Chemical Engineering Communications
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gcec20

THE MODIFIED DIFFERENTIAL QUADRATURES AND THEIR APPLICATIONS

CHUEI-TIN CHANG† [a], CHII-SHANG TSAI [a] & TIEN-TSAI LIN [a]

[a] Department of Chemical Engineering, National Cheng Kung University, Tainan, Taiwan, 70101, Republic of China

Version of record first published: 08 Jun 2010

To cite this article: CHUEI-TIN CHANG†, CHII-SHANG TSAI & TIEN-TSAI LIN (1993): THE MODIFIED DIFFERENTIAL QUADRATURES AND THEIR APPLICATIONS, Chemical Engineering Communications, 123:1, 135-164

To link to this article: http://dx.doi.org/10.1080/00986449308936170

Chem. Eng. Comm. 1993, Vol. 123, pp. 135–164
Reprints available directly from the publisher.
Photocopying permitted by license only.

Printed in the United States of America

THE MODIFIED DIFFERENTIAL QUADRATURES AND THEIR APPLICATIONS

CHUEI-TIN CHANG† CHII-SHANG TSAI AND TIEN-TSAI LIN

Department of Chemical Engineering
National Cheng Kung University
Tainan, Taiwan 70101
Republic of China

(Received August 4, 1992; in final form March 2, 1993)

In this paper, a number of modifications are instituted in implementing the quadrature method for solving chemical engineering problems with semi-infinite domains and/or steep gradients. This improvement in the curve-fitting ability of differential quadratures is achieved by adopting trial functions of forms other than the polynomials. Formal criteria are first developed (and proved) for the selection of proper function forms. If the trial functions are restricted to the products of polynomials and some auxiliary functions, explicit formulae are derived to facilitate the calculation of the corresponding modified quadrature coefficients. If, in addition, the grid points are chosen to be the zeros of an orthogonal polynomial, e.g. Jacobi, Laguerre and Hermite, further simplifications can be realized to promote the efficiency and accuracy of the computation procedure. The modified differential quadratures have been applied to various example problems. From the data we have collected so far, it can be concluded that the proposed approach yields more accurate results in regions where most of the variations in the dependent variables occur and tends to lose its edge at locations where negligible changes can be detected in the numerical solutions.
KEYWORDS Differential quadrature Orthogonal collocation Semi-infinite domain Steep gradient.

INTRODUCTION

Nonlinear ordinary and partial differential equations are the most commonly used formulations in chemical engineering models. The quadrature method (Bellman *et al.*, 1972), or, equivalently, the method of collocation (Finlayson and Scriven, 1966) is one of the most popular numerical methods for solving these problems. In earlier papers, some new insights concerning the characteristics of differential quadratures and the corresponding modifications of their implementation procedure have been presented (Quan and Chang, 1989i; 1989ii). Although it has been shown that the proposed techniques are extremely accurate and efficient (Chang, 1992), there are still several interesting problems which require further attention.

The most celebrated drawback of the present approach, which includes both the method of differential quadrature and the method of orthogonal collocation,

† Author to whom all correspondence is to be addressed.

is probably its inability to produce accurate solutions when applied to problems with steep gradients and/or semi-infinite domains, e.g. see Finlayson (1980) and Bellman and Adomian (1985). Although modifications of the collocation method has been proposed in a number of studies to handle certain special chemical engineering models of this type, e.g. Birnbaum and Lapidus (1978) and Caban and Chapman (1981), it is still necessary to develop reliable and efficient numerical techniques for solving the above problems in general.

This paper addresses this need for additional improvements of the quadrature method. In our study, the trial functions used in determining the quadrature coefficients were no longer restricted to polynomials. Formal constraints were developed to identify proper trial funtions, i.e. they belong to a *family* and, also, a *complete set.* More specifically, trial functions formed by the products of polynomials and various auxiliary functions were adopted to enhance the performance of differential quadratures. Further, based on a strategy of placing the grid points on the zeros of an orthogonal polynomial, e.g. the Jacobi, Laguerre and Hermite polynomials, simplified formulae were derived to expediate the calculation of the modified quadrature coefficients. Finally, the concept of boundary layer was introduced to facilitate the implementation of differential quadratures. For comparison purpose, four different schemes, including that of the orthogonal collocation method, were used to map the zeros of the orthogonal polynomials into the computation fields for solving example problems. A number of typical cases, i.e. steady-state and transient problems with steep gradients and/or semi-infinite domains, were studied using the techniques developed in this work. It can be observed that, on the average, the proposed approach yields better results and, in particular, more accurate solutions can be obtained in the region where most of the variation in the dependent variable takes place.

CHOICE OF TRIAL FUNCTIONS

Generally speaking, the independent variables in a chemical engineering model are spatial distances (y) and/or time (t). The spatial derivatives in the governing partial differential equations can usually be approximated by the differential quadratures, i.e. linear combinations of the values of the dependent variable at all grid points. More specifically,

$$\frac{\partial^n u(t, y_i)}{\partial y^n} \cong \sum_{j=1}^{N} \gamma_{ij}^{(n)} u(t, y_j) \qquad (1)$$

$$i = 1, 2, \ldots, N \qquad n = 1, 2, 3, \ldots$$

where u represents the dependent variable, y_i's represent the locations of the grid points, N is the number of grid points and the constants $\gamma_{ij}^{(n)}$'s will be referred to as the nth-order differential-quadrature coefficients. The values of these coefficients can be determined by assuming that, at a given value of t and over an interval in y, a set of trial functions, $f_i(y)$ and $i = 1, 2, \ldots, N$, can be chosen such

that

$$u(t, y) \cong \sum_{i=1}^{N} \vartheta_i(t) f_i(y) \qquad a_1 < y < a_2$$
$$i = 1, 2, \ldots, N \tag{2}$$

where ϑ_i, $i = 1, 2, \ldots, N$, are constants to be determined and a_1 and a_2 are the lower and upper bounds of the interval in which the model is defined. From Eqs. (1) and (2), it was shown (Finlayson, 1980; Bellman and Adomian, 1985) that

$$\mathbf{G}_n^T = \mathbf{F}_0^{-1}\mathbf{F}_n \tag{3}$$

where,

$$\mathbf{G}_n = (\gamma_{ij}^{(n)})_{N\times N}\,\mathbf{F}_0 = (f_i(y_j))_{N\times N}\,\mathbf{F}_n = \left(\frac{d^n}{dy^n} f_i(y_j)\right)_{N\times N}$$

From Eq. (3), it is clear that inversion of the matrix $\mathbf{F}_0$ is needed to determine the quadrature coefficients $\gamma_{ij}^{(n)}$. Bellman and Adomian (1985) pointed out that the following equation can be used to determine the higher-order coefficients from the first-order coefficients without matrix inversion:

$$\mathbf{G}_n = \mathbf{G}_1^n \tag{4}$$

Although Eq. (4) is intuitively correct and, in fact, valid in a large number of situations, it does not hold for all types of functions. The following counter example delineates the need for further clarification.

Example 1 Using two arbitrarily chosen grid points, one can verify that coefficients obtained from the set of trial functions (e^y, ye^y) satisfy Eq. (4). On the other hand, Eq. (4) is not valid based on the set of trial functions (e^y, ye^y, y) with three grid points. Finally, the relation in Eq. (4) is satisfied if one more trial function, $f_4(y) = 1$, is added to the set (e^y, ye^y, y).

Since none of the published studies offer specific explanations, we have thus developed in this work a sufficient condition of Eq. (4), i.e. the trial functions used in differential quadratures have to form a *family*. A proof of this statement is provided in Appendix A. Also, in a previous study (Quan and Chang, 1989i), we have shown that the quadrature method is actually equivalent to the general collocation method, which is a special case of the method of weighted residual (MWR). Therefore, the basic requirement of the trial functions used in MWR, i.e. they are the leading members of a *complete* set of functions (Finlayson, 1972), should also be imposed to ensure the approximation in Eq. (2) converges as $N \to \infty$.

Notice that the trial functions used in most of the previous studies, e.g. Quan and Chang (1989i; 1989ii), are restricted to polynomials that satisfy the above conditions. Although well-behaved problems can be solved satisfactorily by this approach, the use of such functions fails to mimic the system behaviors governed by more difficult models over the entire problem domains, e.g. those defined in semi-infinite intervals and/or those with steep gradients on their solution surfaces. In this work, an *auxiliary function* $r(y)$ is introduced to enhance the performance

of the quadrature method. A different type of trial functions are created by multiplying the polynomials by this auxiliary function, i.e.

$$\tilde{f}_i(y) = r(y)\sum_{j=1}^{N} c_{ij} y^{j-1} \qquad i = 1, 2, \ldots, N \tag{5}$$

Let

$$\tilde{\mathbf{F}}_0 = (\tilde{f}_i(y_j))_{N\times N} \qquad \tilde{\mathbf{F}}_n = \left(\frac{d^n}{dy^n}\tilde{f}_i(y_j)\right)_{N\times N}$$

Notice that

$$\tilde{\mathbf{F}}_0 = \mathbf{C}\mathbf{V}_0\mathbf{R}_0 \qquad \tilde{\mathbf{F}}_n = \mathbf{C}\sum_{p=0}^{n}\binom{n}{p}\mathbf{V}_p\mathbf{R}_{n-p} \tag{6}$$

where,

$$\mathbf{R}_{n-p} = \left(\delta_{ij}\frac{d^{n-p}}{dy^{n-p}}r(x_i)\right)_{N\times N}$$

and the entries, $v_{p,ij}$, of the matrix $\mathbf{V}_p$ can be determined by

$$v_{p,ij} = \begin{cases} 0 & \text{if } p > i-1 \\ \dfrac{y_j^{i-p-1}}{i}\displaystyle\prod_{m=0}^{p}(i-m) & \text{otherwise} \end{cases}$$

From Eq. (3), one can obtain an equation for calculating the quadrature coefficients based on the trial functions defined in Eq. (5):

$$\tilde{\mathbf{G}}_n^T = (\tilde{\gamma}_{ij}^{(n)})_{N\times N}^T = \sum_{p=0}^{n}\binom{n}{p}\mathbf{R}_0^{-1}\mathbf{V}_0^{-1}\mathbf{V}_p\mathbf{R}_{n-p} = \sum_{p=0}^{n}\binom{n}{p}\mathbf{R}_0^{-1}\mathbf{G}_p^T\mathbf{R}_{n-p} \tag{7}$$

where,

$$\mathbf{G}_p^T = (\gamma_{ij}^{(p)})_{N\times N}^T = \mathbf{V}_0^{-1}\mathbf{V}_p$$

It can be shown that, if only polynomials are used as trial functions, the pth-order ($p \geq 1$) quadrature coefficients are exactly the same as the entries in the matrix $\mathbf{G}_p$ (Quan and Chang, 1989i). Thus, in order to calculate the coefficients $\tilde{\gamma}_{ij}^{(n)}$'s, one can make use of the following simple equation:

$$\tilde{\gamma}_{ij}^{(n)} = \frac{1}{r(y_j)}\sum_{p=0}^{n}\binom{n}{p}\gamma_{ij}^{(p)}\frac{d^{n-p}}{dy^{n-p}}r(y_i) \tag{8}$$

where, the zeroth-order coefficients $\gamma_{ij}^{(0)}$'s are the entries of an identity matrix and the higher-order coefficients $\gamma_{ij}^{(p)}$'s ($p \geq 1$) can be determined by the explicit formulae proposed by Quan and Chang (1989i) or the recursive algorithm developed by Villadsen and Michelsen (1978).

From Eq. (2) and (5), it is quite obvious that the value of the auxiliary function $r(y)$ at any point in the problem domain must be finite and non-zero. Notice that the trial functions $\tilde{f}_i(y)$'s may fail to satisfy the two conditions mentioned before, i.e. they form a family and belong to a complete set. However, if one considers $v(y) = u(y)/r(y)$ as a new dependent variable, the trial functions of the

transformed problem are still polynomials. Thus, introducing an auxiliary function simply modifies the behavior of the dependent variable in the problem domain. This function has to be chosen in such a way that $v(y)$ becomes significantly more suitable for approximation by polynomials. The following are some of the potential auxiliary functions and the corresponding formulae of the first- and second-order quadrature coefficients:

1. $r(y) = e^{-\xi y}$

$$\tilde{\gamma}_{ij}^{(1)} = e^{-\xi(y_i - y_j)}[-\xi\delta_{ij} + \gamma_{ij}^{(1)}] \tag{9a}$$

$$\tilde{\gamma}_{ij}^{(2)} = e^{-\xi(y_i - y_j)}[\xi^2\delta_{ij} - 2\xi\gamma_{ij}^{(1)} + \gamma_{ij}^{(2)}] \tag{9b}$$

2. $r(y) = 1/(1 + \xi y)$

$$\tilde{\gamma}_{ij}^{(1)} = \frac{1 + \xi y_j}{1 + \xi y_i}\left(-\frac{\xi}{1 + \xi y_i}\delta_{ij} + \gamma_{ij}^{(1)}\right) \tag{10a}$$

$$\tilde{\gamma}_{ij}^{(2)} = \frac{1 + \xi y_j}{1 + \xi y_i}\left(\frac{2\xi^2}{(1 + \xi y_i)^2}\delta_{ij} - \frac{2\xi}{1 + \xi y_i}\gamma_{ij}^{(1)} + \gamma_{ij}^{(2)}\right) \tag{10b}$$

3. $r(y) = e^{-\xi y^\zeta}$

$$\tilde{\gamma}_{ij}^{(1)} = e^{-\xi(y_i^\zeta - y_j^\zeta)}(-\xi\zeta y_i^{\zeta-1}\delta_{ij} + \gamma_{ij}^{(1)}) \tag{11a}$$

$$\tilde{\gamma}_{ij}^{(2)} = e^{-\xi(y_i^\zeta - y_j^\zeta)}(-\xi\zeta y_i^{\zeta-2}[\zeta - 1 - \xi\zeta y_i^\zeta]\delta_{ij} - 2\xi\zeta y_i^{\zeta-1}\gamma_{ij}^{(1)} + \gamma_{ij}^{(2)}) \tag{11b}$$

From a practical view point, the function form should be simple enough so that the increase in computational effort is acceptable. Since differentiation of the exponential functions does not create extra terms, a general formula of the nth-order coefficients can be derived from Eq. (8). Thus, the coefficients corresponding to the function $e^{-\xi y}$ are the most convenient ones for implementation.

Notice also that solving problems with the new set of quadrature coefficients $\tilde{\gamma}_{ij}^{(n)}$ is actually equivalent to transforming the original models into differential equations with $v(y)$ as the dependent variable and solving them with the original coefficients $\gamma_{ij}^{(n)}$. However, the process of deriving these equations is often tedious and prone to error. Further, after replacing the derivatives by the differential quadratures, the resulting algebraic equations tend to be very complex and nonlinear and, thus, the corresponding iteration computation is more difficult to converge.

Finally, it should be pointed out that the concept of an auxiliary function is not new. Birnbaum and Lapidus (1978) used the function e^{-t} to enhance the performance of a double orthogonal collocation technique for solving a PDE with time as one of the independent variables. Caban and Chapman (1981) adopted the weight function $e^{-\xi y^\zeta}$ to improve the performance of orthogonal collocation method in solving problems concerning mass transfer with reaction in a boundary layer. The specific values of parameters, ξ and ζ, can be extracted from the analytical solution of a limiting case of the mass transfer model. Our study generalized these ideas in the context of the quadrature method, and improved computational techniques have been developed for a wide variety of problems, i.e. steady-state and transient problems with semi-infinite domains and/or steep gradients.

SIMPLIFIED FORMULAE FOR QUADRATURE COEFFICIENTS

Although both the explicit formulae and the recursive algorithm mentioned in the previous section can be utilized to calculate the quadrature coefficients, $\gamma_{ij}^{(n)}$, with equal accuracy and efficiency, it has been established that simpler formulae can be derived if all the grid points are located at the zeros of a Jacobi polynomial (Quan and Chang, 1989i). In addition to the fact that the accuracy of the numerical solutions is near "optimal," the principal incentive for using this approach is due to the simplicity of these formulae. The computation effort of determining the coefficients can be reduced to a minimum of 1/6 of that of the previous procedures (Chang, 1992). Since the magnitude of error in applying the quadrature method is difficult to estimate, a common practice to ensure the accuracy of the solutions is to gradually increase the number of grid points until the numerical answers do not change appreciably. In such cases, the use of the simplified formulae is especially convenient and time-saving.

It has been shown (e.g. Villadsen and Michelsen, 1978) that

$$\gamma_{ij}^{(n)} = \frac{d^n}{dy^n}\bar{f}_j(y_i) \tag{12}$$

where,

$$\bar{f}_j(y) = \frac{\Phi_N(y)}{(y - y_j)[d\Phi_N(y_j)/dy]}$$

$$\Phi_N(y) = \prod_{m=1}^{N}(y - y_m)$$

and y_i's are the locations of the grid points. Notice that this equation is valid as long as linearly independent polynomials are used as the trial functions and, thus, the values of the coefficients are affected only by the distribution of the grid points. If the zeros of a Jacobi polynomial, $P_N^{(\alpha,\beta)}(y)$, are chosen as the grid point locations, then the function $\Phi_N(y)$ in Eq. (12) should be replaced by it and the simplified formulae can then be derived accordingly. These formulae have already been published in an earlier paper (Quan and Chang, 1989i). In this work, the same derivation has been extended to the other two families of classical orthogonal polynomials, i.e. the Laguerre and Hermite polynomials. A summary of these newly-developed simplified formulae are presented in Appendix B of this paper.

COMPUTATIONAL FIELD

Notice that the simplified formulae presented Appendix B are based on the zeros of orthogonal polynomials defined in their respective standard intervals. The positions of these zeros x_i's need to be mapped onto the desired locations where the corresponding values of the dependent variable(s) can be computed. Since the solution approach of differential quadrature method can be viewed as a form of

Lagrange interpolation for approximating the dependent variable, reliable numerical answers should lie only within the interval between the first and the last grid points. In this study, this interval is called the *computational field* of the problem.

Let x_i's ($i = 1, 2, \ldots, N$) be the zeros of an orthogonal polynomial defined in a standard interval with lower bound s_1 and upper bound s_2. Thus,

$$s_1 < x_1 < x_2 < \cdots < x_{N-1} < x_N < s_2$$

Let y_i's ($i = 1, 2, \ldots, N$) be the projected locations of the zeros x_i's in a computational field with lower bound b_1 and upper bound b_2. Notice that, in solving boundary-value problems, it is important to include the end points of the problem domain as grid points so that boundary conditions can be accurately imposed. Depending on which two points (say c_1 and c_2) in the standard interval are mapped onto b_1 and b_2, different grid point placement schemes can be devised, i.e. (I) $c_1 = x_1$ and $c_2 = x_N$, (II) $c_1 = s_1$ and $c_2 = s_2$, (III) $c_1 = s_1$ and $c_2 = x_N$ and (IV) $c_1 = x_1$ and $c_2 = s_2$ (see Figure 1).

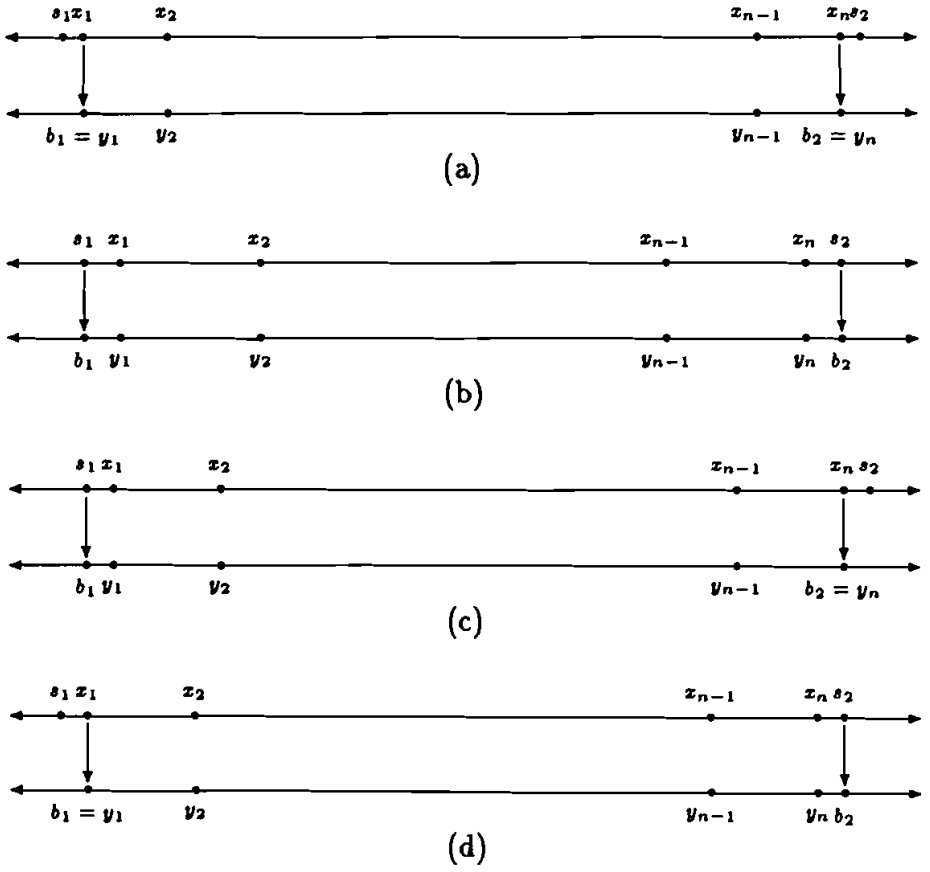

FIGURE 1 Grid Placement Schemes: (a) Scheme I, (b) Scheme(II), (c) Scheme(III), (d) Scheme(IV).

Notice that, in general, the intervals (c_1, c_2) and (b_1, b_2) are not equal. But identical intervals and grid point distributions are shown in Figure 1 just for the convenience of illustration. The simplified formulae presented in Appendix B are applicable only with Scheme I. Thus, the corresponding solution procedure is by far the easiest and most convenient to implement. In the cases of Scheme II, III or IV, one or both of the bounds of the standard interval, s_1 and/or s_2, are mapped onto b_1 and/or b_2. Since both end points of the computational field must be included, extra grid point(s) should be placed at the corresponding boundary location(s). Thus, if grid points are placed according to any of these three schemes, the quadrature coefficients should be computed by the general formulae (Quan and Chang, 1989i) or the recursive algorithm (Villadsen and Michelsen, 1978). Actually, Scheme II is the same as that used in a traditional orthogonal collocation method, and Scheme III and Scheme IV are hybrids of the first two. In certain cases, there may be incentive for using grid point placement strategies other than Scheme I due to the fact that slightly more accurate results can be obtained (e.g. Michelsen and Villadsen, 1991).

Although there are various approaches that can be used to define the mapping relation between (c_1, c_2) and (b_1, b_2), the simplest linear transformation is adopted here. Thus, the projected locations of the zeros can be determined by

$$y_i = \frac{b_2 - b_1}{c_2 - c_1}(x_i - c_1) + b_1 \tag{13}$$

The corresponding nth-order quadrature coefficients based on grid points in the computational field can be calculated by multiplying the standard coefficients by a factor $[(c_2 - c_1)/(b_2 - b_1)]^n$. This fact is particularly useful when the bounds of the computation field, b_1 and/or b_2, themselves are variables to be determined.

APPLICATIONS OF THE GENERALIZED DIFFERENTIAL QUADRATURES

The method of differential quadrature has been applied to a wide range of problems with good results, e.g. Quan and Chang (1989ii). However, it has also been recognized that difficulties may arise when most of the variation in the dependent variable occurs in a small portion of the problem domain. This particular characteristic appears in boundary-value problems defined in semi-infinite intervals and in problems with steep gradients on the solution surfaces. In almost all of the previous studies, polynomials were adopted as the trial functions, and zeros of the Jacobi polynomials were mapped onto the grid points in the computational field. It is not surprising that inaccurate answers were obtained using this approach, since a large number of grid points were not placed in the region where significant change in the dependent variable takes place. In this work, tools such as auxiliary functions and various grid point placement schemes have been utilized to develop improved solution techniques for the problems mentioned above.

BVPs with Semi-Infinite Domains

A large number of chemical engineering models can be written in this form. For example, using similarity transformation, steady-state models of laminar flow in the boundary layer along a flat plate or wedge and dynamic models of heat conduction or mass diffusion in semi-infinite medium can usually be formulated as BVPs with semi-infinite domains. There are several alternatives to solve these problems (Finlayson, 1980), e.g.

1. Transforming the BVP into an integral equation, the approximate solution can be obtained by initially assuming an arbitrary function as the candidate and then substituting it back into the equation. The process is carried out iteratively until termination criteria are satisfied.
2. Recognizing the fact that solution approaches an asymptote as the independent variable approaches infinity, a shooting method can be started at the left end of the domain. Using an implicit method with adjustable step size, one can integrate the equation until the solution does not change significantly. The boundary conditions at the right end can be fitted by varying the conditions at the left end.
3. Approximating the derivatives by linear combinations of the values of dependent variable at grid points, one can transform the BVP into a set of algebraic equations. These equations can then be solved by standard techniques such as the Newton-Raphson method. Notice that various approaches are available for the approximation of derivatives, e.g. the differential quadrature, the orthogonal collocation and the finite difference, etc..

In general, the accuracy of the integral method is unknown and dependent upon the postulated function, and the computational effort involved in implementing the shooting method may be overwhelming if the corresponding ODEs are stiff and it takes a long distance for some of the dependent variables to stabilize. In the present study, the third alternative is adopted using differential quadratures. There is, however, one problem in carrying out this approach, i.e. the upper bound of the problem domain, upon which a boundary condition is imposed, approaches infinity. Since most of the previous developments are concerned with finite computational fields, additional adjustments are needed to overcome this difficulty.

One possible method is to transform the domain, $0 \leq y < \infty$, into finite intervals, e.g. let

$$\eta = e^{-y}$$

As a result, the new independent variable η varies between 0 and 1. The disadvantage of this technique is that too many of the grid points may be placed outside the region of interest. This is due to the facts that the zeros of an orthogonal polynomial are usually densely populated near $\eta = 0$ and the variation of dependent variable is insignificant when $y \to \infty$.

Another approach is to identify appropriate parameters in the auxiliary function $e^{-\xi y^t}$ by reference to the limiting case of the particular system model for

which an analytic solution is available (Caban and Chapman, 1981). This technique has been proven useful in solving problems concerning mass transfer with reaction in a boundary layer. However, the success in deriving an appropriate asymptotic model is not guaranteed for other types of BVPs defined in semi-infinite domains, e.g. those describing the phenomena of laminar flow in thin boundary layers with the stream function as the dependent variable. Even if the parameters in the function $e^{-\xi y^t}$ can be identified, one may still face the laborious tasks of generating the corresponding orthogonal polynomials and locating their zeros. Further, since infinity is considered as the location of the last grid point in this approach (Caban and Chapman, 1981), Eqs. (11) cannot be used and, thus, matrix inversion is unavoidable in determining the quadrature coefficients. As a result, the numerical solutions become unreliable as the dimension of the matrix increases.

Although the use of other auxiliary functions is also feasible, the form $e^{-\xi y}$ is selected to solve BVPs with semi-infinite domains in general. This is due to the fact that the corresponding formulae, Eqs. (9), are the simplest ones among all possible candidates and, thus, accurate values of the modified quadrature coefficients can be determined most efficiently. Further, the parameter ξ in this function can be adjusted in a systematic fashion according to the solution profile of each individual problem. Also, the concept of *boundary layer* has been adopted for the purpose of defining a finite interval $[0, \delta]$ in the semi-infinite domain and using it as the computational field of the problem. The basic idea here is the same as the phenomenological distance δ assumed in the integral method for the approximate analysis of momentum, heat and mass transfer in fluids near solid boundaries. The boundary layer is regarded as the region next to the fluid- solid interface, and no transport via the mechanism of molecular diffusion take place beyond the boundary of this region. In other words, the gradients in velocity, temperature or concentration can be assumed to be negligible outside the boundary layer. Similarly, for BVPs with semi-infinite domains in general, one can postulate such a distance δ from the left end of the interval exists and the boundary conditions originally imposed as $y \to \infty$, i.e.

$$\left.\frac{d^k u}{dy^k}\right|_{y\to\infty} = C \qquad k = 0, 1, \ldots \tag{14}$$

can be assumed to be approximately correct at $y = \delta$. Here, C represents an arbitrary constant. Further, additional conditions can be introduced in a way similar to that of the Pohlausen method (Churchill, 1988) in integral analysis, i.e.

$$\left.\frac{d^{k+1} u}{dy^{k+1}}\right|_{y=\delta} = 0 \qquad k = 0, 1, \ldots \tag{15}$$

These extra constraints are necessary for determining the value of δ in implementing the quadrature method. Notice that the computational field $[0, \delta]$ is now finite and, thus, Eqs. (9) and the formulae presented in Appendix B can be used to compute $\tilde{\gamma}_{ij}^{(n)}$'s accurately and efficiently even with a large number of grid points. Notice that the accuracy in the numerical solutions may tend to

deteriorate near $y = \delta$ due to the approximations made in Eqs. (14) and (15). However, this drawback is outweighed by the improvements in the overall performance. The implementation procedure of the proposed techniques is illustrated in the following example:

Example 2 Consider the problem involving the mass transfer from a rotating disk with bimolecular, irreversible chemical reaction, where a species R diffusing from the surface of the disk reacts with a species S present in the solution according to

$$R + \nu S \xrightarrow{k} P$$

where ν is a stoichiometric coefficient and k is a rate constant. By assuming that the diffusivities of R and S are equal, one can formulate the governing equations of the system (Caban and Chapman, 1981):

$$f_R'' + 3x^2 f_R' - \varphi f_R^r f_S^s = 0 \tag{16a}$$

$$f_S'' + 3x^2 f_S' - \nu\varphi f_R^r f_S^s = 0 \tag{16b}$$

subject to

$$f_R = 1 \qquad f_S' = 0 \qquad x = 0 \tag{16c}$$

$$f_R = 0 \qquad f_S = 1 \qquad x \to \infty \tag{16d}$$

where f_R and f_S denote the dimensionless concentration of species R and S respectively, φ is the dimensionless rate constant, r and s are the orders of irreversible homogeneous reactions of species R and S, and x represents the radial distance from the surface of the rotating disk. The values of the parameters in this model are:

$$r = 1 \qquad s = 1 \qquad \nu = 1 \qquad \varphi = 5$$

Conceptually, the concentrations of the two species R and S may approach the free stream values (i.e. $f_R = 0$ and $f_S = 1$) at different speeds. Thus, two boundary layers of different thicknesses should be assumed for f_R and f_S respectively. This is not feasible, since two sets of grid points will be generated accordingly. In this example, the same boundary layer is adopted for both variables, and their variations outside are assumed to be negligible. Based on Eq. (14) and Eq. (15), the following conditions can be imposed on the edge of the layer:

$$f_R(\delta) = 0 \qquad f_S(\delta) = 1 \tag{17a}$$

$$f_R'(\delta) = f_S'(\delta) = 0 \tag{17b}$$

Note that the two conditions given in Eq. (17b) are extra constraints not included in the original model. Incorporation of one or both of these conditions into the

problem formulation facilitates the estimation of δ and, also, may enhance the accuracy of the numerical solution near the edge of the boundary layer.

Let us next introduce the following transformations:

$$y = \frac{x}{\delta} \qquad f_T = 1 - f_S \tag{18}$$

Thus, the governing equations, Eq. (16), can be approximated by

$$\frac{d^2 f_R}{dy^2} + 3y^2\delta^3 \frac{df_R}{dy} - \varphi\delta^2 f'_R(1 - f_T)^s = 0 \tag{19a}$$

$$\frac{d^2 f_T}{dy^2} + 3y^2\delta^3 \frac{df_T}{dy} + \nu\varphi\delta^2 f'_R(1 - f_T)^s = 0 \tag{19b}$$

$$f_R(0) = 1 \qquad f'_T(0) = 0 \tag{19c}$$

$$f_R(1) = 0 \qquad f_T(1) = 0 \qquad f'_R(1) = 0 \tag{19d}$$

The purpose of introducing the new dependent variable f_T is to convert the corresponding solution profile into a shape that matches the general trend of the auxiliary function $e^{-\xi y}$ for this example.

The method of differential quadrature can then be applied to Eq. (19), i.e.

$$\sum_{j=1}^{N} \gamma_{ij}^{(2)} f_{R_j} + 3y_i^2\delta^3 \sum_{j=1}^{N} \gamma_{ij}^{(1)} f_{R_j} - \varphi\delta^2 f'_{R_i}(1 - f_{T_i})^s = 0 \tag{20a}$$

$$\sum_{j=1}^{N} \gamma_{ij}^{(2)} f_{T_j} + 3y_i^2\delta^3 \sum_{j=1}^{N} \gamma_{ij}^{(1)} f_{T_j} + \nu\varphi\delta^2 f'_{R_i}(1 - f_{T_i})^s = 0 \tag{20b}$$

$$i = 2, 3, \ldots, N-1$$

$$f_{R_1} = 1 \tag{20c}$$

$$\sum_{j=1}^{N} \gamma_{1j}^{(1)} f_{T_j} = 0 \tag{20d}$$

$$f_{R_N} = 0 \tag{20e}$$

$$f_{T_N} = 0 \tag{20f}$$

$$\sum_{j=1}^{N} \gamma_{Nj}^{(1)} f_{R_j} = 0 \tag{20g}$$

There are $2N+1$ equations and $2N+1$ unknowns (i.e. δ, f_{R_i}, f_{T_i} and $i = 1, 2, \ldots, N$) in the above formulation and, thus, Eq. (20) can be solved simultaneously by a standard technique such as the Newton-Raphson method.

In order to assess the performance of various approaches in applying the quadrature method, the exact solution of the governing equations needs to be used as the basis for comparison. Since the given problem is nonlinear, only numerical answers can be obtained. As a result, one must first produce numerical solutions with extremely high accuracy to be used as substitutes. These solutions

were generated by implementing the conventional differential quadratures with a large number of grid points. In this example, zeros of the Legendre polynomials were projected to the interval [0, 1] according to Scheme I.

As mentioned before, the number of grid points N necessary to guarantee a good numerical solution is not known. Thus, the near exact solution was obtained by gradually increasing the grids points until the difference between the solutions corresponding to two successive values of N is insignificant. Since the value of δ and the locations of zeros vary as N increases, one faces the problem of comparing numerical solutions at different sets of grid points. In this example, the relative deviations of the interpolated values of two set of numerical solutions were computed and compared at equal intervals. This approach is theoretically sound, since it has been established that the quadrature method can be viewed as the approximation of the dependent variable(s) by Lagrange interpolation (Quan and Chang, 1989i).

For the present problem, it was found that the solutions corresponding to 26 grid points can be used as the basis for comparison (see Figure 2 and Table I). From Table I, it can be observed that the magnitude of deviation in f_R, Δ_R, starts to increase as x goes beyond 1.2 and finally reaches a level of 2.7%. Thus, solutions outside the interval $0 \leq x \leq 1.2$ may be unreliable. On the other hand, deviations Δ_R and Δ_S at locations inside this region are all very small. Notice also that most of the variations in the dependent variables occur before $x = 1.2$, i.e.

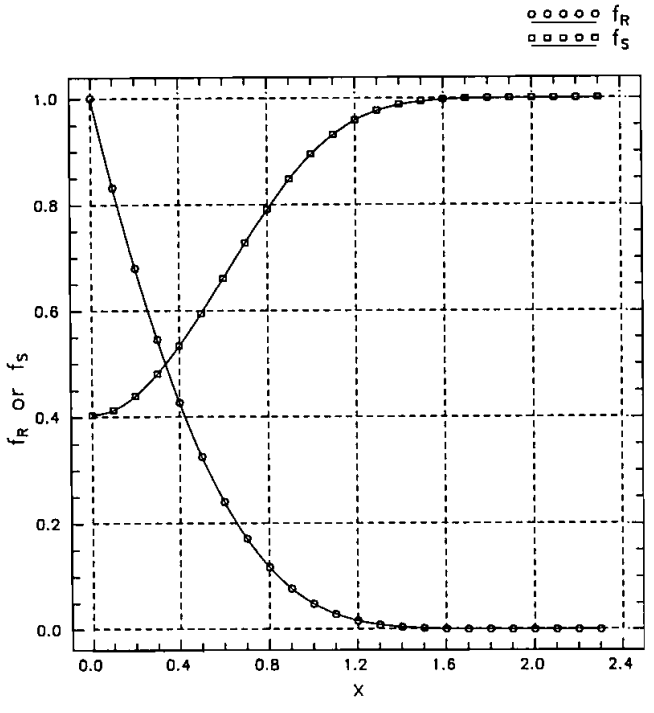

FIGURE 2 Near Exact Solution.

TABLE I

Near exact solution

x	f_R	f_S	Δ_R	Δ_S
0.00000000	1.00000000	0.40302187	0.000000E-00	2.064404E-07
0.10000000	0.83073248	0.41254670	6.379912E-09	1.662842E-07
0.20000000	0.67920932	0.43919156	1.074779E-08	1.268239E-07
0.30000000	0.54438808	0.48032739	1.432801E-08	9.410248E-08
0.40000000	0.42608216	0.53321283	1.642876E-08	6.695363E-08
0.50000000	0.32440398	0.59463732	1.849546E-08	4.641485E-08
0.60000000	0.23933419	0.66083804	1.838434E-08	3.011328E-08
0.70000000	0.17042464	0.72768950	1.877663E-08	1.855187E-08
0.80000000	0.11665160	0.79112011	1.714507E-08	9.733035E-09
0.90000000	0.07642054	0.84764414	1.439404E-08	3.303273E-09
1.00000000	0.04769825	0.89484923	8.386052E-09	7.822546E-10
1.10000000	0.02822550	0.93168108	0.000000E-00	3.756650E-09
1.20000000	0.01575272	0.95843151	3.174055E-08	5.842880E-09
1.30000000	0.00824579	0.97644173	7.276439E-08	6.759236E-09
1.40000000	0.00402474	0.98763239	1.987706E-07	7.593919E-09
1.50000000	0.00182071	0.99491933	5.492369E-07	8.048133E-09
1.60000000	0.000075864	0.99735121	1.449955E-06	8.021247E-09
1.70000000	0.00028932	0.99893179	3.801974E-06	7.908448E-09
1.80000000	0.00010035	0.99961005	1.295511E-05	8.203199E-09
1.90000000	0.00003145	0.99987191	4.451694E-05	7.901012E-09
2.00000000	0.00000885	0.99996237	1.808237E-04	7.500282E-09
2.10000000	0.00000222	0.99999018	4.953393E-04	6.400063E-09
2.20000000	0.00000049	0.99999774	3.035208E-03	4.200009E-09
2.30000000	0.00000010	0.99999956	2.683179E-02	8.000004E-10

99% for f_R and 93% for f_S. Thus, if one is mainly interested in the general system behavior adjacent to the surface of disk, then the near exact solutions of f_R and f_S in [0; 1.2] should be considered adequate for use as the basis to compare the performances of various different approaches.

In addition, the correctness of the data presented in Table I was also confirmed independently by using the multiple shooting methods implemented in the IMSL subroutines. With a tolerance of 10^{-8}, almost identical solutions wer obtained. When comparing the numerical values of f_R and f_S with those presented in Table I, it can be observed that they differ only by the 8th digit below the decimal point.

After establishing the reference values of f_R and f_S, they were then compared with those obtained by implementing the conventional differential quadratures with 9 grid points. Zeros of four different orthogonal polynomials were projected into the interval $0 < y < 1$ according to the four different grid point placement schemes described in the previous section. Three of them are special cases of the Jacobi polynomials, i.e. $P_N^{(1,1)}(x)$, $P_N^{(0,0)}(x)$ (the Legendre polynomial) and $P_N^{(-(1/2),-(1/2))}(x)$ (the Chebyshev polynomial of the first kind). The last one is the Laguerre polynomial $L_N^{(0)}(x)$. Corresponding to each case, the interpolated values of the dependent variables at equal intervals were again determined by Lagrange interpolation, and the arithmetic average of the absolute values of "errors" was computed as a measure of the overall accuracy. These results are summarized in

TABLE IIa

Average absolute errors in solutions obtained by using the conventional differential Quadratures, (f_R).

	Scheme(I)	Scheme(II)	Scheme(III)	Scheme(IV)
$P_n^{(1,1)}(x)$	0.000349	0.000096	0.001822	0.000282
$P_n(x)$	0.000230	0.000120	0.001557	0.000716
$T_n(x)$	0.000165	0.000180	0.001218	0.004473
$L_n(x)$	0.010367	*	0.014518	*

Table IIa and Table IIb. Notice that the upper bound s_2 of the domain of the Laguerre polynomials approaches infinity and, according to Eq. (13), all the grid points in the computational field are required to be placed upon the origin if Scheme II or IV is implemented. Therefore, numerical solutions corresponding to these two cases are not reported. From Table IIa and IIb, it can be observed that Scheme II is by far the best grid point placement strategy. If one is concerned with the accuracy in f_R, then zeros of the Jacobi polynomial $P_7^{(1,1)}(x)$ are probably the most suitable choice. If zeros of a Legendre polynomials are selected, implementation of the conventional differential quadrature using Scheme II yields the most accurate f_S. Also, notice that the worst results among all the cases considered here are those obtained by adopting the zeros of Laguerre polynomials as the grid points.

In this example, two auxiliary functions of the form $e^{-\xi y}$ were introduced simultaneously to enhance the curve-fitting ability of the quadrature method. Two individual parameters, i.e. ξ_R for f_R and ξ_T for f_T, were assigned to these two functions respectively. Thus, two sets of modified quadrature coefficients, $(\tilde{\gamma}_{ij}^{(n)})_R$ for $d^n f_R/dy^n$ and $(\tilde{\gamma}_{ij}^{(n)})_T$ for $d^n f_T/dy^n$, should be adopted to replace the original coefficients, $\gamma_{ij}^{(1)}$ and $\gamma_{ij}^{(2)}$, in Eq. (20).

Naturally, the appropriate values of ξ_R and ξ_T are unknown to us before the start of the solution process. In this study, these parameters were set to zero as the initial guess and, thus, the first pass of calculations are the same as those performed in the conventional quadrature method. Next, the parameters, ξ_R and ξ_T, need to be estimated in such a way that the general trends of the two auxiliary functions follow those of f_R and f_T. Since these functions are only required to

TABLE IIb

Average absolute errors in solutions obtained by using the conventional differential Quadratures, (f_S).

	Scheme (I)	Scheme (II)	Scheme (III)	Scheme (IV)
$P_n^{(1,1)}(x)$	0.004530	0.000689	0.020039	0.000428
$P_n(x)$	0.002632	0.000340	0.017436	0.004315
$T_n(x)$	0.001641	0.000417	0.013518	0.036883
$L_n(x)$	0.025041	*	0.031977	*

* not applicable

mimic the approximate behaviors of the dependent variables, a simple procedure for determining ξ_R and ξ_T has been developed by assuming that

$$\frac{f(y)-f(\infty)}{f(0)-f(\infty)} \approx e^{-\xi y}, \qquad y \geq 0 \tag{21}$$

where, f represents the dependent variable, f_R or f_T, and ξ is the corresponding parameter to be estimated. Thus, as long as the values of the dependent variable(s) are available, the following equation can be used for our purpose:

$$\xi \approx -\sum_{j=2}^{N-l} \ln\left(\frac{f(y_j)-f(y_N)}{f(0)-f(y_N)}\right) \Big/ \sum_{j=2}^{N-l} y_j = -\sum_{j=2}^{N-l} \ln(f(y_j)) \Big/ \sum_{j=2}^{N-l} y_j \tag{22}$$

Notice that, since the solutions near the right end of the computational field are sometimes unreliable, grid points outside the domain of interest (i.e. $y_i\delta > 1.2$ and $i = N-l+1, N-l+2, \ldots, N$) are not included in Eq. (22). Usually, if appropriate combination of grid point placement scheme and the corresponding auxiliary function is selected, the accuracy of the results obtained by using the first estimates of the parameters can be increased significantly. Equation (22) can also be applied repeatedly to improve the estimation until a predetermined limit is reached. However, since this improvement is often marginal, the convergence criterion need not be very strict, say

$$\frac{\xi^{(k+1)}-\xi^{(k)}}{\xi^{(k)}} \leqslant 10^{-2}$$

where, $\xi^{(k)}$ represents the kth estimates of ξ. In most cases, three to four iterations are more than enough.

Average absolute errors in the numerical solutions obtained by various approaches are again computed and presented in Table IIIa and Table IIIb. Several interesting phenomena can be observed. First, the introduction of auxiliary functions of the form $e^{-\xi y}$ is not helpful in enhancing the performance of the quadrature method if the zeros of a Jacobi polynomial are used as the grid points. Results corresponding to the three special cases of the Jacobi polynomials, i.e. $P_N^{(1,1)}(x)$, the Legendre polynomials and the Chebyshev polynomials of the first kind, are less accurate than those obtained without auxiliary functions.

On the other hand, the accuracy in the solutions corresponding to the Laguerre polynomials is dramatically increased. This improvement is also demonstrated in

TABLE IIIa

Average absolute errors in solutions obtained by using the modified differential quadratures, (f_R).

	Scheme (I)	Scheme (II)	Scheme (III)	Scheme (IV)
$P_n^{(1,1)}(x)$	0.013466	0.005705	0.001476	†
$P_n(x)$	0.011115	0.009673	0.000309	0.039777
$T_n(x)$	0.009093	0.008077	0.000446	0.029618
$L_n(x)$	0.000079	*	0.000231	*

TABLE IIIb

Average absolute errors in solutions obtained by using the modified differential quadratures, (f_S).

	Scheme (I)	Scheme (II)	Scheme (III)	Scheme (IV)
$P_n^{(1,1)}(x)$	0.055354	0.039424	0.011088	†
$P_n(x)$	0.51359	0.004137	0.000450	0.107576
$T_n(x)$	0.047276	0.024881	0.001640	0.089990
$L_n(x)$	0.000317	*	0.000991	*

* not applicable
† fails to converge

Figure 3a and Figure 3b. If compared with those presented in Table IIa and Table IIb, the present results are better than all the solutions without the aid of auxiliary functions. To get a deeper insight, two sets of data are plotted in Figure 4a and Figure 4b. They are the local errors of the best numerical solutions in Tables III, i.e. those corresponding to the Laguerre polynomials using Scheme I with auxiliary functions, and the optimal solutions in Tables II, i.e. those obtained by the conventional quadrature method using Scheme II and the zeros of the Jacobi polynomials, $P_N^{(1,1)}(x)$, for placement of grid points. It can be seen clearly that the errors of the solutions obtained by the former approach are smaller in the left region of the domain and tend to lose its edge near the right end. This is not surprising, since the grid points of the former are sparsely distributed in the region close to $x = \delta$ and the absolute error at $x = \delta$ is found to be of the same magnitude of the exact solution itself. This characteristic of the method, however, is desirable, since most of the changes in the dependent variables occur in the left part of the domain.

Problems with Steep Gradients

Some prior knowledge about the system behavior must be obtained before solving this type of problem. The region of rapid change in the dependent variable can be identified with the help of physical insights of the system and/or mathematical techniques such as those used in the singular perturbation method for locating the boundary layer (Nayfeh, 1972). The modified differential quadratures can then be implemented in such intervals with satisfactory performance. This approach was applied to various problems and following is an example:

Example 3 Consider the problem of diffusion and reaction of a component A in a spherical porous catalyst pellet. The first-order reaction in the catalyst is

$$A \rightarrow B$$

The corresponding system model can be found in Finlayson (1980):

$$\frac{d^2c}{dr^2} + \frac{2}{r}\frac{dc}{dr} = \phi^2 c \exp\left(\sigma - \frac{\sigma}{1 + \omega - \omega c}\right) \tag{23a}$$

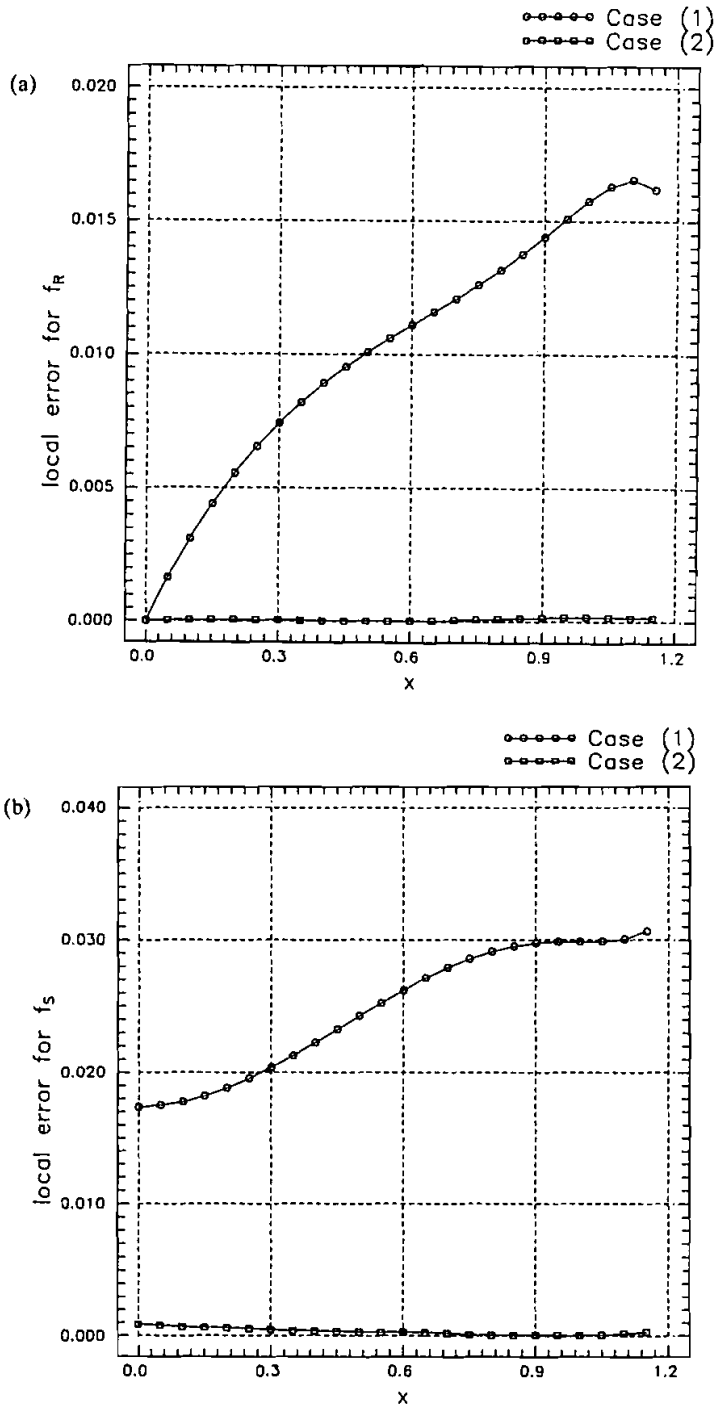

FIGURE 3a Effects of the Auxiliary Function on f_R. Case (1): Laguerre Polynomials, $L_9^{(0)}(y)$; $r(y) = 1.0$; Scheme I Case (2): Laguerre Polynomials, $L_9^{(0)}(y)$; $r(y) = e^{-\xi y}$; Scheme I. 3b Effects of the Auxiliary Function on f_S. Case (1): Laguerre Polynomials, $L_9^{(0)}(y)$; $r(y) = 1.0$; Scheme I Case (2): Laguerre Polynomials, $L_9^{(0)}(y)$; $r(y) = e^{-\xi y}$; Scheme I.

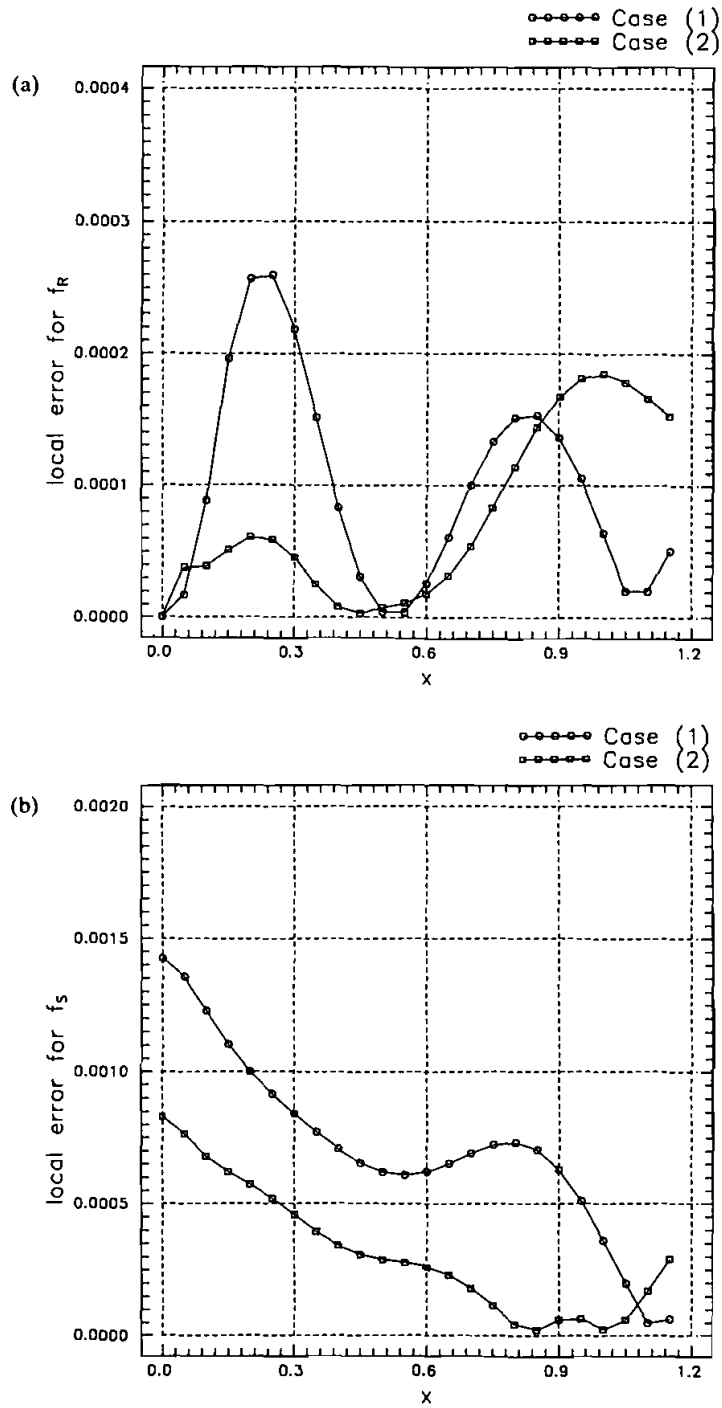

FIGURE 4a Comparison between Two Sets of Optimal Solutions for f_R. Case (1): Jacobi Polynomials, $P_7^{(1,1)}(y)$; $r(y) = 1.0$; Scheme II Case (2): Laguerre Polynomials, $L_9^{(0)}(y)$; $r(y) = e^{-\xi y}$; Scheme I. 4b Comparison between Two Sets of Optimal Solutions for f_S. Case (1): Jacobi Polynomials, $P_7^{(1,1)}(y)$; $r(y) = 1.0$; Scheme II Case (2): Laguerre Polynomials, $L_9^{(0)}(y)$; $r(y) = e^{-\xi y}$; Scheme I.

subject to the boundary conditions

$$\frac{dc}{dr}(0) = 0 \tag{23b}$$

$$c(1) = 1 \tag{23c}$$

where c denotes the dimensionless concentration of A, r denotes the dimensionless radial distance from the center of the sphere, ϕ is the Thiele modulus, σ represents the dimensionless activation energy and ω represents the dimensionless heat of reaction. The parameter values used for this example are

$$\phi = 15 \qquad \omega = 0.02 \qquad \sigma = 20$$

Since the value of Thiele modulus is quite large, the reaction rate inside the catalyst must be very high and, thus, the concentration decreases rapidly to zero within a short distance from the solid surface.

The near exact solution was obtained by a "backward" shooting method from $r = 1$ (Finlayson, 1980) using IMSL subroutines. Note that, as the system equations being integrated from $r = 1$ to $r = 0$, both the concentration and its gradient are supposed to approach zero at a distance not far from the right end of the domain and remain so until the origin is reached. This requirement makes it extremely difficult for the shooting procedure to converge. After numerous attempts, the near exact solution was obtained by setting a tolerance of 10^{-8} with initial guesses close to the actual values of $c(1)$ and $c'(1)$ (Figure 5). In this example, the near exact solution in the interval $0.7 \leq r \leq 1.0$ was selected

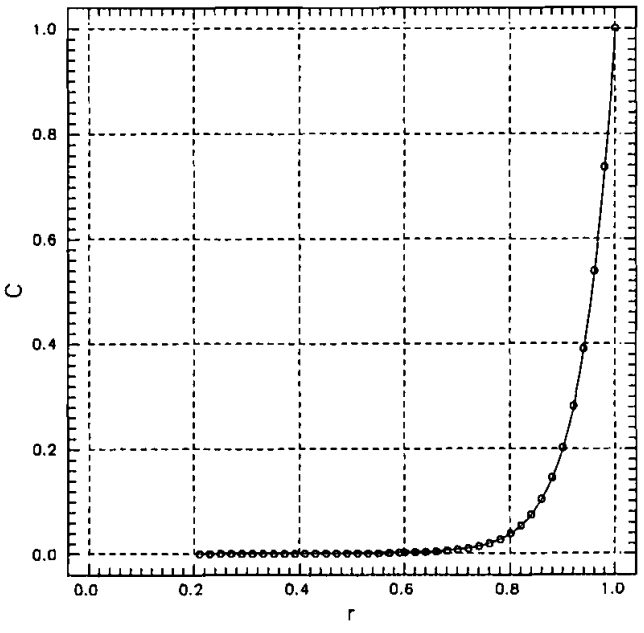

FIGURE 5 Near Exact Solution.

(somewhat arbitrarily) as the basis for comparison. This is due to the fact that most of the variation in c (99.3%) occurs in this region. As a result of the approximations made in Eqs. (14) and (15), one would expect the accuracy in the numerical solutions obtained by the quadrature method to deteriorate significantly at locations close to the edge of the boundary layer, i.e. $r<0.7$. However, if one is interested mainly in the general system behavior, less emphasis can be placed upon the accuracy of solutions in this part of the problem domain.

Next, the existence of a boundary layer adjacent the right end of the problem domain is assumed. At the left edge of the layer, the boundary condition originally imposed at the origin, i.e. $c'=0$, is considered to be valid. To facilitate the implementation of the quadrature method, let us introduce the following transformation:

$$y=\frac{1-r}{\delta}$$

where, δ is the thickness of the boundary layer. Then, Eqs. (23) can be approximated by

$$\frac{1}{\delta^2}\frac{d^2c}{dy^2}-\frac{2}{1-y\delta}\frac{1}{\delta}\frac{dc}{dy}=\phi^2 c\exp\left(\sigma-\frac{\sigma}{1+\omega-\omega c}\right) \tag{24a}$$

with

$$\frac{dc}{dy}(\delta)=0 \tag{24b}$$

$$c(0)=1 \tag{24c}$$

Again, an extra boundary condition is needed

$$c(\delta)=0 \tag{24d}$$

By replacing the spatial derivatives with differential quadratures, Eqs. (24) can be changed into a set of algebraic equations:

$$\frac{1}{\delta^2}\sum_{j=1}^{N}\gamma_{ij}^{(2)}c_j-\frac{2}{1-y_i\delta}\frac{1}{\delta}\sum_{j=1}^{N}\gamma_{ij}^{(1)}c_j=\phi^2 c_i\exp\left(\sigma-\frac{\sigma}{1+\omega-\omega c_i}\right) \tag{25a}$$

$$i=2,3,\ldots,N-1$$

$$\sum_{j=1}^{N}\gamma_{Nj}^{(1)}c_j=0 \tag{25b}$$

$$c_1=1 \tag{25c}$$

$$c_N=0 \tag{25d}$$

Equations (25) have been solved using nine grid points. Two different approaches were adopted for placing these grid points. First, Scheme II was used to determine the grid point locations according to the zeros of a Jacobi

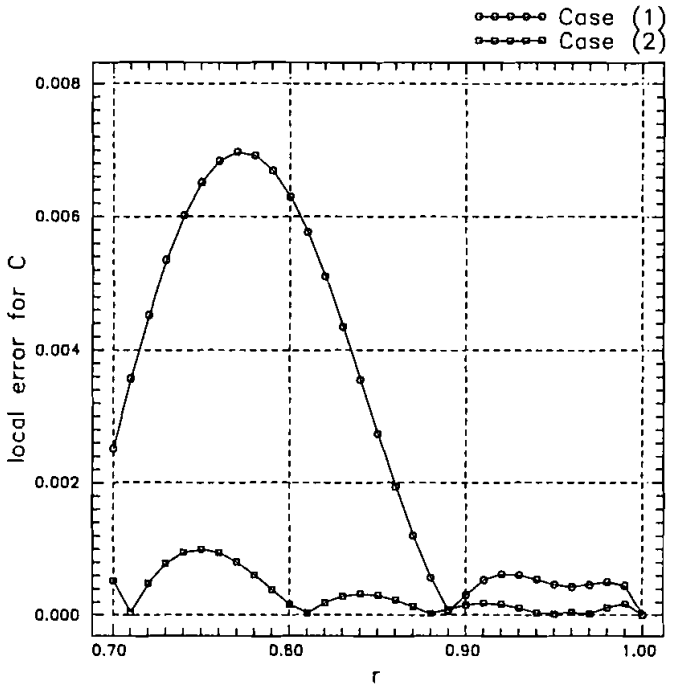

FIGURE 6 Comparison between Two Sets of Optimal Solutions. Case (1): Jacobi Polynomials, $P_7^{(1,0)}(y)$; $r(y) = 1.0$; Scheme II Case (2): Laguerre Polynomials, $L_9^{(0)}(y)$; $r(y) = e^{-\xi y}$; Scheme I.

polynomial $P_7^{(1,0)}(x)$. Only the conventional differential quadratures were adopted for this case. Then, Scheme I was applied to map the zeros of a Laguerre polynomial $L_9^{(0)}(x)$ into the interval $[0, 1]$. An auxiliary function of the form $e^{-\xi y}$ was used to enhance the performance of the curve-fitting ability of the differential quadrature method.

Implementation of either method produces satisfactory results. The average absolute error of the former is 0.001269 and that of the latter is 0.000251. Again, the performance the modified differential quadratures is better and, further, considerably more accurate solutions can be obtained in a region where most of the reaction occurs (see Figure 6). Finally, it should be pointed out that the proposed approach has also been applied successfully to other types of BVPs with steep gradients, e.g. the boundary layer problem presented in Nayfeh (1972), and, thus, can be considered as a useful alternative for solving these problems in general. Following is a simple example:

Example 4

$$\epsilon \frac{d^2f}{dy^2} + (1 + \epsilon^2)\frac{df}{dy} + (1 - \epsilon^2)f = 0 \tag{26a}$$

with the boundary conditions

$$f(0) = \alpha \qquad f(1) = \beta \tag{26b}$$

In this example, the following values are assigned to the parameters:

$$\epsilon = 0.01 \qquad \alpha = 0.0 \qquad \beta = 1.0$$

The corresponding boundary layer can be easily identified by the method of matched asymptotic expansions to be next to the origin. From the analytic solution of the problem, one can determine that the value of f increases from 0 at the left end of the interval to a maximum of 2.592 at $y = 0.047$.

In applying the quadrature method to solving the present problem, the interval $0 \leq y \leq 1$ is divided into two elements $[0, \delta]$ and $[\delta, 1]$. The thickness of boundary layer δ is still a variable to be determined. In this example, five grid points were placed in each interval and, thus, a total of nine points were used. In the interval $\delta \leq y \leq 1$, the grid points were selected according to Scheme II and the zeros of the Jacobi polynomial $P_3^{(1,1)}(x)$. The two approaches adopted here to determine the grid point distribution within the boundary layer are the same as those used in Example 3. Again, the results corresponding to the zeros of Laguerre polynomial $L_5^{(0)}(x)$ with the aid of auxiliary function $e^{-\xi y}$ are superior. The thickness of the boundary layer was determined to be 0.048 and the average absolute error in the layer is approximately 0.16347. The results corresponding to the first grid point placement strategy used in the previous example are less satisfactory, i.e. the average absolute error was found to be 0.20462 and $\delta = 0.036$.

Transient Problems with Steep Gradients and/or Semi-Infinite Domains

The approach taken in solving the transient problems is essentially the same as that for the steady-state problems. The thickness of the assumed boundary layer, however, may vary with time. This is illustrated in the following example:

Example 5 Let us consider the one-dimensional heat transfer problem in a packed column. Initially, the entire packed bed and the gas stream in the column are all maintained at a constant temperature. Starting from $t = 0$, the inlet gas is suddenly raised to a higher temperature and stay that way until the operation is terminated. The mathematical model of this problem was formulated in Ramachandran and Duduković (1984)

$$\frac{\partial u}{\partial x} = -St(u - v) \tag{27a}$$

$$\frac{\partial v}{\partial t} = u - v \tag{27b}$$

Subject to

$$u(0, t) = 1 \qquad t > 0 \tag{27c}$$

$$v(x, 0) = 0 \qquad x > 0 \tag{27d}$$

where, u and v represent the dimensionless gas and solid temperature respectively. The analytic solution of this problem is available in Jacob (1957). Using a Stanton number of 20, the numerical values of u and v at any location and time

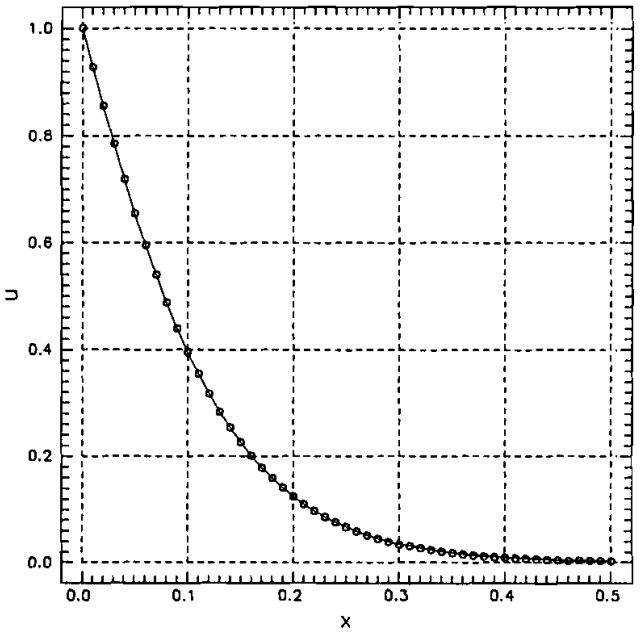

FIGURE 7 Dimensionless gas temperature profile at $t = 1$.

can be determined accordingly. These temperature profiles at $t = 1.0$ in the packed column are plotted in Figure 7.

In this example problem, the penetration depth for the gas temperature, δ is a function of time. Thus, care must be taken in introducing the transformations

$$y = \frac{x}{\delta(t)} \qquad \tau = t$$

Following the techniques suggested by Ramachandran and Duduković (1984) and replacing the spatial derivatives by differential quadratures, Eqs. (27) can be approximated by

$$\sum_{j=1}^{N} (\gamma_{ij}^{(1)})_u \frac{du_j}{d\tau} = -St\left(\frac{du_i}{d\tau} - \frac{dv_i}{d\tau}\right)\delta - St(u_i - v_i)\frac{d\delta}{d\tau}, \qquad i = 2, 3, \ldots, N-1 \quad (28a)$$

$$\frac{dv_i}{d\tau} - \frac{y_i}{\delta}\left(\frac{d\delta}{d\tau}\right)\sum_{j=1}^{N} (\gamma_{ij}^{(1)})_v v_j = u_i - v_i, \qquad i = 1, 2, \ldots, N-1 \quad (28b)$$

$$u_1 = 1 \quad (28c)$$

$$\sum_{j=1}^{N} (\gamma_{Nj}^{(1)})_u \frac{du_j}{d\tau} = 0 \quad (28d)$$

$$u_N = 0 \quad (28e)$$

$$v_N = 0 \quad (28f)$$

It is assumed in this formulation, with Eq. (28d), that there is no heat flow in the gas phase beyond the penetration depth. Since Eqs. (27) imply that the values of

TABLE IV

Average absolute errors in solutions obtained by using the modified differential Quadratures

	$P_N^{(1,0)}(x)$	$L(x)$
$t = 1.0$	0.001249	0.000956
$t = 1.5$	0.001283	0.000637
$t = 2.0$	0.000812	0.000507

u and v approaches zero at locations far away from the origin, the penetration depth δ is thus assumed to be the distance at which both u and v also equal zero. These requirements are specified in Eq. (28e) and Eq. (28f).

Two different approaches were adopted to place seven grid points in the interval $0 \leq y \leq 1$. They are the same as those applied in Example 3. An implicit Euler method with a time step of 0.01 was used to integrate Eqs. (28) from $t = 0$ to $t = 2.5$. The average absolute error of u in intervals where 99% of the change takes place at time 1, 1.5 and 2.0 are presented in Table IV.

It can be seen clearly from these data that both approaches are adequate for obtaining resonable solutions. The local errors of both cases at $t = 1$ are also compared in Figure 8. Again, the accuracy in the results generated by the

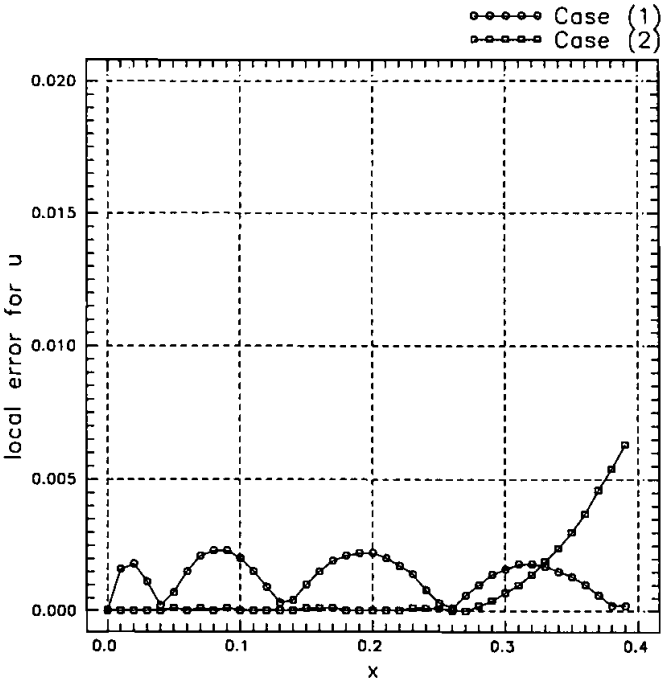

FIGURE 8 Effects of the Auxiliary Function at $t = 1$. Case (1): Jacobi Polynomials, $P_5^{(1,0)}(y)$; $r(y) = 1.0$; Scheme II Case (2): Laguerre Polynomials, $L_7^{(0)}(y)$; $r(y) = e^{-\xi y}$; Scheme I.

suggested approach is higher for almost the entire interval. The same observations can be made at any other instance.

CONCLUSIONS

Modified differential quadratures have been developed in this study to overcome the difficulties encountered in solving problems with semi-infinite domains and/or steep gradients by the conventional approach. Specifically, different forms of trial functions and various grid point placement schemes were adopted to enhance the curve-fitting ability of the quadrature method. Proper trial functions can be selected by the formal constraints proposed in this paper. Simplified formulae, corresponding to the Jacobi, Laguerre and Hermite polynomials, were derived to calculate the modified quadrature coefficients. Due to the simplicity of their forms, accurate results can be obtained efficiently even when the number of grid points is large. To improve the overall quality of the numerical solutions, the concept of "boundary layer" was introduced in solving the above problems. Reduction of the problem domain to such a finite interval forces the grid points to be distributed over the region of interest and, thus, more accurate solutions can be obtained accordingly. Note, however, that this improvement is achieved at the price of sacrificing the performance of the solutions at locations near the edge of the boundary layer. The assumptions made to determine the thickness of boundary layer makes them to be inherently less accurate than those in the rest of the interval.

The modified differential quadratures were tested with a number of example problems. Based on the data we have collected so far, it can be concluded that, on the average, the proposed approach yields better results and, in particular, more accurate solutions can be obtained in the region where most of the change in dependent variable occurs.

ACKNOWLEDGEMENT

This work is supported by the National Science Council of the Republic of China under project NSC79-0402-E006-08.

NOMENCLATURE

English Letters

b_1, b_2	the lower and upper bound of a computational field
c	the dimensionless concentration
$\mathbf{F}_n$	the nth-derivatives matrix of the trial functions
$\tilde{\mathbf{F}}_n$	the modified nth-derivatives matrix of the trial functions

f_i	the i-th trial function
$\tilde{f}_i$	the ith modified trial function
$\bar{f}_i$	the ith Lagrange interpolation function
f_R, f_S	the dimensionless concentrations of R, S
$\mathbf{G}_n$	the nth-order quadrature coefficient matrix
$\tilde{\mathbf{G}}_n$	the modified nth-order quadrature coefficient matrix
$L_N^{(0)}(x)$	the Nth-degree Laguerre polynomial with $\alpha = 0$
N	total number of grid points
$P_N^{\alpha,\beta}(x)$	the Nth-degree Jacobi polynomial
$\mathbf{R}_n$	the nth-derivative matrix of the auxiliary functions
$r(y)$	auxiliary function
s_1, s_2	the lower and upper bound of the standard interval in which an orthogonal polynomial is defined
St	the Stanton number
t	independent variable, $0 \leq t < \infty$
u	dependent variable
$\mathbf{V}_n$	the nth-derivative Vandermonde matrix
x	independent variable in a standard interval
y	independent variable in the interval $a_1 \leq y \leq a_2$

Greek Letters

Δ	local relative deviations between two numerical solutions
Φ_n	a polynomial with N real roots
δ	the thickness of boundary layer
δ_{ij}	the Kronecker delta
$\gamma_{ij}^{(n)}$	the nth-order differential-quadrature coefficients
$\tilde{\gamma}_{ij}^{(n)}$	the modified nth-order differential-quadrature coefficients
φ	a dimensionless rate constant
ϑ_i	coefficient of the i-th trial function
ζ, ξ	the parameters of an auxiliary function

REFERENCES

1. Bellman, R.E., and Adomian, G., *Partial Differential Equations*, pp. 129–147, D. Reidel Publishing Co., Holland (1985).

2. Bellman, R.E., Kashef, B., and Casti, J., "Differential quadrature: a technique for the rapid solution of nonlinear partial differential equations", *J. Comput. Physics,* **10,** 40 (1972).
3. Birnbaum, I., and Lapidus, L., "Studies in approximation method-IV" *Chem. Engng. Sci.,* **33,** 455 (1978).
4. Caban, R., and Chapman, T.W., "Solution of boundary-layer transport problems by orthogonal collocation", *Chem. Engng. Sci.* **36,** 849 (1981).
5. Chang, C.T., "Letter to the Editors", *Comput. & Chem. Engng,* **16,** in press (1992).
6. Churchill, S.W., *Viscous Flows-The Practical Use of Theory,* pp. 271–278, Butterworths, Boston (1988).
7. Finlayson, B.A., *The Method of Weighted Residuals and Variational Principles,* Academic-Press, New York (1972).
8. Finlayson, B.A., *Nonlinear Analysis in Chemical Engineering,* McGraw-Hill, New York (1980).
9. Finlayson, B.A., and Scriven, L.E., "The method of weighted residuals-a review", *Appl. Mech. Rev.,* **19,** 735 (1966).
10. Jacob, M., *Heat Transfer,* **2,** pp. 275, J. Wiley, New York (1957).
11. Michelsen, M.L., and Villadsen, J.V., "Letter to the Editors", *Comput. & Chem. Engng.,* **15,** 145 (1991).
12. Nayfeh, A.H., *Introduction to Perturbation Techniques,* pp. 257–324, Wiley, New York (1972).
13. Quan, J.R., and Chang, C.T., "New insights in solving distributed system equations by the quadrature method-I. analysis", *Comput. & Chem. Engng.,* **13,** 7, 779 (1989i).
14. Quan, J.R., and Chang, C.T., "New insights in solving distributed system equations by the quadrature method-III. numerical experiments", *Comput. & Chem. Engng.,* **13,** 9, 1017 (1989ii).
15. Ramachandran, P.A., and Dudukovi'c, M.P., "A moving finite element collocation method for transient problems with steep gradients", *Chem. Engng. Sci.* **39,** 1321 (1984).
16. Villadsen, J.V., and Michelsen, M.L., *Solution of Differential Equation Models by Polynomial Approximation,* Prentice-Hall, Englewood Cliffs, New Jersey (1978)..

APPENDIX A

To facilitate later discussions, the concept of a *family* must be defined first, i.e.

Definition A *family* of trial functions is a set of linearly independent functions, $f_i(y)$, $i = 1, 2, \ldots, N$, of which any of the functions, $f_i(y)$'s, and its derivatives with respect to y are linear combinations.

Note that a set of functions, $f_i(y)$'s, is said to be *linearly independent* over an interval, $a_1 \le y \le a_2$, if the *Wronskian* of $f_1(y), f_2(y), \ldots, f_N(y)$ is not identically zero in $a_1 \le y \le a_2$. Based on the above definition, the following theorem can be utilized to characterize the relationship between the first- and higher-order quadrature coefficients:

[*Theorem*] If a set of trial functions satisfies the requirements of a family, then

$$\mathbf{G}_n = \mathbf{G}_1^n \tag{4}$$

Proof If the trial functions, $f_i(y)$, $i = 1, 2, \ldots, N$, form a family, then

$$\frac{d\mathbf{f}(y)}{dy} = \mathbf{D}\mathbf{f}(y) \tag{A1}$$

where,

$$\mathbf{f}(y) = [f_1(y), f_2(y), \ldots, f_N(y)]^T$$

and $\mathbf{D}$ is a matrix with constant entries. Differentiate both sides of Eq. (A1) with

respect to y:

$$\frac{d^2\mathbf{f}(y)}{dy^2} = \mathbf{D}\frac{d\mathbf{f}(y)}{dy} = \mathbf{D}^2\mathbf{f}(y) \tag{A2}$$

Thus,

$$\frac{d^n\mathbf{f}(y)}{dy^n} = \mathbf{D}^n\mathbf{f}(y) \tag{A3}$$

From Eq. (A3), one can conclude that

$$\mathbf{F}_n = \left[\frac{d^n\mathbf{f}(y_1)}{dy^n}, \frac{d^n\mathbf{f}(y_2)}{dy^n}, \ldots, \frac{d^n\mathbf{f}(y_N)}{dy^n}\right] = \mathbf{D}^n[\mathbf{f}(y_1), \mathbf{f}(y_2), \ldots, \mathbf{f}(y_N)] = \mathbf{D}^n\mathbf{F}_0 \tag{A4}$$

Substitute Eq. (A4) into Eq. (3) in this paper,

$$\mathbf{G}_n^T = \mathbf{F}_0^{-1}\mathbf{F}_n = \mathbf{F}_0^{-1}\mathbf{D}^n\mathbf{F}_0 = (\mathbf{F}_0^{-1}\mathbf{D}\mathbf{F}_0)^n = (\mathbf{G}_1^T)^n \tag{A5}$$

APPENDIX B

1. The Jacobi Polynomials $(P_N^{(\alpha,\beta)}(x),\ -1 < x < 1)$

For $i \neq j$,

$$\gamma_{ij}^{(1)} = \frac{(1-x_j^2)P_{N-1}^{(\alpha,\beta)}(x_i)}{(x_i-x_j)(1-x_i^2)P_{N-1}^{(\alpha,\beta)}(x_j)} \tag{B1}$$

$$\gamma_{ij}^{(2)} = \frac{[(x_i-x_j)(\beta-\alpha-(\alpha+\beta+2)x_i)+2(1-x_i^2)](1-x_j^2)P_{N-1}^{(\alpha,\beta)}(x_i)}{(x_i-x_j)^2(1-x_i^2)^2P_{N-1}^{(\alpha,\beta)}(x_j)} \tag{B2}$$

For $i = j$,

$$\gamma_{ii}^{(1)} = \frac{(\alpha+\beta+2)x_i+\alpha-\beta}{2(1-x_i^2)} \tag{B3}$$

$$\gamma_{ii}^{(2)} = \frac{1}{3(1-x_i^2)^2}\{[\beta-\alpha-(\alpha+\beta+2)x_i]^2 + (1-x_i^2)[\alpha+\beta+2-N(N+\alpha+\beta+1)] - 2x_i[\beta-\alpha-(\alpha+\beta+2)x_i]\} \tag{B4}$$

Although these simplified formulae have already been presented in an earlier paper (Quan and Chang, 1989i), further simplifications were achieved in this study for several special cases of the Jacobi polynomials, e.g. the Chebyshev polynomials of the first kind and the second kind. Their respective quadrature coefficients can be determined by the following equations:

- *The Chebyshev Polynomials of the First Kind* $(\alpha = \beta = -\frac{1}{2})$

For $i \neq j$,

$$\gamma_{ij}^{(1)} = (-1)^{i-j}\frac{(1-x_j^2)^{1/2}}{(x_i-x_j)(1-x_i^2)^{1/2}} \tag{B5}$$

$$\gamma_{ij}^{(2)} = (-1)^{i-j}\frac{(1-x_j^2)^{1/2}[(x_i-x_j)x_i-2(1-x_i^2)]}{(x_i-x_j)^2(1-x_i^2)^{3/2}} \tag{B6}$$

For $i = j$,

$$\gamma_{ii}^{(1)} = \frac{x_i}{2(1-x_i^2)} \tag{B7}$$

$$\gamma_{ii}^{(2)} = \frac{(N^2+2)x_i^2+(1-N^2)}{3(1-x_i^2)^2} \tag{B8}$$

• *The Chebyshev Polynomials of the Second Kind* ($\alpha = \beta = \frac{1}{2}$)
For $i \neq j$,

$$\gamma_{ij}^{(1)} = (-1)^{i-j} \frac{(1 - x_j^2)}{(x_i - x_j)(1 - x_i^2)} \tag{B9}$$

$$\gamma_{ij}^{(2)} = (-1)^{i-j} \frac{(5x_i^2 - 3x_i x_j - 2)(1 - x_j^2)}{(x_i - x_j)^2 (1 - x_i^2)^2} \tag{B10}$$

For $i = j$,

$$\gamma_{ii}^{(1)} = \frac{3x_i}{2(1 - x_i)} \tag{B11}$$

$$\gamma_{ii}^{(2)} = \frac{(N^2 + 2N + 12)x_i - (N^2 + 2N - 3)}{3(1 - x_i^2)^2} \tag{B12}$$

2. The Laguerre Polynomials ($L_N^{(\alpha)}(x)$, $0 < x < \infty$)
For $i \neq j$,

$$\gamma_{ij}^{(1)} = \frac{x_j L_{N-1}^{(\alpha)}(x_i)}{x_i (x_i - x_j) L_{N-1}^{(\alpha)}(x_j)} \tag{B13}$$

$$\gamma_{ij}^{(2)} = -\frac{x_j[(x_i - x_j)(\alpha + 1 - x_i) + 2x_i] L_{N-1}^{(\alpha)}(x_i)}{x_i^2 (x_i - x_j)^2 L_{N-1}^{(\alpha)}(x_j)} \tag{B14}$$

For $i = j$,

$$\gamma_{ii}^{(1)} = -\frac{\alpha + 1 - x_i}{2x_i} \tag{B15}$$

$$\gamma_{ii}^{(2)} = \frac{(\alpha + 1 - x_i)(\alpha + 2 - x_i) - (N - 1)x_i}{3x_i^2} \tag{B16}$$

3. The Hermite Polynomials ($H_N(x)$, $-\infty < x < \infty$)
For $i \neq j$,

$$\gamma_{ij}^{(1)} = \frac{H_{N-1}(x_i)}{(x_i - x_j) H_{N-1}(x_j)} \tag{B17}$$

$$\gamma_{ij}^{(2)} = \frac{2[x_i(x_i - x_j) - 1] H_{N-1}(x_i)}{(x_i - x_j)^2 H_{N-1}(x_j)} \tag{B18}$$

For $i = j$,

$$\gamma_{ii}^{(1)} = x_i \tag{B19}$$

$$\gamma_{ii}^{(2)} = \frac{4x_i^2 - 2(N - 1)}{3} \tag{B20}$$

Note that the symbols x_i (or x_j) in the above equations represent the ith (or jth) zeros of the corresponding orthogonal polynomial defined in its standard interval.