{dx}\right\rvert^{\mu-1}\frac{dv}{dx}$	Ostwald–de Waele
$A \operatorname{arcsinh}\left(-\frac{1}{B}\frac{dv}{dx}\right)$	Eyring
$-(\varphi_0 + \varphi_1 \lvert\tau\rvert^{\alpha-1})^{-1}\frac{dv}{dx}$	Ellis
$a\left[1 - \exp\left(-\alpha\frac{dv}{dx}\right)\right]$	Taganov

1.5 Types of Nonlinear Boundary Value Problems in Chemical Engineering

1. Calculation of chemical engineering equipment
   (a) Calculation of temperature profiles in countercurrent heat exchangers if the heat-transfer coefficients are dependent on temperature.
   (b) Calculation of concentration and temperature profiles in countercurrently operated packed mass exchangers (rectification columns, absorbers) [28].

   (c) Calculation of concentration profiles in extraction columns [29].
   (d) Calculation of concentration and temperature profiles in tubular reactors with countercurrent cooling.
   (e) Calculation of concentration and temperature profiles in tubular recycle reactors [30].
   (f) Calculation of concentration and temperature profiles in tubular reactors if the inlet concentration and the amount of heat transferred are specified.
   (g) Calculation of concentration and temperature profiles for a tubular reactor with an external heat exchanger [31].
   (h) Calculation of concentration and temperature for a tubular reactor with an internal heat exchanger [31].
   (i) Calculation of concentration and temperature profiles for complex configuration "reactor-heat exchangers": for instance, various types of ammonia reactors (TVA, Casal, Quench, NEC, Fauser-Montecatini, OSAG, Haldor-Topsoe, etc.) [32].
   (j) Design of catalytic convertors with a short bed [33].
2. Chemical reaction engineering problems
   (a) Mass transfer and effectiveness factor evaluation for an isothermal catalytic reaction occurring on a single pellet having nonlinear kinetics [34].
   (b) Heat and mass transfer and effectiveness factor evaluation for a nonisothermal catalytic reaction occurring on a single porous pellet [10, 11].
   (c) Calculation of the characteristics of a laminar flame [35].
   (d) Calculation of the critical dimensions of an explosive sample [1].
   (e) Absorption and chemical reactions with nonlinear kinetics (or nonisothermal) occurring in a liquid film [36].
   (f) Heat transfer in a nonporous catalytic particle.
   (g) Transport phenomena and substrate consumption in a microbial film [37].
   (h) Calculation of optimum temperature and pressure profiles in tubular reactors [38].
   (i) Calculation of optimum "catalyst profiles" in tubular reactors [38].
   (j) Calculation of boundary layer problems with a chemical reaction [39].
3. Problems of heat and mass transfer
   (a) Heat and mass transfer in a plate, cylinder, and sphere if thermal conductivity is dependent on temperature [40] and diffusivity is dependent on concentration [41].
   (b) Radiation problems (e.g., radiation of a sphere or a fin) [20].
   (c) Solution of combined conduction–radiation problems in an optically thick medium [42].
   (d) Heat and mass transfer in boundary layer problems (natural

convection from a vertical wall [43], transpiration cooling [44], massive blowing [45], radiation in the boundary layer at subsonic and supersonic velocities [46], thermal boundary layer on rotating bodies [4], heat transfer in a compressible boundary layer [4], etc.).

1.6 Types of Nonlinear Boundary Value Problems in Physics

1. Problems of hydrodynamics and hydrostatics
   (a) Flow of non-Newtonian fluids on a vertical plate (or Newtonian fluids with variable properties).
   (b) Calculation of the shape of velocity profiles in a non-Newtonian fluid flowing between two rotating cylinders.
   (c) Calculation of boundary layer problems for both Newtonian and non-Newtonian fluids (flow on a flat plate [4], flow on a plate with surface curvature [47], flow through a diverging channel [4], flow caused by rotating disks [4], multidimensional flow [44], flow through a porous structure [9, 48], flow of a compressible fluid [4], problems of a supersonic boundary layer [4], problems of a non-steady-state boundary layer [49]), magnetohydrodynamic hypersonic flow [50].
   (d) Effect of fluid motion on a free surface shape [51].
2. Problems of electrodynamics and electrostatics
   (a) Equilibrium of suspended electrically charged drops [15].
   (b) Breakdown of dielectrics [52].
   (c) Ionic boundary layers [53].
   (d) Problems of calculation of photoionization chambers [54].
   (e) Calculation of semiconductor-device current characteristics [55, 56].
3. Problems of magnetohydrodynamics and plasma theory
   (a) Problems leading to the magnetohydrodynamic boundary layer (Hartmann flow) [57].
   (b) Diffusion of magnetic field into plasma [58].
   (c) Problems of plasma radiation (Troesch equation) [59, 60].
   (d) Problems of radiative magnetohydrodynamic channel flow [61].
   (e) Calculation of the effect of a cold wall on a hot plasma [62].
   (f) Calculation of the flow of weakly ionized gases [63].
4. Problems of classical mechanics: theory of elasticity
   (a) Calculation of N-body trajectories [64, 68].
   (b) Nonlinear oscillations.
   (c) Deformation of thin shells [66].
   (d) Finite bending of thin-walled tubes [65].
   (e) Stress analysis of solid propellant grains [67].