# APPLICATION OF DIFFERENTIAL QUADRATURE TO ENGINEERING PROBLEMS

by

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ABSTRACT

Differential quadrature is a useful numerical technique for solving non-linear partial differential equations. It involves approximating the partial derivatives by a linear combination of functional values and, therefore, provides an easy method of transformation of partial differential equations into a set of ordinary differential equations. The technique is employed for solving boundary value problems which can be represented by partial differential equations.

Most other methods like the finite-difference method involve approximation in terms of functional differences instead of functional values and therefore, require functional evaluation at a large number of points for satisfactory results. It is in this respect that differential quadrature has its major advantages over other methods in terms of both, the computer storage and computational time. However, the success of the method depends largely upon the method of evaluation of weighting coefficients. Three methods are considered in this respect viz.classical quadrature analogy, Legendre polynomial approach and spline approximation.

Differential quadrature is applied to solving several models in engineering with both fixed and moving boundary conditions. A moving boundary condition is specified at a point which itself varies as a function of time. Differential

quadrature is used to solve the isothermal reactor model as well as the adiabatic reactor model. A lot of computer memory and computation time are saved by using this technique.

# CHAPTER I

# DIFFERENTIAL QUADRATURE AND SPLINE APPROXIMATION - A LITERATURE SURVEY

## 1.1 Introduction

Partial differential equations are frequently encountered in the fields of engineering and science. However, the numerical solution of time-dependent non-linear partial differential equations has been a complicated and highly problem dependent process. In general, the solution of slightly different type of partial differential equations may require separate and completely different computer programs. Thus, effective numerical technique in this respect can be very beneficial.

The conventional numerical techniques such as the method of lines, finite difference method, etc. require the function value to be evaluated at a large number of points to obtain satisfactory results. This requires a lot of computer storage and computer time and thus an increased cost and effort.

Quadrature techniques like trapezoidal rule, Simpson's rule have been used since early times to estimate the area under curves. A more common technique is that of Guassian quadrature which can provide a good approximation for integrals. This chapter deals with a recently developed numerical technique known as differential quadrature which is very much similar in principle to that of Guassian quadrature and

can be effectively used for polynomial approximation of partial differentials. The following chapters deal with some of the applications of this method in the field of engineering.

Consider the type of approximation

$$Lu = \sum_i a_i u_i \qquad (1)$$

which is known as quadrature approximation if L is an integral operator. In analogy, the same approximation was named as differential quadrature by Bellman (1) when L is an integral operator. Unlike Guassian quadrature, differential quadrature method is still at an early stage of development. The advantages of the method will be obvious after the discussion of the following chapters.

Differential quadrature method is different from most conventional methods in the sense that the interpolation is expressed in terms of the values of the function instead of the differences of the function. However, the approximation of derivatives by differences provide the basis of many methods of solving differential equations. Interpolation using functional values at certain selected points has been dropped in past due to hazards of roundoff errors, but Bellman and his coworkers has shown that the difficulty can be overcome by first smoothening the data and then differentiating. They have successfully applied the method to the solution of fluid

flow equations, the Hodgkin-Haxley model (2) and other models.

1.2 Differential Quadrature

Consider a linear or non-linear first order partial differential equation of the form

$$U_t = f(t, x, U, U_x) \qquad (2)$$

where x lies in the finite interval (a,b) and the boundary conditions of the problem are in any given form. The initial condition is assumed to be known and is of the form

$$U(o,x) = U^o(x) \qquad (3)$$

Assuming the function U to be sufficiently smooth in the interval (a,b) we can write the following approximate solution (3)

$$U_x(t, x_i) = \sum a_{ij} U(t,x_j), \quad = 1, 2, \ldots ;N \qquad (4)$$

where, N is the number of mesh points selected and $a_{ij}$ is the matrix of weighting coefficients of order NXN. N is also known as the order of differential quadrature method. Substituting equation (4) into equation (2), we get,

$$U(t,x_i) = f(t,x_i, U(t,x_i), \sum_{j=1}^{N} a_{ij} U(t,x_j)),$$

$$i = 1, 2, \ldots ;N \qquad (5)$$

which is a set of N ordinary differential equations with initial conditions

$$U(0,x_i) = U^o(x_i), \; i = 1, 2, \ldots ;N \qquad (6)$$

Thus, the solution of equation (2) can be obtained by solving the set of ordinary differential equations (5) with initial condition (6). The boundary conditions for eqn.(2) can be reduced to a set of algebric equations by using approximation (2) and the result can be used in order to eliminate two of the N variables, $U(t,x_i)$, i=1, 2, .....,N in equations (5). Thus, the solution is obtained by solving the (N-2) ordinary differential equations and the remaining two functional values can, therefore, be evaluated using the boundary conditions of the problem.

For approximation of higher order methods, the same idea can be extended. Considering equation (2) as a linear transformation of U, we can write

$$U_x = AU \tag{7}$$

Then, the second order derivatives can be approximated as

$$U_{xx} = (U_x)_x = A\,(AU) = A^2U \tag{8}$$

The higher order derivatives can similarly be found by iterating the linear transformation A. Writing equation (8) in the sense of equation (4), we have,

$$U_{xx}(t,x_i) = \sum_{k=1}^{N} \sum_{j=1}^{N} a_{ik}\, a_{kj}\, U_j\,(t),$$

$$i = 1, 2, ....,N \tag{9}$$

Similarly,

$$U_{xxx}(t,x_i) = \sum_{i=1}^{N} \sum_{k=1}^{N} \sum_{j=1}^{N} a_{il}\, a_{lk}\, a_{kj}\, U_j(t),$$

$$i = 1, 2, ....,N \tag{10}$$

and so on.

Therefore, it can be seen that success of differential quadrature method depends largely upon the values of weighting coefficients $a_{ij}$'s. The method which have been used in the past by Bellman and his coworkers (4,5,6) are discussed in the next section.

## 1.3 Determination of Weighting Coefficients $a_{ij}$'s

### 1.3.1 By analogy with the classical quadrature case

The coefficients $a_{ij}$'s in the approximation,

$$U_x(x_i) = \sum_{j=1}^{N} a_{ij} U(x_i), \quad i = 1, 2, \ldots, N \tag{11}$$

can be easily determined by analogy with the classical quadrature case which demands that equation (2) be exact for all polynomials of degree less than or equal to (N-1). Considering the test function,

$$g_k(x) = x^k, \qquad k = 1, 2, \ldots, N \tag{12}$$

For arbitrary points $x_i$, i=1, 2, . . . . ,N this leads to a set of linear algebric equations

$$\sum_{j=1}^{N} a_{ij} x_j^{k-1} = (k-1) x_i^{k-1}, \quad k = 1, 2, \ldots, N, \quad i = 1, 2, \ldots, N \tag{13}$$

Thus, choosing N and $x_i$, i = 1, 2, . . . . ,N the values of the weighting coefficients $a_{ij}$'s can be uniquely determined.

1.3.2 By analogy with Lagrange's interpolation formula

Instead of solving a set of algebric equations in the previous case, the coefficients $a_{ij}$'s can also be determined by properly selecting $x_i$'s i.e. if we consider x to be the root of shifted Lagendre polynomial of degree N, $P_N^*(x)$ with orthogonality range of (0,1), the legendre polynomial $P_N^*(x)$ being defined as

$$P_N^*(x) = P_N(1-2x) \tag{14}$$

By analogy with lagrange's interpolation formula the trial function is taken of the form,

$$\mathcal{E}_k(x) = P_N^*(x) \Big/ \left[(x-x_k)\, P_N^{*\prime}(x_k)\right] \tag{15}$$

Since $P_N^*(x)$ is a polynomial of degree N, $\mathcal{E}_k(x)$ will be a polynomial of degree (N-1) such that

$$\mathcal{E}_k(x_j) = \mathcal{E}_{kj}, \quad \begin{matrix} k = 1, 2, \ldots, N \\ j = 1, 2, \ldots, N \end{matrix} \tag{16}$$

Assuming that the equation,

$$U_x(x_i) = \sum_{j=i}^{N} a_{ij}\, U(x_j), \quad i = 1, 2, \ldots, N \tag{17}$$

is exact for $U(x)=\mathcal{E}_k(x)$, we have

$$a_{ik} = \frac{P_N^{*\prime}(x_k)}{(x_i - x_k)\, P_N^*(x_k)} \tag{18}$$

For i=k we use the L'Hospital rule and the fact that $P_N^*(x)$ satifies the differential equation

$$x(1-x^2)P_N^{*''}(x) + (1+2x)P_N^{*'}(x) + N(N-1)P_N^{*}(x) = 0 \qquad (19)$$

which gives,

$$a_{mm} = (1-2x_m) \Big/ [2x_m(x_m-1)] \qquad (20)$$

Thus the weighting coefficients $a_{ij}$'s can be calculated by equation (18) and (20).

A better approach to the determination of weighting coefficients is given by smoothening the data. Spline approximation is one of the best methods in this respect. It is discussed in the following section.

## 1.4 Spline Approximation

### 1.4.1 Introduction

A spline in its simplest form can be understood from analogy with a draftsman spline which is a thin strip of wood or some other material used for fitting smooth curves passing through certain points. These splines are anchored in place by applying lead weights called "ducks" at points along the spline and the spline can thus be made to pass through certain points by adjusting the position of these weights. Regarding this spline as a simple beam, the Bernoulli-Euler law can be stated as

$$M(x) = \frac{EI}{R(x)} \qquad (21)$$

where,

M(x) is the bending moment; E is the Young's modulus for the material of the beam; I is the geometric moment of inertia which depends on the dimensions of the beam and R(x) is the radius of curvature for the curve formed. Assuming small deflection

$$R(x) = \frac{1}{y''(x)} \qquad (22)$$

where, y(x) denotes the beam elastica.

In analogy, the definition of a mathematical spline can be stated in the words of Ahlberg, Nelson and Walsh (7) as follows:

> "The mathematical spline is the result of replacing the draftman's spline by its elastica and approximating the latter by a piecewise cubic (normally a different cubic between each pair of adjacent ducks) with certain discountinuities of derivatives permitted at the junction points (the ducks where two cubic join)".

A mathematical spline is continuous and has a continuous first derivative as well as a continuous second derivative. Thus, spline interpolating functions are a class of piecewise interpolating polynomial functions satisfying certain continuity properities at the interpolating points. The idea of spline approximation was first pointed out in 1946 by Schoenberg (8). In 1949, Sard (9) generalised the classical approach by means of searching the best approximating function

of order M, where $1 \leq M \leq N$ such that equation (1) is exact for polynomials of degree (M-1) or less. He then fixed the (N-M) degrees of freedom in determining the coefficients by effectively requiring that

$$\int_a^b U^{M}(x)^2 \, dx = \text{minimum} \qquad (23)$$

where, $U^{M}(x)$ is the $M^{th}$ derivative of the approximating function. Schoenberg (8) proved among other properties that the spline interpolation formula is the "Best" interpolation formula in the sense of Sard.

The simplest kind of spline function for interpolation is the cubic spline. It has already proved to be of great use in approximation theory and system identification. Its properties are discussed in (7). The concept is extended to curves that are composed of segments of polynomials curves of an arbitrary degree and the spline function so fitted are known as polynomial splines. The theory has also been applied to approximation in two dimensions. For the purpose of present discussion we will only consider the spline approximation as applied to differential quadrature method.

1.4.2 Natural Splines

This is a subclass of splines used by Bellman, Kashef and Vasudevan (3) for the evaluation of weighting coefficients in equation (4). Natural spline of degree (2M-1) is defined

by the following condition.

i) S is a polynomial of degree 2M-1 in each interval $(x_i, x_{i+1})$, $i = 1, 2, \ldots, N-1$.

ii) S is a polynomial of degree M-1 outside the region (a,b).

This is the boundary condition requirement.

iii) $S, S', \ldots, S^{(2M-2)}$ are continuous at $x_1, x_2, \ldots, x_N$

iv) $S(x_i) = u(x_i)$ for $i=1, 2, \ldots, N$.

An equivalent definition in the sense of Schoenberg is given by

i) $\int_a^b S^M(x)^2 dx$ exists and is minimised subject to the following two conditions.

ii) $S, S^1, \ldots, S^{(M-1)}$ are continuous in (a,b)

iii) $S(x_i) = u(x_i)$, $i=1, 2, \ldots, N$

Both the above definitions of spline uniquely specify function S(x) on the interval (a,b). As can be seen these functions have strong convergence properties and for this reason, these can be effectively employed in the approximate process of interpolation, integration and differentiation.

1.4.3 Cardinal Spline

Cardinal spline is also called "fundamental spline" and is a spline for which exactly one defining value is one and all others are zero i.e. cardinal spline is a natural spline function with the interpolating conditions,

$$C_i(x_j) = \delta_{ij} , \quad i = 1, 2, \ldots , N \qquad (24)$$

consider cubic spline and M=2, then the natural spline function S(x) which interpolates u(x) can be expressed as

$$S(x) = \sum_{i=1}^{N} U(x_i)\, C_i(x) \qquad (25)$$

The arbitrary function U(x) can be approximated as

$$U(x) = \sum_{i=1}^{N} U(x_i)\, C_i(x) \qquad (26)$$

Now, by operating with L on the function S(x) of equation (25), we get

$$L\, S(x) = L \sum_{i=1}^{N} U(x_i)\, C_i(x) \qquad (27)$$

Since $U(x_i)$ is given for a particular value of $x_i$, the operator L can be taken inside the summation and therefore, eq$^n$(27) can be written as

$$L\, S(x) = \sum_{i=1}^{N} U(x_i) L\, C_i(x)$$

$$= \sum_{i=1}^{N} (LC_i(x))\, U(x_i) \qquad (28)$$

comparing equation (28) with equation (1),

$$A_i(x) = L\, C_i(x) \qquad (29)$$

The procedure can be applied to determine the weighting coefficients of differential quadrature method as follows:

1.4.4 Computational Scheme for Weighting Coefficients $a_{ij}$'s

The complete set of cardinal splines which span the

whole space depends on the boundary conditions of the problem. Let us assume that the boundary conditions of the problem under consideration are known in the form

$$\frac{\partial U(x)}{\partial x}\Big|_{x=x_1} = b_1 \tag{30}$$

and,

$$\frac{\partial U(x)}{\partial x}\Big|_{x=x_N} = b_2 \tag{31}$$

where the function U(x) is approximated at the points $x_1$, $x_2$, ....., $x_N$ using the approximation

$$\frac{\partial U(x_i)}{\partial x} \cong \sum_{j=1}^{N} a_{ij}\, U(x_j), \quad i = 1, 2, \ldots, N \tag{32}$$

Defining a vector Y as

$$\underset{\sim}{Y} = (U_1', U_1, U_2, \ldots, U_N, U_N') \tag{33}$$

where,

$$U_1' = \frac{U(x)}{x}\Big|_{x=x_1} \tag{34}$$

$$U_N' = \frac{U(x)}{x}\Big|_{x=x_N} \tag{35}$$

Then, the (N+2) cardinal splines which completely span the space are given as

$$C_i(x_j) = \delta_{ij}\ ; \qquad C_i'(x_1) = C_2'(x_N) = 0$$

$$C_o(x_j) = 0\ ; \qquad C_o'(x_j) = \delta_{ij}$$

$$C_{N+j}(x_j) = 0\ ; \qquad C_{N+1}'(x_j) = \delta_{Nj}$$

for $i = 1, 2, \ldots, N$

$j = 1, 2, \ldots, N$ (36)

where $\delta_{ij}$ is the kronoker delta defined as

$$\delta_{ij} = 1 \quad \text{for } i=j \tag{37}$$

$$0=0 \quad \text{otherwise}$$

The spline interpolating function here is

$$S(x) = \sum_{i=1}^{N} U(x_i)\, C_i(x) + U_1'\, C_0(x) + U_2'\, C_{N+1}(x) \tag{38}$$

Representing the N+2 elements of Y as $Y_i$'s, i= 0, 1, 2, . . . . ,N+1 and considering the N+2 cardinal splines as $C_i(x)$, i=0, 1, . . . . N+1 equation (38) can be written as

$$S(x) = \sum_{i=1}^{N+1} Y_i\, C_i(x) \tag{39}$$

Now, operating S(x) by L, we get

$$LS(x) = \sum_{i=0}^{N+1} \left[ LC_i(x) \right] Y_i \tag{40}$$

comparison of equation (40) with equation (4) gives

$$a_{ij} = \left[ LC_i(x) \right]_{x=x_j} \quad i,j=0, 1, 2, . . . . ,N+1 \tag{41}$$

Similarly, if the boundary conditions are defined as

$$\frac{\partial^2 U(x)}{\partial x^2} \Big|_{x=x_0} = B_1 \tag{42}$$

$$\frac{\partial^2 U(x)}{\partial x^2} \Big|_{x=x_N} = B_2 \tag{43}$$

the complete set of cardinal splines over the whole space can be defined as

$$C_i(x_i) = \delta_{ij} \; ; \qquad C_i''(x_i) = C_i''(x_N) = 0$$

$$C_o(x_j) = 0 \quad ; \qquad C_o''(x_j) = \delta_{ij}$$

$$C_{N+1}(x_j) = 0 \quad ; \qquad C''_{N+1}(x_j) = \delta_{Nj}$$

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

$$j = 1, 2, \ldots, N \qquad (44)$$

The weighting coefficients can be determined in a similar way as in the case of first order derivatives.

1.4.5 Construction of cubic spline using raw data

A cubic spline in the interval (0,1) is constructed by considering the N+1 mesh points $x_0, x_1, \ldots\ldots, x_N$ in the interval (0,1) such that

$$0 = x_0 < x_1 < x_2 < \ldots\ldots < x_N = b \qquad (45)$$

with each value of $x_1$ is associated a data point $y_i$ which is assumed to be given or known. Then the spline S(x) with respect to interval 0 to b should have the following properties

i) S (x) is continuous, together with its first and second derivatives on $(0 \leq x \leq b)$

ii) S (x) is cubic polynomial within each subinterval

$x_{i-1} < x < x_1$, i=1, 2, . . . . ,N

Analytically, the spline can be represented over each sub-interval $(x_{i-1}, x_i)$ as

$$S''(x) = M_{i-1} \frac{(x_i - x)}{h_i} + M_i \frac{(x - x_{i-1})}{h_i} \qquad (46)$$

Integrating equation (46) twice and evaluating the

constants of integration, we obtain

$$S(x)=M_{i-1}\frac{(x_i-x)^3}{6h_i}+M_i\frac{(x-x_{i-1})^3}{6h_i}+\left(y_{i-1}-\frac{M_{i-1}h_i^2}{6}\right)\frac{(x_i-x)}{h_i}$$

$$+\left(y_i-\frac{M_ih_i^2}{6}\right)\frac{(x-x_{i-1})}{h_i} \qquad (47)$$

From equation (46) and (47), it can be seen that S (x) and S" (x) are continuous on (0,b). The continuity of S (x) at $x_i$ requires

$$\frac{h_i}{6}M_{i-1}+\frac{h_i+h_{i+1}}{3}M_i+\frac{h_{i+1}}{6}M_{i+1}=\frac{y_{i+1}-y_i}{h_{i+1}}-\frac{y_i-y_{i-1}}{h_i} \qquad (48)$$

1.4.5.1 Computational Scheme

From equation (47), it is clear that calculation of spline S(x) requires the calculation of moments $M_i(x)$, i=0, 1, 2, . . . . ,N. This is carried out as follows.

Step 1. Define and Calculate the following parameters.

$$C_i=\frac{h_{i+1}}{h_i+h_{i+1}}$$

$$a_i=1-C_i$$

$$d_i=\frac{6[(y_{i+1}-y_i)/h_{i+1}-(y_i-y_{i-1})/h_i]}{h_i+h_{i+1}}$$

$$i=0, 1, 2, . . . . ,N \qquad (49)$$

Step 2. Initialize $Q_0=0, U_0=0$ (50)

Step 3. Let $P_k = 2 + a_k \cdot Q_{k-1}$

then calculate $Q_k = -c_k / P_k$ , $k = 1, 2, \ldots, N$ (51)

and $U_k = \dfrac{d_k - a_k U_{k-1}}{P_k}$, $k = 1, 2, \ldots, N$ (52)

Step 4. The moments $M_i$ can then be calculated using the following equations:

$$M_N = \frac{d_N - a_N U_{N-1}}{2 + a_N Q_{N-1}}$$

$$M_k = Q_k M_{k+1} + U_k , \quad k = N-1, \ldots, 2, 1$$

$$M_0 = \frac{(d_0 - c_0 M_1)}{2} \qquad (53)$$

Thus, the spline can be determined using equation (47). Theoretical discussion for the above algorithm is given in (7) and (10).

## 1.5 Concluding Remarks

Differential Quadrature method could prove to be a very useful tool for the solution of non-linear partial differential equations since it provides approximation to partial derivatives in terms of functional values. Moreover, it provides a simpler way of conversion of partial differential equations to ordinary differential equations. In most of the cases boundary conditions are reducible to simple algebraic equations. The method is applied to the solution

of packed bed reactor problems as well as to a simple case of moving boundary value problem. The results are discussed in the following chapters. For the evaluation of weighting coefficients, the method of splines approximation was found to be too involved in mathematics and could not be experimented with in the present study. Therefore, the weighting coefficient for the differential quadrature approximation are evaluated using the analogy with the classical quadrature case.

## CHAPTER II

## DIFFERENTIAL QUADRATURE AND THE ISOTHERMAL REACTOR WITH AXIAL MIXING

### 2.1 Introduction

To illustrate the method of previous chapter, let us consider the case of a chemical reactor, tubular in form and which is filled with a packing material. Such a reactor is called a fixed bed reactor. The transient reaction taking place inside the reactor is of the form

$$A + A \longrightarrow 2B \tag{1}$$

For the sake of simplicity, we consider the case of an isothermal reactor only in this chapter. The equations for the adiabatic case will be dealt with in the following chapter. Assuming that the packing material has no influence on the reaction taking place inside the reactor except its contribution to the axial mixing. The transient equations for this type of reactor can be given as

$$\frac{1}{N_{Pe}} \frac{\partial^2 p}{\partial z^2} - \frac{\partial p}{\partial z} - r p^2 = \frac{\partial p}{\partial t} \tag{2}$$

where p is the partial pressure of reactant A in the interstitial fluid; z is the dimensionless reactor length; t is the dimensionless time, and $N_{Pe}$ and r are the peclet group and the reactor rate group respectively defined as follows

$$N_{Pe} = \frac{Dv}{D} \tag{3}$$

$$r = \frac{k\ Dp}{v} \tag{4}$$

$$Z = \frac{x}{Dp} \tag{5}$$

$$t = \theta\ \frac{v}{Dp} \tag{6}$$

where Dp is the average diameter of the packing particle v is the average interstitial velocity, D and k are respectively the effective axial diffusion constant and the chemical rate constant, and x and $\theta$ being the reactor length variable and time variable respectively. The boundary conditions for p(z,t) are

$$P_e = P(o,t) - \frac{1}{N_{Pe}}\ \frac{\partial P}{\partial Z}, \quad a^t\ Z = 0,\ t > 0 \tag{7}$$

$$\frac{\partial P}{\partial Z} = 0 \qquad a^t\ Z = Z_f,\ t > 0 \tag{8}$$

where $z_f$ is the total dimensionless length of the reactor and $P_e$ is the concentration of A before entering the reactor. The initial condition for p(z,t) is

$$p(z,0) = p^o, \quad a^t\ t=0,\ 0 < z < z_f \tag{9}$$

The above problem was solved by Lee (15) using the generalized Newton-Raphson method. The same numerical data was used in the present context for the sake of comparison of results.

2.2 Differential Quadrature approximation:

Using approximation (1) and (2) of Chapter I, the partial derivatives of p can be represented as

$$\frac{\partial P_i(t)}{\partial Z} = \sum_{j=1}^{N} a_{ij} P_j(t), \text{ for } i = 1, 2, \ldots, N \tag{10}$$

Where N is the number of selected points $Z_1 Z_2, \ldots, Z_N$ and $a_{ij}$'s are the weighting coefficients and the notation $P_j(t)$ refers to the function 1 value of $p(Z,t)$ at $Z=Z_j$. Similarly, for the second order derivatives of p

$$\frac{\partial^2 P_i(t)}{\partial Z^2} = \sum_{k=1}^{N} \sum_{j=1}^{N} a_{ik} a_{kj} P_j(t), \quad i = 1, 2, \ldots, N \tag{11}$$

Using (10) and (11), equation (2) becomes

$$\frac{1}{N_{Pe}} \sum_{k=1}^{N} \sum_{j=1}^{N} a_{ij} a_{kj} P_j(t) - \sum_{j=1}^{N} a_{ij} P_j(t) - r P_i^2(t)$$

$$= \frac{d P_i(t)}{dt}, \quad i = 1, 2, \ldots, N \tag{12}$$

If the points $Z_1, Z_2, \ldots, Z_N$ are so selected that $Z_1=0$ and $Z_N=Z_f$ the boundary conditions (7) and (8) can be represented as

$$Pe = P_j(t) - \frac{1}{N_{Pe}} \sum_{j=1}^{N} a_{ij} P_j(t), \quad Z=Z_1=0, \; t>0 \tag{13}$$

$$\sum_{j=1}^{N} a_{Nj} P_j(t) = 0, \quad Z=Z_N=Z_f, \quad t > 0 \tag{14}$$

and, the initial condition is

$$P_i(o) = P_i^{\,o}, \quad i = 1, 2, \ldots, N \tag{15}$$

Equation (12) represents a set of N ordinary differential equations in N variables $P_1(t), P_2(2), \ldots, P_N(t)$ subject to the boundary conditions (13) and (14) and the

initial condition given by equation (15). Equations (13) and (14) are ordinary algebraic equations in N variables and therefore, can be solved simultaneously for two variables say, $P_1(t)$ and $P_2(t)$ in terms of other (N-2) variables i.e. using (13) and (14), we can obtain

$$P_1(t) = f_1(t, P_3, P_4, \ldots, P_N) \qquad (16)$$

$$P_2(t) = f_2(t, P_3, P_4, \ldots, P_N) \qquad (17)$$

Substituting equations (16) and (17) into equation (12), we can obtain a set of (N-2) ordinary differential equations in (N-2) variables

$$\frac{dP_i(t)}{dt} = f_i(t, P_3, P_4, \ldots, P_N) \qquad i = 3, 4, \ldots, N \qquad (18)$$

Equations (18) can be solved with the given initial conditions (15). Fourth order Range-Kutta method was used for this purpose in the present analysis.

2.3 Computational Procedure

Step 1. Select N appropriate points between 0 and $Z_f$ representing the values of $Z_1, Z_2, \ldots, Z_N$ such that $Z_1=0$, $Z_N=Z_f$.

Step 2. Calculate the weighting coefficients $a_{ij}$'s by solving the set of algebraic equations

$$\sum_{j=1}^{N} Z_j^{k-1} a_{ij} = (k-i) Z_1^{k-2}, \quad k = 1, 2, \ldots, N \quad i = 1, 2, \ldots, N \qquad (19)$$

Step 3. To start, let t = 0. Initialize $P_1$, $P_2$, . . . . ,$P_N$ using equations (15). Let k = 1.

Step 4. Set $t_k=t_{k-1}+\Delta t$. Solve equations (13) and (14) for $P_1(1)$ and $P_2(t)$ using the values of $P_3(t)$, $P_4(t)$, . . . . , $P_N(t)$.

Step 5. Calculate the co-efficients for Range-Kutta method as

$$m_{i1} = f_i(P_3(t_1),\ P_4(t_k),\ \ldots,P_N(t_k))$$

$$m_{i2} = f_i(P_3(t_k) + \tfrac{1}{2}m_{31},\ P_4(t_k) + \tfrac{1}{2}m_{41},\ \ldots,\ P_N(t_k)+\tfrac{1}{2}m_{N1})$$

$$m_{i3} = f_i(P_3(t_k)+\tfrac{1}{2}m_{32},\ P_4(t_k)+\tfrac{1}{2}m_{42},\ \ldots,P_N(t_k)+\tfrac{1}{2}m_{N2})$$

$$m_{i4} = f_i(P_3(t_k)+m_{33},\ P_4(t_k)+m_{43},\ \ldots,P_N(t_k)+m_{N3})$$

$$i = 3, 4, \ldots, N \qquad (20)$$

Step 6. $$P_i(t_k)=P_i(t_{k-1})+\frac{1}{6}(m_{i1}+2m_{i2}+2m_{i3}+m_{i4}),$$

$$i = 3, 4, \ldots, N \qquad (21)$$

Step 7. Set k=k+1. and repeat step 4 through 7 til a steady state is reached.

2.4 Numerical Results

The following numerical data was used for the problem

$P_e = 0.07$ ; $Z_f = 48$

$N_{Pe} = 20$ ; $t_f = 80$

$r = 1.0$ ; $P_i(o) = P_i^{\,o} = 0$

$$t = 0.2 \; ; \qquad i = 1, 2, \ldots, N$$

Three different experiments were conducted using $7^{th}$, $9^{th}$, and $11^{th}$ order differential quadrature approximation. The assumed points for the three cases are as follows:

a)N=7; $Z_1=0$, $Z_2=5$, $Z_3=10$, $Z_4=20$, $Z_5=30$, $Z_6=40$, $Z_7=48$

b)N=9; $Z_1=0$, $Z_2=2$, $Z_3=5$, $Z_4=6$, $Z_5=10$, $Z_6=20$, $Z_7=30$, $Z_8=40$, $Z_9=48$

c)N=11; $Z_1=0$, $Z_2=2$, $Z_3=5$, $Z_4=6$, $Z_5=8$, $Z_6=10$, $Z_7=15$, $Z_8=20$, $Z_9=30$, $Z_{10}=40$, $Z_{11}=48$

The results from the experiments are shown in tables 2.1, 2.2,2.3 for cases (a), (b) and (c) respectively. Figures 2.1, 2.2, and 2.3 show the respective plots of partial pressure in the reactor versus the dimensionless reactor length. The results of the finite difference method (20) are plotted in figure 2.4.

## 2.5 Discussion

As may be seen, the results from the differential quadrature method are quite encouraging. The results from the seventh order differential quadrature approximation differ slightly from those of finite difference method but those from differential quadrature method of order 9 very closely agree with the results of the finite difference method. However, finite difference method requires functional evaluation

for about 480 different points. Thus, besides the simplicity of differential quadrature method, major advantage is obtained in computation time which is much less than that required by finite difference method. Only about half a minute of computation time is required by $9^{th}$ order differential quadrature. The result from the $11^{th}$ order method are similar to those from $9^{th}$ order but required more computation time. Moreover, instability problems arises with higher order methods. Thus, it can be concluded that differential quadrature of order 9 is good enough for the solution of the model of Isothermal Reactor model with axial mixing.

Table 2.1

Isothermal Reactor with axial mixing by 7th order Differential Quadrature

| T | P(t,0) | P(t,5) | P(t,10) | P(t,20) | P(t,30) | P(t,40) | P(t,48) |
|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 0.0651 | 0.0280 | 0.0094 | -0.0003 | 0.0001 | -0.0000 | 0.0000 |
| 10 | 0.0679 | 0.0451 | 0.0241 | 0.0024 | -0.0003 | 0.0001 | -0.0000 |
| 20 | 0.0687 | 0.0568 | 0.0447 | 0.0197 | 0.0034 | -0.0003 | 0.0000 |
| 30 | 0.0675 | 0.0502 | 0.0420 | 0.0308 | 0.0166 | 0.0039 | -0.0000 |
| 40 | 0.0625 | 0.0292 | 0.0319 | 0.0315 | 0.0222 | 0.0158 | 0.0030 |
| 50 | 0.0488 | -0.0401 | -0.0149 | 0.0283 | 0.0208 | 0.0219 | 0.0095 |
| 60 | -0.0026 | -0.3410 | -0.2712 | -0.0229 | 0.0196 | 0.0199 | 0.0142 |

Table 2.2

Isothermal Reactor with Axial Mixing by $9^{th}$ order Differential Quadrature

| t | P(t,0) | P(t,2) | P(t,5) | P(t,6) | P(t,10) | P(t,20) | P(t,30) | P(t,40) | P(t,48) |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 0.0681 | 0.0535 | 0.0256 | 0.0181 | 0.0021 | 0.0009 | -0.0011 | 0.0012 | -0.0007 |
| 10 | 0.0688 | 0.0644 | 0.0536 | 0.0484 | 0.0245 | -0.0008 | 0.0009 | -0.0010 | 0.0006 |
| 20 | 0.0683 | 0.0604 | 0.0496 | 0.0470 | 0.0405 | 0.0206 | -0.0003 | 0.0015 | -0.0008 |
| 30 | 0.0675 | 0.0594 | 0.0517 | 0.0496 | 0.0419 | 0.0288 | 0.0168 | 0.0011 | 0.0002 |
| 40 | 0.0679 | 0.0604 | 0.0513 | 0.0488 | 0.0408 | 0.0298 | 0.0222 | 0.0144 | 0.0019 |
| 50 | 0.0675 | 0.0591 | 0.0506 | 0.0484 | 0.0411 | 0.0297 | 0.0222 | 0.0202 | 0.0091 |
| 60 | 0.0676 | 0.0594 | 0.0506 | 0.0483 | 0.0406 | 0.0297 | 0.0222 | 0.0200 | 0.0136 |
| 70 | 0.0677 | 0.0597 | 0.0509 | 0.0485 | 0.0408 | 0.0294 | 0.0225 | 0.0194 | 0.0149 |
| 80 | 0.0677 | 0.0598 | 0.0510 | 0.0487 | 0.0410 | 0.0294 | 0.0225 | 0.0192 | 0.0151 |

Table 2.3

Isothermal Reactor with Axial Mixing by $11^{th}$ order Differential Quadrature

| t | p(t,0) | p(t,2) | p(t,5) | p(t,6) | p(t,8) | p(t,10) | p(t,15) | p(t,20) | p(t,30) | p(t,40) | p(t,48) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 0.0724 | 0.0619 | 0.0259 | 0.0170 | 0.0059 | 0.0014 | -0.0000 | 0.0000 | -0.0016 | 0.0055 | -0.0055 |
| 10 | 0.0634 | 0.0533 | 0.0530 | 0.0500 | 0.0392 | 0.0255 | 0.0034 | 0.0003 | 0.0006 | -0.0042 | 0.0031 |
| 20 | 0.0655 | 0.0591 | 0.0560 | 0.0531 | 0.0462 | 0.0402 | 0.0322 | 0.0203 | 0.0031 | -0.0097 | 0.0080 |
| 30 | 0.0688 | 0.0652 | 0.0549 | 0.0508 | 0.0437 | 0.0392 | 0.0347 | 0.0292 | 0.0184 | -0.0049 | 0.0052 |
| 40 | 0.0701 | 0.0653 | 0.0516 | 0.0478 | 0.0427 | 0.0400 | 0.0351 | 0.0291 | 0.0230 | 0.0138 | 0.0008 |
| 50 | 0.0694 | 0.0619 | 0.0494 | 0.0468 | 0.0434 | 0.0411 | 0.0347 | 0.0291 | 0.0219 | 0.0224 | 0.0049 |
| 60 | 0.0680 | 0.0588 | 0.0493 | 0.0474 | 0.0446 | 0.0418 | 0.0343 | 0.0293 | 0.0216 | 0.0227 | 0.0087 |
| 70 | 0.0670 | 0.0577 | 0.0504 | 0.0487 | 0.0454 | 0.0418 | 0.0340 | 0.0295 | 0.0221 | 0.0204 | 0.0118 |
| 80 | 0.0670 | 0.0585 | 0.0517 | 0.0496 | 0.0454 | 0.0414 | 0.0341 | 0.0296 | 0.0228 | 0.0183 | 0.0142 |

Isothermal Reactor with Axial Mixing by $7^{th}$ order Differential Quadrature

$Z_i$=(0,5,10,20,30,40,48)

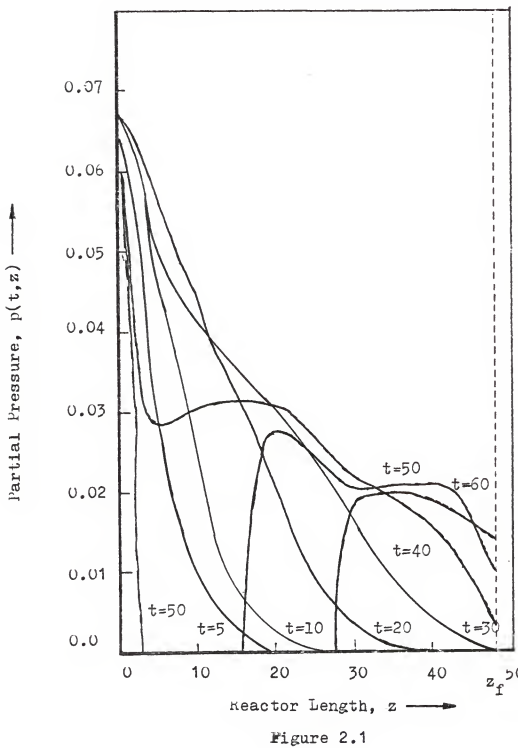


Figure 2.1

Isothermal Reactor with Axial Mixing by 9$^{th}$ order Differential Quadrature

$Z_i$=(0,2,5,6,10,20,30,40,48)

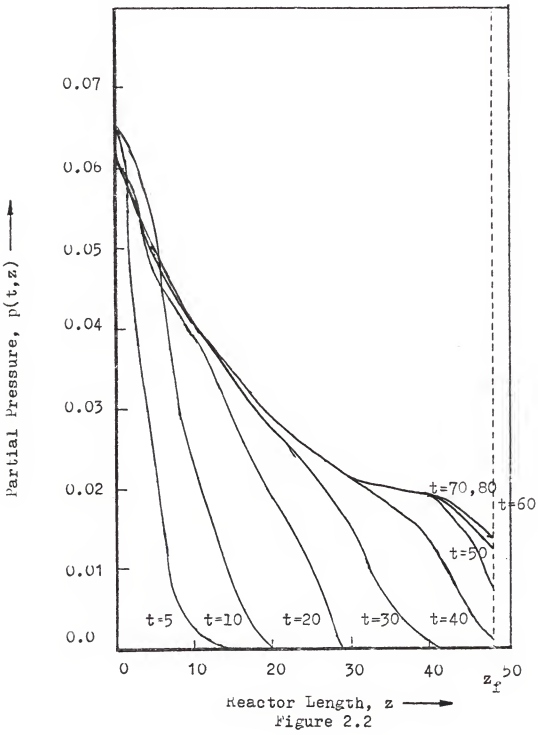


Figure 2.2

Isothermal Reactor with Axial Mixing by $11^{th}$ order Differential Quadrature

$Z_i$=(0,2,5,6,8,10,15,20,30,40,48)

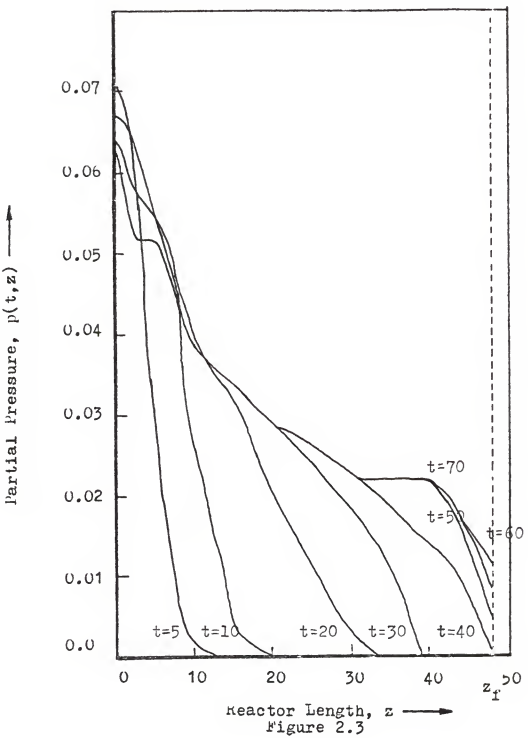


Figure 2.3

Isothermal Reactor with Axial Mixing by
Finite-Difference Method

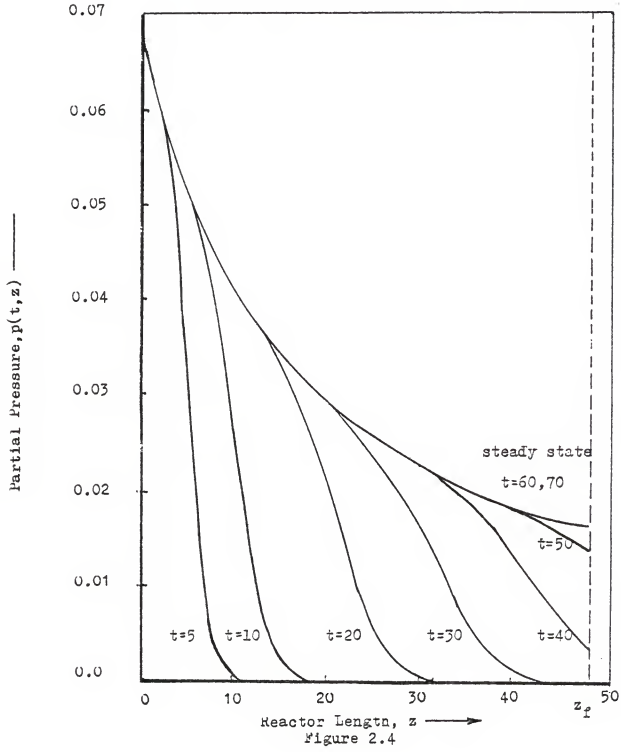


Figure 2.4

## CHAPTER III

## DIFFERENTIAL QUADRATURE AND THE ADIABATIC REACTOR WITH AXIAL MIXING

### 3.1 Introduction

A more general case of packed bed reactor is the one where energy balance is also the criterion in addition to mass balance. Such is the case of an adiabatic reactor with axial mixing. The differential quadrature method of Chapter I proved to be an effective tool to solve this problem for steady state like in the case of an isothermal reactor. Assuming the same chemical reaction and the same role of the packing material as in the case of an isothermal reactor, the equations representing the dynamics of an adiabatic reactor with axial mixing can be given as follows

$$\frac{1}{N_{Pe}} \frac{\partial^2 P}{\partial Z^2} - \frac{\partial P}{\partial Z} - r_o P^2 \exp\left(-\frac{E}{RT}\right) = \frac{\partial P}{\partial t} \qquad (1)$$

$$\frac{1}{N_{Pe}} \frac{\partial^2 T}{\partial Z^2} - \frac{\partial T}{\partial Z} + Q\, r_o P^2 \exp(-E/RT) = \frac{\partial T}{\partial t} \qquad (2)$$

where,

$$r_o = \frac{DP\, k_o}{v} \qquad (3)$$

$$Q = \frac{H}{c_f P_f} \qquad (4)$$

$k_o$ frequency factor constant in the Arrhenious equation.

$\Delta H$ Heat of the reaction.

$c_f$ Specific heat of the reaction mixture.

$\rho_f$ Density of the reaction mixture.

Other variables have the same meaning as in the case of the isothermal reactor. The mas axial diffusion co-efficient is assumed to be equal to the thermal axial diffusion constant. The boundary conditions for equation (1) and equation (2) are respectively,

$$P_e = P(0,t) - \frac{1}{N_{Pe}} \frac{\partial P}{\partial Z}, \text{ at } Z=0,\ t>0 \qquad (5)$$

$$\frac{\partial P}{\partial Z} = 0 \quad \text{at } Z=Z_f,\ t>0 \qquad (6)$$

and,

$$T_e = T(0,t) - \frac{1}{N_{Pe}} \frac{\partial T}{\partial Z}, \text{ at } Z=0,\ t>0 \qquad (7)$$

$$\frac{\partial T}{\partial Z} = 0 \quad \text{at } Z=Z_f,\ t>0 \qquad (8)$$

where, $T_e$ represents the temperature of the reaction mixture before entering the reactor. The initial conditions for (1) and (2) are

$$P(Z,0) = P^o(Z), \text{ at } 0<Z<Z_f,\ t>0 \qquad (9)$$

$$T(Z,0) = T^o(Z), \text{ at } 0<Z<Z_f,\ t>0 \qquad (10)$$

The solution of the above problem was obtained by Liu and Amundson (16) using finite difference method and by Lee (15) using the generalized Newton-Raphson method for the same numerical data. The results are shown in figures 3.13 and 3.14.

The solution of this problem was obtained using differential quadrature method following the procedure given in the next section.

3.2 Problem Formulation

By using equations (4) and (9) of Chapter I, the partial differential equations for the adiabatic reactor (equations (1) and (2), (5)-(10)) can be reduced to a set of 2N ordinary differential equation. Defining,

$$P(Z_i,t) = P_i(t) \quad , \quad i = 1, 2, 3, \ldots, N$$

$$T(Z_i,t) = T_i(t) \quad , \quad i = 1, 2, 3, \ldots, N$$

Equations (1) and (2) can be represented as

$$\frac{1}{N_{Pe}} \sum_{k=1}^{N} \sum_{j=1}^{N} a_{ik}\, a_{kj}\, P_j(t)) - \sum_{j=1}^{N} a_{ij}\, P_j(t) - r_o(P_i(t))^2 \exp(-\frac{E}{RT}) = \frac{P_i(t)}{dt} \quad , \; i=1, 2, \ldots, N \tag{11}$$

$$\frac{1}{N_{Pe}} \sum_{k=1}^{N} \sum_{j=1}^{N} a_{ik}\, a_{kj}\, T_j(t)) - \sum_{j=1}^{N} a_{ij}\, T_j(t) - a\, r_o(P_i(t))^2 \exp(-\frac{E}{RT}) = \frac{dT_i(t)}{dt} \quad , \; i = 1, 2, \ldots, N \tag{12}$$

Assuming $Z_1=0$ and $Z_N=Z_f$, the boundary conditions of the problem can be represented as

$$P_e = P_1(t) - \frac{1}{N_{Pe}} \sum_{j=1}^{N} a_{ij}\, P_j(t)), \text{ at } Z=Z_1=0 \; t > 0 \tag{13}$$

$$\sum_{j=1}^{N} a_{Nj} P_j(t) = 0, \quad \text{at } Z=Z_N=Z_f, \ t > 0 \quad (14)$$

$$T_e = T_1(t) - \frac{1}{N_{Pe}} \sum_{j=1}^{N} a_{1j} T_j(t)), \text{ at } Z=Z_1=0, \ t > 0 \quad (15)$$

$$\sum_{j=1}^{N} a_{Nj} T_j(t) = 0, \quad \text{at } Z=Z_N=Z_f, \ t > 0 \quad (16)$$

which gives a set of four algebraic equations. Similarly, the initial conditions (9) and (10) can be represented as

$$P_i(Z,0) = P_i^{o}(Z), \quad i = 1, 2, \ldots, N, \ t > 0 \quad (17)$$

$$T_i(Z,0) = T_i^{o}(Z), \quad i = 1, 2, \ldots, N, \ t > 0 \quad (18)$$

The set of equations (11) and (12) can be solved subject to boundary conditions (13)-(17) and initial conditions (18) and (19) by following the computational procedure as given below.

3.3 Computational Procedure

Step 1. Select N and $Z_i$, i=1, 2, . . . . ,N.

Step 2. Determine the weighting co-efficients $a_{ij}$, i=1, 2, . . . . ,N and j=1, 2, . . . . ,N by using the selected values of $Z_i$ and solving the set of following algebraic equations

$$\sum_{j=1}^{N} Z_j^{k-1} a_{ij} = (k-1) Z_i^{k-2}, \quad k= 1, 2, \ldots, N \quad i = 1, 2, \ldots, N \quad (19)$$

Step 3. Solve equations (13)-(16) to obtain

$$P_1(t) = f_1 (P_3, P_4, \ldots, P_N) \qquad (20)$$

$$P_2(t) = f_2(P_3, P_4, \ldots, P_N) \qquad (21)$$

$$T_1(t) = F_1(T_3, T_4, \ldots, T_N) \qquad (22)$$

$$T_2(t) = F_2(T_3, T_4, \ldots, T_N) \qquad (23)$$

Step 4. Substitute equations (20)-(23) in (11) and (12) to get a set of (2N-4) ordinary differential equations

$$\frac{d P_i(t)}{dt} = f_i' (P_3, P_4, \ldots, P_N, T_i), \quad i = 3, 4, \ldots, N \qquad (24)$$

$$\frac{dT_i(t)}{dt} = F_i' (T_3, T_4, \ldots, T_N, P_i), \quad i = 3, 4, \ldots, N \qquad (25)$$

Step 5. Solve equations (24) and (25) with initial conditions given by equations (17) and (18).

Step 6. Calculate $P_1, P_2, T_1, T_2$, $t > 0$ by using the results from step 5 and equations (20)-(23).

Step 7. Repeat steps 3-6 till a steady state is reached.

3.4 Numerical Results

The numerical data used was taken from that used by Lee (15) and also by Liu and Amundson (16) and is given below:

$$P_e = 0.07 \text{ atm.} \quad ; \quad E/R = 22{,}000^\circ R$$

$T_e = 1250^oR$ ; $Q = 0.1 \times 10^4\ ^oR/atm.$

$N_{Pe} = 2.0$ ; $r_o = 0.5 \times 10^8\ (atm)^{-1}$

$t = 0.2$ ; $Z_f = 48$

At t=0

$P^o(Z) = 0$ ; $T^o(Z) = 1270^oR$

A number of experiments were done in order to analyse the behavior of these equations. The order of differential quadrature approximation used and the selected points in each case is given below:

a) N=7; $Z_1=0$, $Z_2=5$, $Z_3=10$, $Z_4=20$, $Z_5=30$, $Z_6=40$, $Z_7=48$

b) N=9; $Z_1=0$, $Z_2=2$, $Z_3=5$, $Z_4=6$, $Z_5=10$, $Z_6=20$, $Z_7=30$, $Z_8=40$, $Z_9=48$

c) N=11; $Z_1=0$, $Z_2=2$, $Z_3=5$, $Z_4=6$, $Z_5=8$, $Z_6=10$, $Z_7=15$, $Z_8=20$, $Z_9=30$, $Z_{10}=40$, $Z_{11}=48$

d) N=9; $Z_1=0$, $Z_2=0.5$, $Z_3=1.0$, $Z_4=5.0$, $Z_5=10$, $Z_6=20$, $Z_7=30$, $Z_8=40$, $Z_9=48$

e) N=9; $Z_1=0$, $Z_2=0.1$, $Z_3=1.0$, $Z_4=5.0$, $Z_5=10$, $Z_6=20$, $Z_7=30$, $Z_8=40$, $Z_9=48$

f) N=12; $Z_1=0$, $Z_2=0.5$, $Z_3=5$, $Z_4=10$, $Z_5=15$, $Z_6=20$, $Z_7=25$, $Z_8=30$, $Z_9=35$, $Z_{10}=40$, $Z_{11}=45$, $Z_{12}=48$

g) N=12; $Z_1$=0, $Z_2$=0.5, $Z_3$=1, $Z_4$=5, $Z_5$=10, $Z_6$=15, $Z_7$=20, $Z_8$=25, $Z_9$=30, $Z_{10}$=35, $Z_{11}$=40, $Z_{12}$=48

h) N=9; $Z_1$=0, $Z_2$=0.5, $Z_3$=1, $Z_4$=5, $Z_5$=15, $Z_6$=25, $Z_7$=35, $Z_8$=45, $Z_9$=48,

i) N=9; $Z_1$=0, $Z_2$=0.8, $Z_3$=2, $Z_4$=6, $Z_5$=10, $Z_6$=20, $Z_7$=30, $Z_8$=39, $Z_9$=48

The results from experiments (a)-(e) and (i) are tabulated in tables 3.1 - 3.12 respectively and the respective plots are shown in fig. 3.1 - 3.12. The results of the approximation for the rest of the experiments were found to be quite unstable and in the first few iterations only, the fluctuations were high enough to exceed the overflow limits of the computer. The result obtained from the finite difference method are plotted in figures 3.13 and 3.14.

3.5 Discussion

As may be seen the same distribution of node points as in the case of isothermal reactor, did not prove to be equally good here. In fact, the selection of node points plays a very important role in the case of adiabatic reactor. A seven point differential quadrature approximation was not found to be satisfactory. The results obtained by using $7^{th}$ order

differential quadrature method (fig. 3.1 and 3.2) do not agree with those from the finite difference method. Therefore, the number of points were increased to 9 in further experimentation. In experiments (a)-(b) and (c), the initial boundary slope of the curve obtained changes with time, as a result of which wide fluctuations are produced as the reactor length increases. Experimentation was also done using $11^{th}$ order and $12^{th}$ order differential quadrature method (exp. e, f, g) but this was not found to be of much help, due to the increased round off and truncation errors in the computations. Therefore, the $9^{th}$ order differential quadrature method was used and the initial points were kept close to each other (cases d, e, and i) in order to maintain a constant slope. Variations were considered based on the experimental judgement. Steady state conditions were best obtained in experiment (i). The results obtained (fig. 3.11 and fig. 3.12) agree very closely with those from the finite difference method (fig. 3.13 and fig. 3.14). The computation time required was found to be less than a minute while it requires several minutes of computation time by the finite difference method. Thus, it can be concluded that with the proper selection of node points, $9^{th}$ order differential quadrature method gives as accurate results as the finite difference method does.

Table 3.1

Transient in Partial Pressure, Adiabatic Reactor by $7^{th}$ order Differential Quadrature

| T | P(t,0) | P(t,5) | P(t,10) | P(t,20) | P(t,30) | P(t,40) | P(t,48) |
|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 0.0649 | 0.0272 | 0.0093 | -0.0003 | 0.0001 | -0.0000 | 0.0000 |
| 10 | 0.0677 | 0.0435 | 0.0234 | 0.0023 | -0.0003 | 0.0001 | -0.0000 |
| 20 | 0.0677 | 0.0503 | 0.0382 | 0.0175 | 0.0032 | -0.0002 | 0.0000 |
| 30 | 0.0664 | 0.0411 | 0.0299 | 0.0221 | 0.0136 | 0.0036 | 0.0000 |
| 40 | 0.0633 | 0.0292 | 0.0247 | 0.0190 | 0.0137 | 0.0124 | 0.0026 |
| 50 | 0.0564 | -0.0050 | 0.0028 | 0.0191 | 0.0106 | 0.0128 | 0.0070 |

Table 3.2

Transient in Temperature, Adiabatic Reactor by $7^{th}$ order Differential Quadrature

| t | T(t,0) | T(t,5) | T(t,10) | T(t,20) | T(t,30) | T(t,40) | T(t,48) |
|---|---|---|---|---|---|---|---|
| 0 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 |
| 5 | 1251.5 | 1262.4 | 1267.5 | 1270.1 | 1270.0 | 1270.0 | 1270.0 |
| 10 | 1251.1 | 1260.0 | 1265.3 | 1269.5 | 1270.0 | 1270.0 | 1270.0 |
| 20 | 1254.2 | 1277.7 | 1280.5 | 1271.7 | 1269.4 | 1270.0 | 1270.0 |
| 30 | 1254.5 | 1288.5 | 1302.9 | 1295.3 | 1276.4 | 1269.6 | 1270.0 |
| 40 | 1249.0 | 1259.9 | 1285.6 | 1314.3 | 1301.7 | 1279.9 | 1270.4 |
| 50 | 1223.5 | 1130.5 | 1191.6 | 1300.2 | 1314.5 | 1310.0 | 1278.9 |

Table 3.3

Transient in Partial Pressure, Adiabatic Reactor with Axial Mixing by $9^{th}$ order Differential Quadrature

| t | p(0,t) | p(2,t) | p(5,t) | p(6,t) | p(10,t) | p(20,t) | p(30,t) | p(40,t) | p(48,t) |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 0.0673 | 0.0511 | 0.0250 | 0.0178 | 0.0021 | 0.0009 | -0.0010 | 0.0012 | -0.0007 |
| 10 | 0.0677 | 0.0603 | 0.0487 | 0.0440 | 0.0229 | -0.0008 | 0.0009 | -0.0011 | 0.0006 |
| 20 | 0.0689 | 0.0617 | 0.0477 | 0.0434 | 0.0318 | 0.0170 | -0.0002 | 0.0012 | -0.0006 |
| 30 | 0.0659 | 0.0532 | 0.0433 | 0.0414 | 0.0356 | 0.0202 | 0.0123 | 0.0014 | -0.0001 |
| 40 | 0.0686 | 0.0622 | 0.0509 | 0.0471 | 0.0332 | 0.0202 | 0.0145 | 0.0098 | 0.0020 |
| 50 | 0.0666 | 0.0546 | 0.0427 | 0.0401 | 0.0338 | 0.0213 | 0.0127 | 0.0127 | 0.0051 |
| 60 | 0.0679 | 0.0608 | 0.0515 | 0.0484 | 0.0357 | 0.0197 | 0.0148 | 0.0101 | 0.0082 |
| 70 | 0.0675 | 0.0571 | 0.0443 | 0.0411 | 0.0334 | 0.0225 | 0.0129 | 0.0119 | 0.0074 |
| 80 | 0.0671 | 0.0582 | 0.0497 | 0.0471 | 0.0366 | 0.0200 | 0.0156 | 0.0100 | 0.0083 |

Table 3.4

Transient in Temperature, Adiabatic Reactor with Axial Mixing by $9^{th}$ order Differential Quadrature

| t | T(t,0) | T(t,2) | T(t,5) | T(t,6) | T(t,10) | T(t,20) | T(t,30) | T(t,40) | T(t,48) |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 |
| 5 | 1251.5 | 1257.5 | 1264.2 | 1265.8 | 1269.4 | 1269.9 | 1270.0 | 1270.0 | 1269.9 |
| 10 | 1255.3 | 1268.6 | 1272.5 | 1271.8 | 1268.4 | 1270.6 | 1269.1 | 1271.2 | 1267.7 |
| 20 | 1248.6 | 1248.8 | 1262.9 | 1269.0 | 1289.8 | 1278.2 | 1268.2 | 1271.9 | 1266.7 |
| 30 | 1255.4 | 1273.5 | 1285.7 | 1286.6 | 1283.1 | 1296.8 | 1284.9 | 1267.5 | 1269.2 |
| 40 | 1250.4 | 1251.3 | 1258.7 | 1262.9 | 1284.8 | 1301.7 | 1298.2 | 1290.8 | 1265.9 |
| 50 | 1251.9 | 1264.5 | 1282.1 | 1285.4 | 1286.9 | 1296.2 | 1307.9 | 1304.6 | 1282.7 |
| 60 | 1251.5 | 1253.7 | 1256.5 | 1258.7 | 1275.5 | 1303.8 | 1298.1 | 1318.8 | 1295.3 |
| 70 | 1249.9 | 1257.5 | 1275.7 | 1280.2 | 1286.0 | 1290.3 | 1307.8 | 1306.5 | 1308.4 |

Table 3.5

Transient in Partial Pressure, Adiabatic Reactor with Axial Mixing by $11^{th}$ order Differential Quadrature

| t | p(t,0) | p(t,2) | p(t,5) | p(t,6) | p(t,8) | p(t,10) | p(t,15) | p(t,20) | p(t,30) | p(t,40) | p(t,48) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 0.0716 | 0.0620 | 0.0253 | 0.0167 | 0.0058 | 0.0014 | 0.0000 | 0.0000 | -0.0014 | 0.0048 | -0.0050 |
| 10 | 0.0629 | 0.0487 | 0.0460 | 0.0437 | 0.0351 | 0.0235 | 0.0033 | 0.0004 | -0.0003 | -0.0016 | 0.0005 |
| 20 | 0.0576 | 0.0393 | 0.0480 | 0.0488 | 0.0450 | 0.0376 | 0.0245 | 0.0166 | 0.0025 | -0.0101 | 0.0061 |
| 30 | 0.0598 | 0.0634 | 0.0779 | 0.0718 | 0.0524 | 0.0350 | 0.0226 | 0.0213 | 0.0214 | -0.0365 | 0.0283 |

Table 3.6

Transient in Temperature, Adiabatic Reactor with Axial Mixing by $11^{th}$ order Differential Quadrature

| t | T(t,0) | T(t,2) | T(t,5) | T(t,6) | T(t,8) | T(t,10) | T(t,15) | T(t,20) | T(t,30) | T(t,40) | T(t,48) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 |
| 5 | 1251.6 | 1257.3 | 1264.2 | 1266.0 | 1268.5 | 1269.6 | 1270.0 | 1270.1 | 1268.8 | 1268.8 | 1255.1 |
| 10 | 1253.1 | 1270.8 | 1280.3 | 1278.5 | 1273.1 | 1269.4 | 1269.4 | 1269.6 | 1272.1 | 1257.6 | 1258.6 |
| 20 | 1273.0 | 1317.1 | 1289.2 | 1277.3 | 1265.7 | 1270.1 | 1290.7 | 1278.0 | 1275.0 | 1252.3 | 1256.1 |
| 30 | 1298.1 | 1316.2 | 1211.4 | 1205.0 | 1229.7 | 1271.7 | 1308.0 | 1292.3 | 1263.8 | 1344.8 | 1152.3 |

Table 3.7

Transient in Partial Pressure, Adiabatic Reactor with Axial Mixing by $9^{th}$ order Differential Quadrature

| t | p(0,t) | p(0.1,t) | p(1,t) | p(5,t) | p(10,t) | p(20,t) | p(30,t) | p(40,t) | p(48,t) |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 0.0681 | 0.0676 | 0.0626 | 0.0284 | 0.0002 | 0.0025 | -0.0028 | 0.0043 | -0.0009 |
| 10 | 0.0672 | 0.0666 | 0.0623 | 0.0465 | 0.0235 | -0.0017 | 0.0011 | 0.0008 | 0.0021 |
| 20 | 0.0675 | 0.0670 | 0.0627 | 0.0465 | 0.0336 | 0.0170 | -0.0007 | 0.0033 | 0.0026 |
| 30 | 0.0675 | 0.0670 | 0.0627 | 0.0466 | 0.0335 | 0.0207 | 0.0106 | 0.0043 | 0.0031 |
| 40 | 0.0675 | 0.0670 | 0.0627 | 0.0466 | 0.0335 | 0.0197 | 0.0124 | 0.0114 | 0.0044 |
| 50 | 0.0675 | 0.0670 | 0.0627 | 0.0466 | 0.0335 | 0.0197 | 0.0120 | 0.0116 | 0.0069 |
| 60 | 0.0675 | 0.0670 | 0.0627 | 0.0466 | 0.0335 | 0.0196 | 0.0121 | 0.0111 | 0.0071 |
| 70 | 0.0675 | 0.0670 | 0.0627 | 0.0466 | 0.0335 | 0.0196 | 0.0121 | 0.0111 | 0.0071 |
| 80 | 0.0675 | 0.0670 | 0.0627 | 0.0466 | 0.0335 | 0.0197 | 0.0122 | 0.0108 | 0.0066 |

Table 3.8

Transient in Temperature, Adiabatic Reactor with Axial Mixing by $9^{th}$ order Differential Quadrature

| t | T(t,0) | T(t,0.1) | T(t,1) | T(t,5) | T(t,10) | T(t,20) | T(t,30) | T(t,40) | T(t,48) |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 |
| 5 | 1252.2 | 1252.7 | 1256.6 | 1266.6 | 1269.1 | 1274.0 | 1260.9 | 1307.4 | 1249.7 |
| 10 | 1251.7 | 1252.1 | 1256.4 | 1272.6 | 1270.2 | 1278.9 | 1252.4 | 1328.5 | 1248.5 |
| 20 | 1251.4 | 1251.7 | 1255.8 | 1275.8 | 1285.0 | 1298.1 | 1246.8 | 1336.0 | 1270.2 |
| 30 | 1251.4 | 1251.7 | 1255.8 | 1275.9 | 1285.4 | 1317.7 | 1271.5 | 1326.9 | 1285.3 |
| 40 | 1251.4 | 1251.8 | 1255.8 | 1275.6 | 1285.5 | 1319.1 | 1292.9 | 1349.9 | 1278.7 |
| 50 | 1251.3 | 1251.6 | 1255.7 | 1276.0 | 1285.2 | 1320.5 | 1292.9 | 1379.0 | 1299.7 |
| 60 | 1251.4 | 1251.6 | 1255.7 | 1275.9 | 1285.5 | 1320.5 | 1295.4 | 1377.1 | 1335.9 |
| 70 | 1251.5 | 1251.8 | 1255.9 | 1275.6 | 1285.5 | 1319.1 | 1297.1 | 1375.5 | 1335.0 |
| 80 | 1251.5 | 1251.8 | 1255.9 | 1275.6 | 1285.5 | 1318.2 | 1297.2 | 1375.5 | 1344.2 |

Table 3.9

Transient in Partial Pressure, Adiabatic Reactor with Axial Mixing by $9^{th}$ order Differential Quadrature

| t | p(0,t) | p(0.5,t) | p(1,t) | p(5,t) | p(10,t) | p(20,t) | p(30,t) | p(40,t) | p(48,t) |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 0.0681 | 0.0656 | 0.0626 | 0.0283 | 0.0002 | 0.0023 | -0.0024 | 0.0023 | -0.0014 |
| 10 | 0.0672 | 0.0645 | 0.0622 | 0.0465 | 0.0236 | -0.0022 | 0.0019 | 0.0023 | 0.0007 |
| 20 | 0.0675 | 0.0650 | 0.0625 | 0.0466 | 0.0339 | 0.0163 | 0.0003 | 0.0002 | -0.0006 |
| 30 | 0.0674 | 0.0649 | 0.0625 | 0.0467 | 0.0337 | 0.0206 | 0.0122 | 0.0012 | -0.0007 |
| 40 | 0.0674 | 0.0649 | 0.0625 | 0.0467 | 0.0337 | 0.0203 | 0.0140 | 0.0101 | 0.0011 |
| 50 | 0.0674 | 0.0649 | 0.0625 | 0.0467 | 0.0337 | 0.0205 | 0.0134 | 0.0119 | 0.0057 |
| 60 | 0.0674 | 0.0649 | 0.0625 | 0.0467 | 0.0337 | 0.0204 | 0.0136 | 0.0109 | 0.0076 |
| 70 | 0.0674 | 0.0649 | 0.0625 | 0.0467 | 0.0337 | 0.0202 | 0.0137 | 0.0106 | 0.0078 |
| 80 | 0.0674 | 0.0649 | 0.0625 | 0.0467 | 0.0337 | 0.0203 | 0.0137 | 0.0106 | 0.0077 |

Table 3.10

Transient in Temperature, Adiabatic Reactor with Axial Mixing by $9^{th}$ order Differential Quadrature

| t | T(t,0) | T(t,0.5) | T(t,1) | T(t,5) | T(t,10) | T(t,20) | T(t,30) | T(t,40) | T(t,48) |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 |
| 5 | 1252.6 | 1255.0 | 1257.2 | 1265.8 | 1269.9 | 1269.7 | 1270.3 | 1266.7 | 1267.1 |
| 10 | 1252.6 | 1255.0 | 1257.6 | 1270.9 | 1271.5 | 1268.6 | 1271.2 | 1264.7 | 1264.3 |
| 20 | 1252.7 | 1255.3 | 1257.9 | 1273.0 | 1286.1 | 1278.8 | 1268.0 | 1267.3 | 1258.9 |
| 30 | 1252.6 | 1255.1 | 1257.5 | 1273.3 | 1286.1 | 1297.1 | 1282.9 | 1264.9 | 1257.9 |
| 40 | 1252.6 | 1255.1 | 1257.5 | 1273.3 | 1286.3 | 1299.6 | 1301.8 | 1282.1 | 1258.4 |
| 50 | 1252.5 | 1255.0 | 1257.4 | 1273.5 | 1286.2 | 1300.5 | 1303.9 | 1305.2 | 1269.7 |
| 60 | 1252.4 | 1254.9 | 1257.3 | 1273.6 | 1286.2 | 1301.7 | 1303.4 | 1310.4 | 1287.1 |
| 70 | 1252.5 | 1255.0 | 1257.4 | 1273.5 | 1286.3 | 1301.2 | 1305.6 | 1307.3 | 1297.7 |
| 80 | 1252.6 | 1255.1 | 1257.5 | 1273.3 | 1286.3 | 1300.1 | 1306.7 | 1306.5 | 1299.6 |

Table 3.11

Transient in Partial Pressure, Adiabatic Reactor with Axial Mixing by $9^{th}$ order Differential Quadrature

| t | p(t,0) | p(t,0.8) | p(t,2) | p(t,6) | p(t,10) | p(t,20) | p(t,30) | p(t,39) | p(t,48) |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 0.0685 | 0.0645 | 0.0555 | 0.0191 | 0.0010 | 0.0017 | -0.0018 | 0.0020 | -0.0013 |
| 10 | 0.0669 | 0.0626 | 0.0576 | 0.0428 | 0.0234 | -0.0017 | 0.0016 | -0.0019 | 0.0012 |
| 20 | 0.0677 | 0.0640 | 0.0586 | 0.0438 | 0.0336 | 0.0164 | 0.0002 | 0.0002 | -0.0002 |
| 30 | 0.0674 | 0.0634 | 0.0578 | 0.0432 | 0.0337 | 0.0206 | 0.0121 | 0.0024 | -0.0001 |
| 40 | 0.0674 | 0.0633 | 0.0579 | 0.0437 | 0.0338 | 0.0201 | 0.0142 | 0.0105 | 0.0017 |
| 50 | 0.0674 | 0.0634 | 0.0579 | 0.0435 | 0.0337 | 0.0204 | 0.0134 | 0.0116 | 0.0057 |
| 60 | 0.0674 | 0.0634 | 0.0580 | 0.0437 | 0.0338 | 0.0203 | 0.0137 | 0.0109 | 0.0073 |
| 70 | 0.0674 | 0.0634 | 0.0580 | 0.0437 | 0.0338 | 0.0203 | 0.0137 | 0.0108 | 0.0076 |
| 80 | 0.0674 | 0.0634 | 0.0580 | 0.0436 | 0.0338 | 0.0204 | 0.0138 | 0.0108 | 0.0076 |

Table 3.12

Transient in Temperature, Adiabatic Reactor with Axial Mixing by $9^{th}$ order Differential Quadrature

| t | T(t,0) | T(t,0.8) | T(t,2) | T(t,6) | T(t,10) | T(t,20) | T(t,30) | T(t,39) | T(t,48) |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 | 1270 |
| 5 | 1252.3 | 1255.6 | 1259.6 | 1266.6 | 1269.7 | 1270.0 | 1270.1 | 1269.8 | 1270.5 |
| 10 | 1253.4 | 1258.5 | 1264.4 | 1272.7 | 1270.4 | 1269.8 | 1270.2 | 1269.5 | 1270.9 |
| 20 | 1252.8 | 1256.8 | 1261.6 | 1274.5 | 1286.0 | 1279.8 | 1267.6 | 1272.0 | 1269.9 |
| 30 | 1252.3 | 1256.1 | 1261.9 | 1277.6 | 1286.8 | 1296.8 | 1284.5 | 1267.8 | 1272.3 |
| 40 | 1252.7 | 1256.8 | 1262.3 | 1276.1 | 1286.0 | 1300.3 | 1302.1 | 1288.6 | 1271.4 |
| 50 | 1252.3 | 1256.1 | 1261.5 | 1276.4 | 1286.4 | 1300.2 | 1305.3 | 1307.4 | 1283.1 |
| 60 | 1252.3 | 1255.9 | 1261.3 | 1275.9 | 1285.7 | 1301.1 | 1304.7 | 1311.0 | 1298.1 |
| 70 | 1252.4 | 1256.1 | 1261.5 | 1275.9 | 1285.6 | 1300.3 | 1306.0 | 1309.7 | 1307.3 |
| 80 | 1252.5 | 1256.5 | 1261.9 | 1276.2 | 1285.9 | 1299.5 | 1306.2 | 1309.5 | 1311.0 |

Transient in Partial Pressure, Adiabatic Reactor with Axial Mixing by $7^{th}$ order Differential Quadrature

$Z_i$=(0,5,10,20,30,40,48)

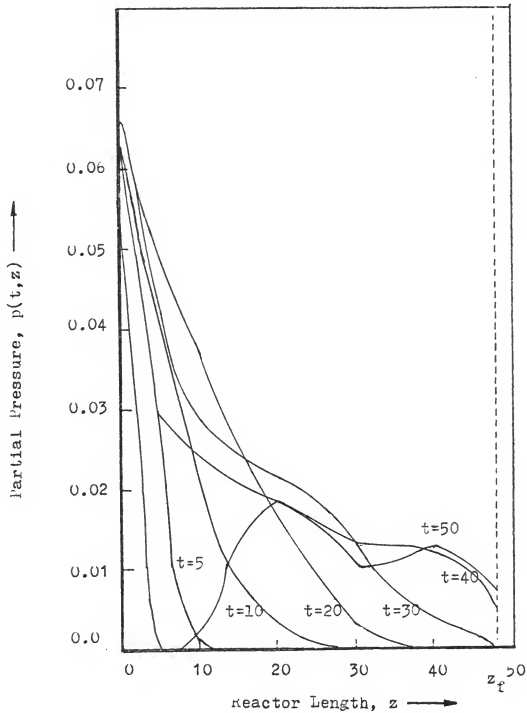


Figure 3.1

Transient in Temperature, Adiabatic Reactor with Axial Mixing by $7^{th}$ order Differential Quadrature

$Z_i=(0,5,10,20,30,40,48)$

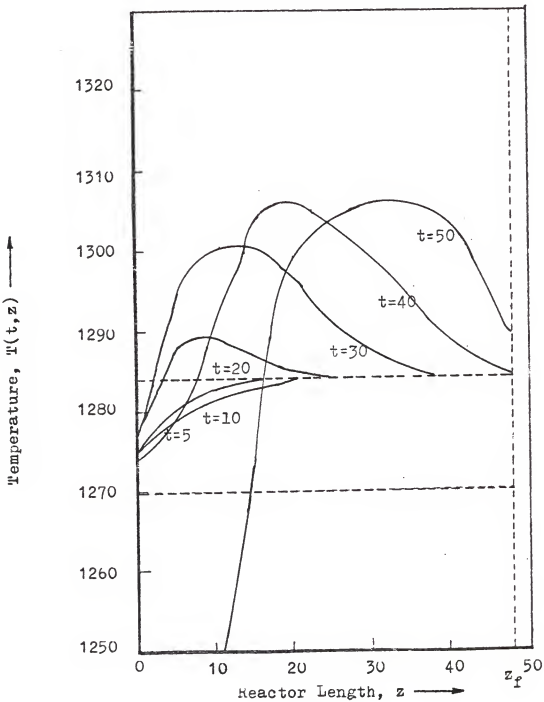


Figure 3.2

Transient in Partial Pressure, Adiabatic Reactor with Axial Mixing by 9$^{th}$ order Differential Quadrature

$Z_i$=(0,2,5,6,10,20,30,40,48)

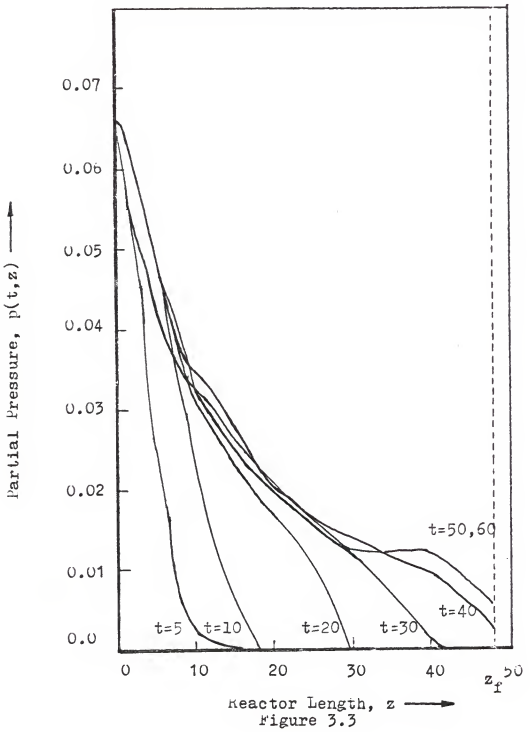


Figure 3.3

Transient in Temperature, Adiabatic Reactor with Axial Mixing by $9^{th}$ order Differential Quadrature

$Z_i=(0,2,5,6,10,20,30,40,48)$

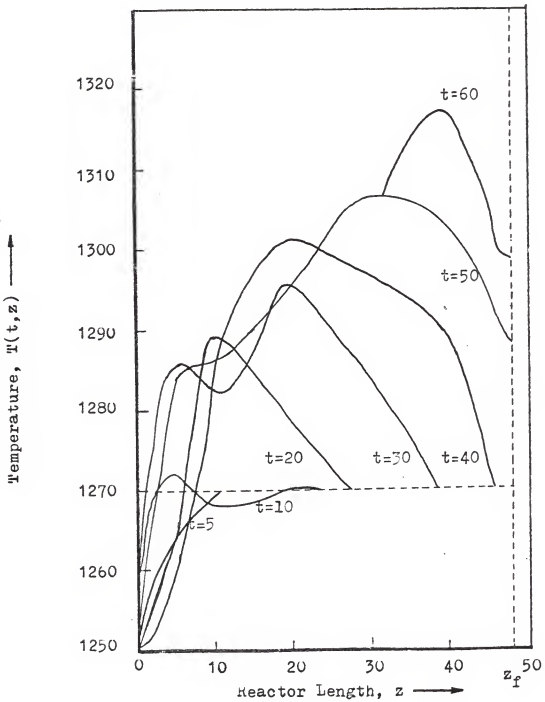


Figure 3.4

Transient in Partial Pressure, Adiabatic Reactor with Axial Mixing by 11$^{th}$ order Differential Quadrature

$Z_i$=(0,2,5,6,8,10,15,20,30,40,48)

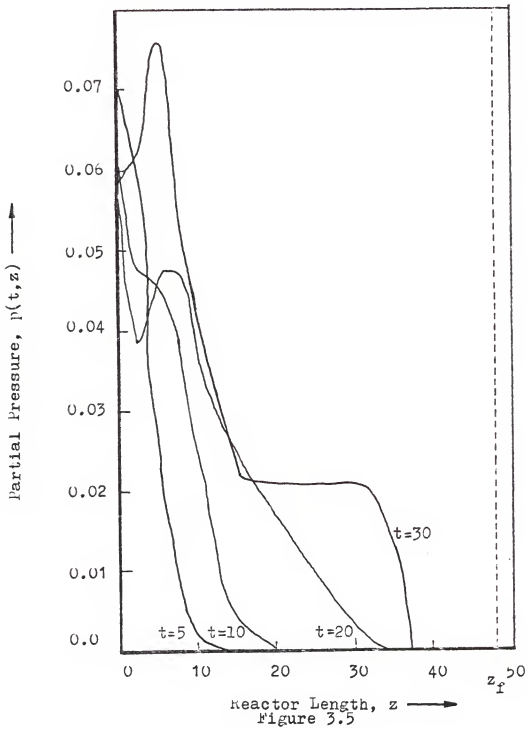


Figure 3.5

Transient in Temperature, Adiabatic Reactor with Axial Mixing by $11^{th}$ order Differential Quadrature

$Z_i$=(0,2,5,6,8,10,15,20,30,40,48)

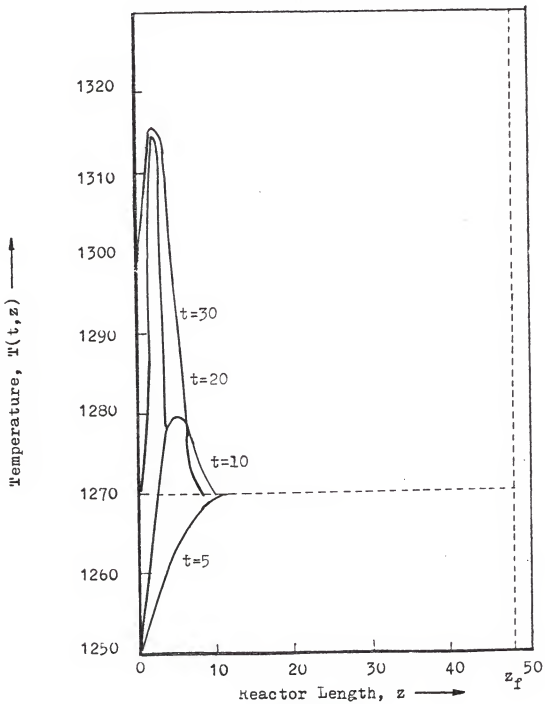


Figure 3.6

Transient in Partial Pressure, Adiabatic Reactor with Axial Mixing by $9^{th}$ order Differential Quadrature
$Z_i$=(0,0.1,1.5,10,20,30,40,48)

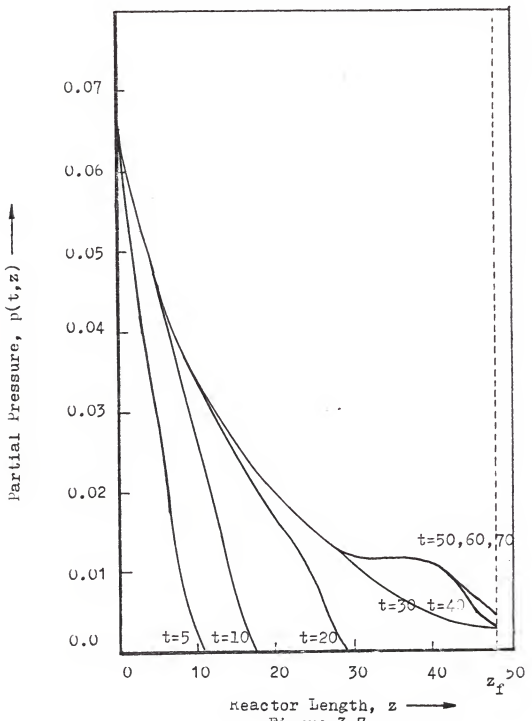


Figure 3.7

Transient in Temperature, Adiabatic Reactor with Axial Mixing by $9^{th}$ order Differential Quadrature

$Z_i$=(0,0.1,1,5,10,20,30,40,48)

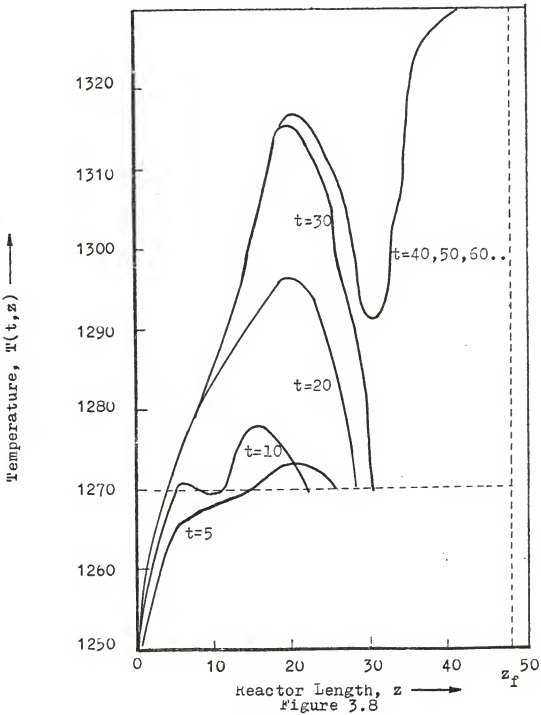


Figure 3.8

Transient in Partial Pressure, Adiabatic Reactor with Axial Mixing by $9^{th}$ order Differential Quadrature

$Z_i$=(0,0.5,1,5,10,20,30,40,48)

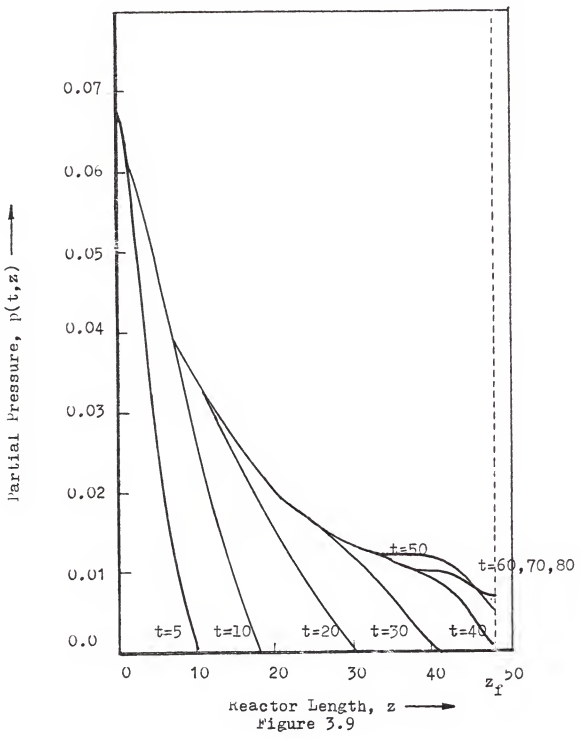


Figure 3.9

Transient in Temperature, Adiabatic Reactor with Axial Mixing by $9^{th}$ order Differential Quadrature

$Z_i$=(0,0.5,1,5,10,20,30,40,48)

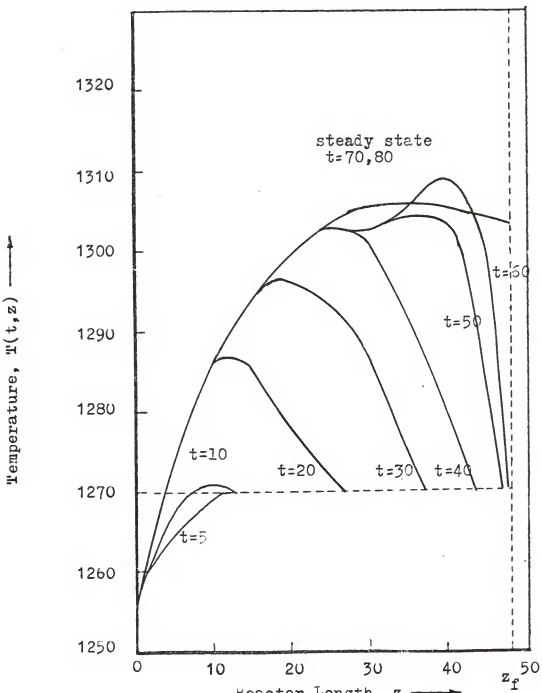


Figure 3.10

Transient in Partial Pressure, Adiabatic Reactor with Axial Mixing by $9^{th}$ order Differential Quadrature
$Z_i$=(0,0.8,2,6,10,20,30,39,48)

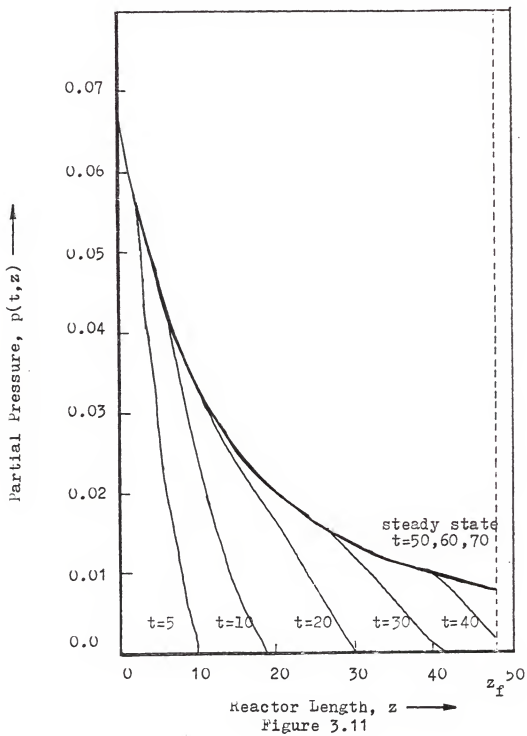


Figure 3.11

Transient in Temperature, Adiabatic Reactor with Axial Mixing by $9^{th}$ order Differential Quadrature

$Z_i$=(0,0.8,2,6,10,20,30,39,48)

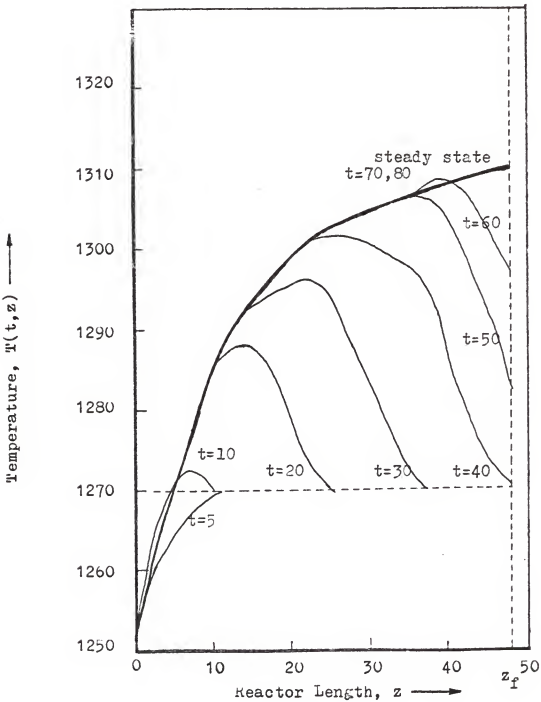


Figure 3.12

Transient in Partial Pressure, Adiabatic Reactor with Axial Mixing by Finite-Difference Method

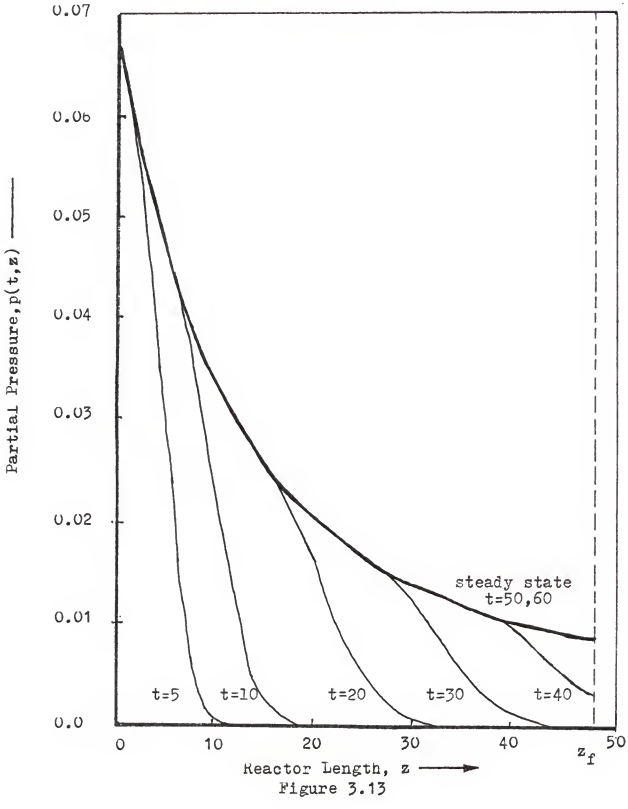


Figure 3.13

Transient in Temperature, Adiabatic Reactor with Axial Mixing by Finite-Difference Method

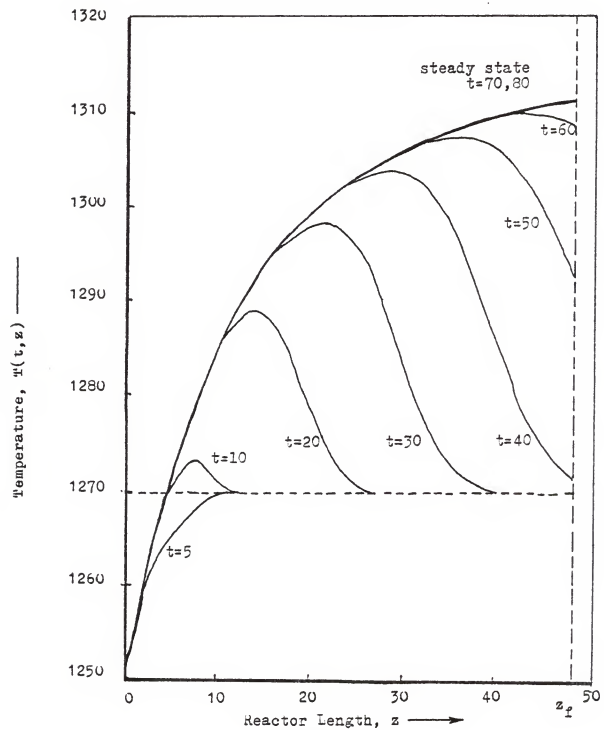


Figure 3.14

# CHAPTER IV

## CONCLUSIONS

Differential quadrature was found to be an excellent tool for the solution of non-linear partial differential equations. Results for both, the isothermal reactor as well as the adiabatic reactor are encouraging in this respect. Although, much experimentation was required in order to arrive at accurate results but it is mainly due to the values of the weighting coefficients used in the approximation. But in practice, these coefficients need to be determined only once for a particular type of problems. Therefore, if the optimal values are known, the method can be conveniently applied. Besides its advantages in terms of savings in computational time and computer storage, the comparison of the method with finite-difference method shows that differential quadrature is much easier to apply in practice. Differential quadrature using spline approximation may enhance its chances of success and may enable the successful solution of more general cases of packed-bed reactors without any instability problems. Thus, more research in this field may prove to be beneficial.

## REFERENCES


1. Bellman, R., 'A New Approach for the Identification of Systems', Math. Biosciences 5, 201(1969).

2. Bellman, R. and Kashef, B., 'Solution of the partial differential equations of the Hodgkin-Huxley Model using Differential Quadrature!, Mathematical Biosciences 19, 1(1974).

3. Bellman, R., Kasef, B. and Vasudevan, R., 'Differential Quadrature and Splines', Technical Report No. USCEF-RB75-3, University of Southern California, April, 1975.

4. Lee, E.S., Bellman, R., Kasef, B. and Vasudevan, R. 'Solving Hard Problems by Easy Methods. Differential and Integral Quadrature', Comp. and Maths. with Appl. 1, 133 (1975).

5. Bellman, R., Kasef, B. and Vasudevan, R., 'Splines via Dynamic Programming', Jour. of Math. Anal. and Appl. 38, 471(1972).

6. Bellman, R., Kasef, B.G. and Casti, J., 'Differential Quadrature: A Technique for the Rapid Solution of Non-Linear Partial Differential Equations', Journal of Computational Physics 10, 40(1972).

7. Ahlberg, J.H., Nilson, E.L. and Walsh, J.L. 'The Theory of Splines and Their Applications', Academic Press, N.Y., 1967.

8. Schoenberg, 'On Best Approximation of Linear Operators', Indag. Math. 26, 155(1964).

9. Sard, A., 'Linear Approximation', (Math. Surveys No. 9), Amer. Math, Soc., Providence, Rhode Island, 1963.

10. Bellman R. and Roth, R.S., 'The use of Splines with unknown End Points in the Identification of Systems', Journal of Mathematical Analysis and Applications 34, No. 1, April, 1971.

11. Bellman R. and Angel E., 'Dynamic Programming and Partial Differential Equations', Academic Press, N.Y.(1972).

12. Lanczos, C., 'Applied Analysis', Prentice Hall, Inc., N.J.(1956).

13. Bellman R., Kalaba, R.E. and Lockett, J.A., 'Numerical Inversion of the Laplace Transform', American Elsevier Pub. Co. Inc., N.Y.(1966).

14. Bellman, R. and Casti, J., 'Differential Quadrature and Long-Term Integration', Journal of Mathematics Anal. and Appl. 34, No. 2, 235(1971).

15. Lee, E.S., 'A Generalised Newton-Raphson Method for Non-Linear Partial Differential Equations- Packed-Bed Reactor with Axial Mixing', Chemical Engineering Sciences 21, 143(1966).

16. Liu, S.L. and Amundson, N.R., 'Stability of Adiabatic Packed Bed Reactors', Industr. Engrg. Chem. Fund. 2, 183 (1963).

17. Yagi, S. and Kunii D., 5th International symposium on Combustion, Reinhold, N.Y., 231(1955).

18. Wang, K., 'Boundary Value Problems and Invariant Imbedding with Applications', Ph.D. Dissertation, Kansas State University (1975).

19. Ghizzetti, A. and Ossicini A., 'Quadrature Formulae', Academic Press, 1968.

20. Lee, E.S., 'Quasilinearization and Invariant Imbedding', Academic Press, 1968.

# APPLICATION OF DIFFERENTIAL QUADRATURE TO ENGINEERING PROBLEMS

by

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AN ABSTRACT OF A MASTER'S THESIS

submitted in partial fulfillment of
the requirements of the degree

MASTER OF SCIENCE

Department of Industrial Engineering
KANSAS STATE UNIVERSITY
Manhattan, Kansas
1978

ABSTRACT

Differential quadrature is a useful numerical technique for solving non-linear partial differential equations. It involves approximating the partial derivatives by a linear combination of functional values and, therefore, provides an easy method of transformation of partial differential equations into a set of ordinary differential equations. The technique is employed for solving boundary value problems which can be represented by partial differential equations.

Most other methods like the finite-difference method involve approximation in terms of functional differences instead of functional values and therefore, require functional evaluation at a large number of points for satisfactory results. It is in this respect that differential quadrature has its major advantages over other methods in terms of both, the computer storage and computational time. However, the success of the method depends largely upon the method of evaluation of weighting coefficients. Three methods are considered in this respect viz.classical quadrature analogy, Legendre polynomial approach and spline approximation.

Differential quadrature is applied to solving several models in engineering with both fixed and moving boundary conditions. A moving boundary condition is specified at a point which itself varies as a function of time. Differential

quadrature is used to solve the isothermal reactor model as well as the adiabatic reactor model. A lot of computer memory and computation time are saved by using this technique.