A Moving Collocation method for the Solution of the Transient Convection-Diffusion-Reaction Problems

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Abstract. An adaptive collocation method is introduced for simulating the short time diffusion-convection-reaction problem. The method is based on dividing the solution domain into active and inactive zones in such away that the collocation points remain concentrated in regions of solution variation. The numerical results show that the proposed method is efficient in simulating the sharp profile at short time for the convective-dominant case. The adaptive scheme performance is found compatible with the high-order finite difference method, the QUICK method in term of the CPU time and average numerical errors.

Introduction

A variety of numerical methods have been presented for the numerical solution of time-dependent partial differential equations which involve steep spatial gradients of species moving with time (Finlayson 1992, Wouwer et. Al. 2001). The problems of transient heat conduction or material diffusion in simple and complicated geometries, convection-diffusion-reaction problems in chemical reactors are examples of such problem. Finlayson (1980) presents some of the numerical method used for solving the transient conduction or diffusion problems including finite difference, finite element and orthogonal collocation. The collocation method which is one of the methods of weighted residuals has several important advantages over the other discretization methods. It provides a high order of convergence, gives continuous approximate solutions, and easily handles general boundary conditions while still being simple to program. The collocation method appears in different forms depending on the basis function used to approximate the solution of the differential equations. The orthogonal collocation method uses series expansion based on orthogonal basis functions such as the *Legendre* polynomial where the coefficients are determined by minimization of some criteria (Villadsen & Michelson (1978)). Soliman(1992) developed a spline collocation method for steady state diffusion-convection problems. Direct collocation methods such as the differential quadrature method have been applied for complex convection-diffusion nonlinear problems (Chen and T. & Zhong, (1998)). Several attempts have been made to draw guidelines of implementing the collocation method to chemical engineering problems (Lefervre *et. al.* 2000).

Adaptive numerical schemes are found to gain significant improvement in accuracy over traditional fixed grid methods. Significant improvement has been made by adapting the numerical method discretization nodes so that they are concentrated about these areas of large gradients. Villadsen and Michelsen (1978) pointed the need of applying special techniques for short time period since the steepness of profile necessitates the use of large number of collocation points which in turn increases the stiffness of the differential equations. An initial attempt for alleviating this problem was presented by Soliman and Ibrahim (1999). They divided the solution domain for short time into active and inactive zones. The knowledge of the asymptotic solution was used to develop an equation which determines the speed by which the solution in the active zone advances with time. Another scheme based on the moving coordinate systems was presented by Yoshida, *et.al*. (1975) to solve the problem of gas-solid reaction system where solid disappearance creates sharp moving fronts. Huang and Russell (1996) have introduced a moving collocation method based on moving mesh concept and applied it to time-dependent partial differential equations having large solution variation. Their numerical experiments found that the moving collocation method produces more accurate results for small number of mesh points.

In this work we apply the same concept of dividing the domain for short time into active and an inactive zone in order to capture the moving steepness fronts observed for transient convection-diffusion reaction problems at short times. We apply the proposed method to reaction flow models arising from homogenous chemical reactions in tubular reactors. These models describe the chemical transformations and transport of species inside the reactors. In our previous work (Alhumaizi et. al. 2003) we have analyzed the resulted set of one dimensional reaction-diffusion-convection system using different reduction techniques (finite difference method, orthogonal collocation, and finite element methods). For convection-dominated problems we have shown that the fixed grid global collocation method is not appropriate of predicting the dynamics of the studied system. In addition, the method of fixed grid collocation on finite elements proved to be much better than the global method but introduced unphysical oscillations before and after the moving fronts.

Moving Collocation Method Formulation

A moving collocation method will be used in this paper for the solution of transient diffusion convection reaction problems which involve steep profiles. Initial attempts indicated that the moving grid global collocation method as the one presented in Soliman and Ibrahim (1999) is not suitable and produce unacceptable oscillations around the sharp profiles. In this work we propose to use the spline collocation method (Carey & Finlayson (1975), Soliman (1992)), rather than the global collocation method within the moving zones. The presented scheme is based on estimating the moving coordinate which differentiate between the active and the dead zones. This represents a case in which the elements of the collocation method move in time but their movement is estimated simultaneously with the determination of the solution of the collocation method discretized problem.

In this section we present the derivation of the proposed method to a single diffusion-convection-reaction problem:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} - v\frac{\partial u}{\partial x} - f(u), \qquad x \in [0,1] \tag{1}$$

The boundary and initial conditions for this problem are given as

$$u(0,t) = u_o, \qquad \frac{\partial u(1,t)}{\partial x} = 0, \qquad u(x,0) = u_{ss} \tag{2}$$

First, we make use of the following transformation

$$r = \frac{mx}{\lambda(t)} \qquad \textit{for} \qquad 0 \le x \le \lambda \tag{3}$$

Where m is the number of splines over the new domain $r \in [0,m]$ and λ(t) is the moving zone location. Notice that the r takes the value of 1,2,…..m at $x = \frac{\lambda}{m}, \frac{2\lambda}{m}, ..., \lambda$.

Let $\overline{u}(r,t)$ to be the state variable in the new domain (r). The accumulation parts in the new domain and the original domain are related by:

$$\frac{\partial u}{\partial t} = \frac{\partial \overline{u}}{\partial t} + \frac{\partial \overline{u}}{\partial r}\cdot\frac{\partial r}{\partial \lambda}\cdot\frac{d\lambda}{dt} \tag{4}$$

Substituting equation (1) in (4) leads to

$$\frac{\partial \overline{u}}{\partial t} = D\frac{\partial^2 u}{\partial x^2} - v\frac{\partial u}{\partial x} - f(u) + \frac{r}{\lambda}\frac{\partial \overline{u}}{\partial r}\cdot\frac{\partial \lambda}{\partial t} \tag{5}$$

This equation can written in term of the new domain variable as

$$\frac{\partial \overline{u}}{\partial t} = \frac{1}{\lambda^2}\left[Dm^2\frac{\partial^2 \overline{u}}{\partial r^2} - vm\lambda\frac{\partial \overline{u}}{\partial r} + \frac{r}{2}\frac{\partial \overline{u}}{\partial r}\left(\frac{d\lambda^2}{dt}\right) - \lambda^2 f(\overline{u})\right] \tag{6}$$

Equation (6) will be solved using splines collocation in the zones $i \le r \le i+1, \quad i = 1,2,......,m-1$. The initial and boundary conditions for equation (6) are:

$$\bar{u}(0,t) = u_0, \qquad \bar{u}(r,0) = u_{ss} \tag{7}$$

The equation which determines boundary of the moving zones is

$$\bar{u}(0,m) = u_{ss} \quad \text{(Initial value of u)} \tag{8}$$

That is to say we have added this extra equation in the new formulation to determine the change of the moving front λ with time. We also have the following condition at *r=m*:

$$\left.\frac{\partial \bar{u}}{\partial r}\right|_{r=m} = 0 \tag{9}$$

The following continuity equations hold between the elements of the moving zones *i=1,2,….,m-1* ,

$$\bar{u}\big|_{r=i-} = \bar{u}\big|_{r=i^+}, \qquad \left.\frac{\partial \bar{u}}{\partial r}\right|_{r=i^-} = \left.\frac{\partial \bar{u}}{\partial r}\right|_{r=i^+} \tag{10}$$

We notice that equation (6) becomes singular as λ approaches zero. This necessitates for the quantity between brackets in the R.H.S of equation (6) to be zero. In fact this sets up the initial conditions for $\bar{u}$ and the time derivative of λ for the new equation (6) by letting $\lambda \to 0$ to obtain

$$0 = \left[Dm^2 \frac{\partial^2 \bar{u}}{\partial r^2} + \frac{r}{2}\frac{\partial \bar{u}}{\partial r}\Lambda \right] \tag{11}$$

where $\Lambda = \frac{d\lambda^2}{dt}\big|_{t=0}$ is the initial condition for the moving zone. The steady state equation needs to be solved in the zones ($i \le r \le i+1, \quad i = 1,2,......,m-1$) together with the continuity conditions;

$$\bar{u}\big|_{r=i-} = \bar{u}\big|_{r=i^+} \quad \text{and} \quad \left.\frac{\partial \bar{u}}{\partial r}\right|_{r=i^-} = \left.\frac{\partial \bar{u}}{\partial r}\right|_{r=i^+} \qquad i = 1,2,..........,m-1 \tag{12}$$

and the boundary conditions

$$\bar{u}\big|_{r=m} = u_{ss}, \quad \left.\frac{\partial \bar{u}}{\partial r}\right|_{r=m} = 0, \qquad u(0)=u_o. \tag{13}$$

These equations will be solved for the initial conditions for u and for the initial condition for the moving zone $\left.\frac{d\lambda^2}{dt}\right|_{t-0}$.

When λ takes the value of one, the moving zone covers the whole domain, and it stops moving. Thus dλ/dt becomes zero, and we will be having a fixed grid spline collocation method.

The discretized model is defined using the orthogonal collocation method (Villadsen & Michelsen 1978) which makes use of orthogonal polynomials in each interval and let the equations to be satisfied at the zeros of these polynomials. There are families of polynomials that obey the orthogonality condition. *Legendre, Chebyshev, Hermite* and *Laguerre polynomials* are the most widely used orthogonal polynomials. In the present study we use the *Legendre* polynomials. The collocation points are chosen in each interval as the zeros of the *Legendre* polynomials .

The position derivatives of the state variable at the collocation points are discretized by applying the orthogonal collocation method to equation (6) using n collocation points in the interior of each zone. This can be expressed as

$$\frac{\partial \overline{u}_{i-1+k(n+1)}}{\partial t} = \frac{1}{\lambda^2}\left[\begin{array}{l} Dm^2 (B_{i1}\overline{u}^* + \sum_{j=2}^{n+2} B_{ij}\overline{u}_{j-1+k(n+1)}) - \\ \left(vm\lambda - \frac{r}{2}\left(\frac{d\lambda^2}{dt}\right)\right)(A_{i1}\overline{u}^* + \sum_{j=2}^{n+2} A_{ij}\overline{u}_{j-1+k(n+1)}) - \lambda^2 f(\overline{u}_{i-1+k(n+1)}) \end{array}\right]$$

$$i = 2,3,...,n+1$$
$$k = 0,1,....,m-1 \qquad (14)$$

where A's and B's are the weights of discretized first and second derivatives respectively (Villadsen & Michelsen 1978). For the first spline *(k=0*), the value of u at the first collocation point (r=0) in equation (14) is given as

$\overline{u}^* = u_0$

while for the other splines ($k \neq 0$),

$\overline{u}^* = \overline{u}_{k(n+1)}$

Equation (14) constitutes a set of $m \times n$ nonlinear ordinary differential equations whose describe the dynamic behavior of the state variable $\overline{u}$ at n collocation points in each spline.

The continuities of the derivatives become

$$A_{n+2,1}\overline{u}^{*}+\sum_{j=2}^{n+2}A_{n+2,j}\overline{u}_{j-1+k(n+1)}=\sum_{j=1}^{n+2}A_{1,j}\overline{u}_{j-1+(k+1)(n+1)} \qquad k=0,1,....,m-2 \tag{15}$$

We have also the boundary conditions written in the following discretized form;

$$A_{n+2,1}\overline{u}^{*}+\sum_{j=2}^{n+2}A_{n+2,j}\overline{u}_{j-1+k(n+1)}=0, \qquad k=m-1 \tag{16}$$

The boundary of the moving zone is given by

$$\overline{u}_{m(n+1)}=u_{ss} \tag{17}$$

So we have a total of *m(n+1)+1* unknowns; u_j, *(j=1,…,m(n+1))* variables, and the unknown moving zone λ. Notice also that the continuity of u condition was inserted in the above equations to reduce the number of variables and hence the equations.

Applying the collocation method to the steady-state equation (11) gives

$$0=\left[Dm^{2}(B_{i1}\overline{u}^{*}+\sum_{j=2}^{n+2}B_{ij}\overline{u}_{j-1+k(n+1)})+\left(\frac{r}{2}\Lambda\right)(A_{i1}\overline{u}^{*}+\sum_{j=2}^{n+2}A_{ij}\overline{u}_{j-1+k(n+1)})\right] \qquad i=2,3,...,n-1 \quad k=0,1,....,m-1 \tag{18}$$

Similar equations can be written for the continuity conditions and the boundary condition (Equations12-13)

Initially we solve the algebraic steady state equation (Eq.18) to define the initial condition for the moving zone location. The system of the differential algebraic equations generated via the collocation method (Eq.14-17) is usually stiff, implicit or semi-implicit integration schemes are preferable. In this work we use the efficient Petzold's Fortran-based DASSL code which is designed for the numerical solution of implicit systems of differential/algebraic equations written in the form F(t,y,y')=0, where F, y, and y' are vectors, and initial values for y and y' are given. This code uses the backward differentiation formulas of orders one through five to approximate the derivatives and the resulting nonlinear system at each time step is solved by Newton’s method.

Reacting Flow Problem

We consider a well-documented autocatalytic reaction model in which the mutant competes with the autocatalyst (Alhumaizi & Abasaeed, 2000). The chemical scheme of the autocatalytic reaction, which takes place in a continuous flow tubular reactor, consists of the following steps:

Replication of B: $A + 2B \xrightarrow{k_1} 3B$

Death of B: $B \xrightarrow{k_2} P_1$

Mutation of B into C: $A + 2B \xrightarrow{\alpha k_1} 2C + B$

Replication of C: $A + 2C \xrightarrow{\beta k_1} 3C$

Death of C: $C \xrightarrow{k_2/\beta} P_2$

where k_1, and k_2 are the rate constants, and the parameters α, and β are the mutation constant and mutation efficiency, respectively.

Results of the calculations shown in this study are numerical solutions of the equations of transport balance for the reacting species A, B, and C with concentrations denoted u_1, u_2, and u_3, respectively. In order to simplify the problem, the species have been assumed to have constant flow velocities along the reactor. The transport balance equations for the three reacting species are in one dimension as follows.

For A: $$\frac{\partial u_1}{\partial t} + v\,\frac{\partial u_1}{\partial x} = \bar{D}_1 \frac{\partial^2 u_1}{\partial x^2} - k_1(1+\alpha)u_1u_2^2 - k_1\beta u_1 u_3^2 \qquad (19.a)$$

For B: $$\frac{\partial u_2}{\partial t} + v\frac{\partial u_2}{\partial x} = \bar{D}_2 \frac{\partial^2 u_2}{\partial x^2} + k_1(1-\alpha)u_1u_2^2 - k_2 u_2 \qquad (20.a)$$

For C: $$\frac{\partial u_3}{\partial t} + v\,\frac{\partial u_3}{\partial x} = \bar{D}_3 \frac{\partial^2 u_3}{\partial x^2} + k_1\beta u_1 u_3^2 + 2k_1\alpha u_1 u_2^2 - \frac{k_2}{\beta} u_3 \qquad (21.a)$$

where t is time, and x is spatial coordinate.

Written in dimensionless form, Eqs. (18.a)-(20.a) become

$$\frac{\partial U_1}{\partial T} + V\frac{\partial U_1}{\partial X} = D_1\frac{\partial^2 U_1}{\partial X^2} + (1+\alpha)(1-U_1)U_2^2 + \beta(1-U_1)U_3^2 \qquad (19.b)$$

$$\frac{\partial U_2}{\partial T} + V\frac{\partial U_2}{\partial X} = D_2\frac{\partial^2 U_2}{\partial X^2} + (1-\alpha)(1-U_1)U_2^2 - \gamma U_2 \qquad (20.b)$$

$$\frac{\partial U_3}{\partial T} + V\frac{\partial U_3}{\partial X} = D_3\frac{\partial^2 U_3}{\partial X^2} + \beta(1-U_1)U_3^2 + 2\alpha(1-U_1)U_2^2 - \frac{\gamma}{\beta}U_3 \qquad (21.b)$$

and with the initial conditions

$$U_1 = 1, \quad U_2 = 0, \quad U_3 = 0; \quad T = 0 \qquad \text{(Clean system)}$$

where

$$U_1 = \frac{u_f - u_1}{u_f}, \quad U_2 = \frac{u_2}{u_f}, \quad U_3 = \frac{u_3}{u_f}$$

$$X = \frac{x}{L},\ T = k_1 u_f^2 t,\ V = \frac{v}{k_1 u_f^2 L},\ \gamma = \frac{k_2}{k_1 u_f^2}$$

$$D_1 = \frac{\bar{D}_1}{k_1 u_f^2 L^2},\ D_2 = \frac{\bar{D}_2}{k_1 u_f^2 L^2},\ D_3 = \frac{\bar{D}_3}{k_1 u_f^2 L^2}$$

u_f is the feed substrate concentration, U_i (i = 1,2,3) is the dimensionless concentration of species i, and U_{if} is the concentration of species i at the reactor inlet. L is the length of the tubular reactor. The model equations (19b-21b) are in the form of the original equation (1) which need to be transformed to the modified form (equation 6) using the transformation of equation (3).

Results and Discussion

The calculation results correspond to the case of a *clean system* for which the concentrations of all reacting species inside the reactor were initially set to zero. The initial dimensionless concentration of species A, U_1, is equal to unity by virtue of its definition. The kinetic parameters were kept constant with $\alpha = 0.065$, $\beta = 2.0$, and $\gamma = 0.0250$ (Alhumaizi, et. al. 2003) and the feed concentrations adopted for species A, B, and C are $U_{1f} = 0$, $U_{2f} = 0.67$, and $U_{3f} = 0$, respectively, for all simulation runs.

The exact solutions of dynamic and steady-state problem for the model considered here is not available. In a previous work (Alhumaizi 2004) we have shown that the three-point upstream finite difference method QUICK developed by Leonard (1979) is the fastest method to achieve a given accuracy. First, we define the closest solution to the exact by using QUICK method with large number of grids. Figure 1 shows the calculated concentrations profiles for all species at initial times along the reactor using the QUICK method with 500 grids for the convection-dominated case V=1.0 (*Pe*=10000). High Peclet numbers correspond to low residence times of the species in the reactor, which means more time is needed to consume the reactant A along the reactor. It can be seen in Figure 1 that with the considered parameter values, steep variations in species concentrations are spread over small number of grids number. So even with large number of grid cells the numerical solution exhibits unphysical oscillations after and before the front. Figure 1 shows values higher than unity for the substrate conversion U1 which is physically unacceptable. Figure 2 shows the simulation results for the same case with lower number of grids at t=0.5. Reducing the number of grids reduces the CPU time but results in less sharp profiles and higher errors.

In the following we compare the results of the new method with the output of the QUICK method with 200 grids at t=0.5 for the convective-dominant case V=1.0. Solving the dynamic equations using the proposed moving collocation method for different grid orientations are illustrated as follows; the first case with 16 intervals and 2 collocation points gives oscillatory behavior and is unable to provide enough smoothing in the active zone as shown in Figure 3. On the other hand it eliminates the unacceptable overshoot exhibited by the finite difference method after the front in the dead zone. In the second case, we reduce the number of intervals to 12 and increase the collocation points in each interval to 4. Figure 4 shows the results for this case. We obtained similar results to the first case. With increasing both the number of the intervals and collocation points in the third case, we have found there is a clear gain in numerical accuracy. Figure 5 shows the results for the case M=24 and Ncol=4. For this case we show that the developed method take care of the difficulties found before and is found able to capture the steep profile and provide enough smoothing in the active zone. There is hardly any difference visible between the QUICK solution and the moving method numerical approximation. A comparison between Figures 3, 4 and 5 shows the significant accuracy improvement obtained by increasing the number of intervals and collocation points.

In figure 6 we compare the results of the proposed method with the results corresponding to QUICK method for low velocity value (V=0.1). The moving collocation method for the two cases which fail to yield the right dynamics for V=1.0, is found successful in solving the low velocity problem without any oscillations.

Table (1) compares the performance of the proposed moving collocation method and the finite difference method for the convection-dominated case V=1.0 (*Pe*=10000). In order to compare the methods, we calculate the error which is defined as the average difference between the computed concentration of the reactant A and its high accuracy solution found using QUICK method with 500 points. The error was computed for the whole reactor length at a certain time (t=0.5). In the first and second columns of Table 1 we show the maximum local error and the average error. The finite difference methods exhibits its maximum error at the front locations while the collocation method suffer from high undershoot behavior before the front. Large local errors are observed for both methods when low number of nodes is used. The moving collocation method with 24 intervals and 4 collocation points show a comparable performance to the QUICK method with 200 grids but it consumes less CPU time.

Conclusion

In this paper, we developed a moving collocation method and applied to simulate the dynamics of a convection-diffusion-reaction model. We used the developed method to simulate the steep profiles exhibited by such models. The results were compared with one of the most efficient methods to solve such problems. The application of the method was illustrated for two different cases; for the difficult high convection velocity case, we found that the moving collocation method can capture the sharp profiles with fine tuning of the number of collocation splines and points. For the low velocity case, the method simulates the dynamic profiles of the systems with less number of collocation intervals and points.

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Notation

A	substrate concentration
B	autocatalyst concentration
C	mutant concentration
D, $\overline{D}$	species dimensionless diffusion coefficient/ species diffusion coefficient
k	kinetic rate constants
L	reactor dimensionless length
M	number of intervals
N	number of grids for finite difference method
Ncol	number of collocation points
T	dimensionless time
u	species concentration
U	dimensionless species concentration
V	convection dimensionless coefficient
x	axial coordinate
X	dimensionless axial direction

Greek letters

α, β	mutation efficiency coefficients
γ	dimensionless kinetic parameter
λ	Dimensionless distance of the zones boundary.

Subscripts

1, 2, 3	species identifiers
f	feed

Method	Max error %	Ave. Error %	CPU time (sec)
QUICK, N= 50	70.4	21.7	0.87
QUICK, N= 100	71.9	18.9	1.88
QUICK, N= 200	3.0	2.0	4.386
MC, M=16, Ncol=2	120	18.1	0.80
MC, M=12, Ncol=4	82.2	12.4	1.64
MC, M=24, Ncol=4	9.3	1.12	3.52

Table (1): Comparison of the results of the moving collocation method and QUICK method for the case *Pe*=10000.

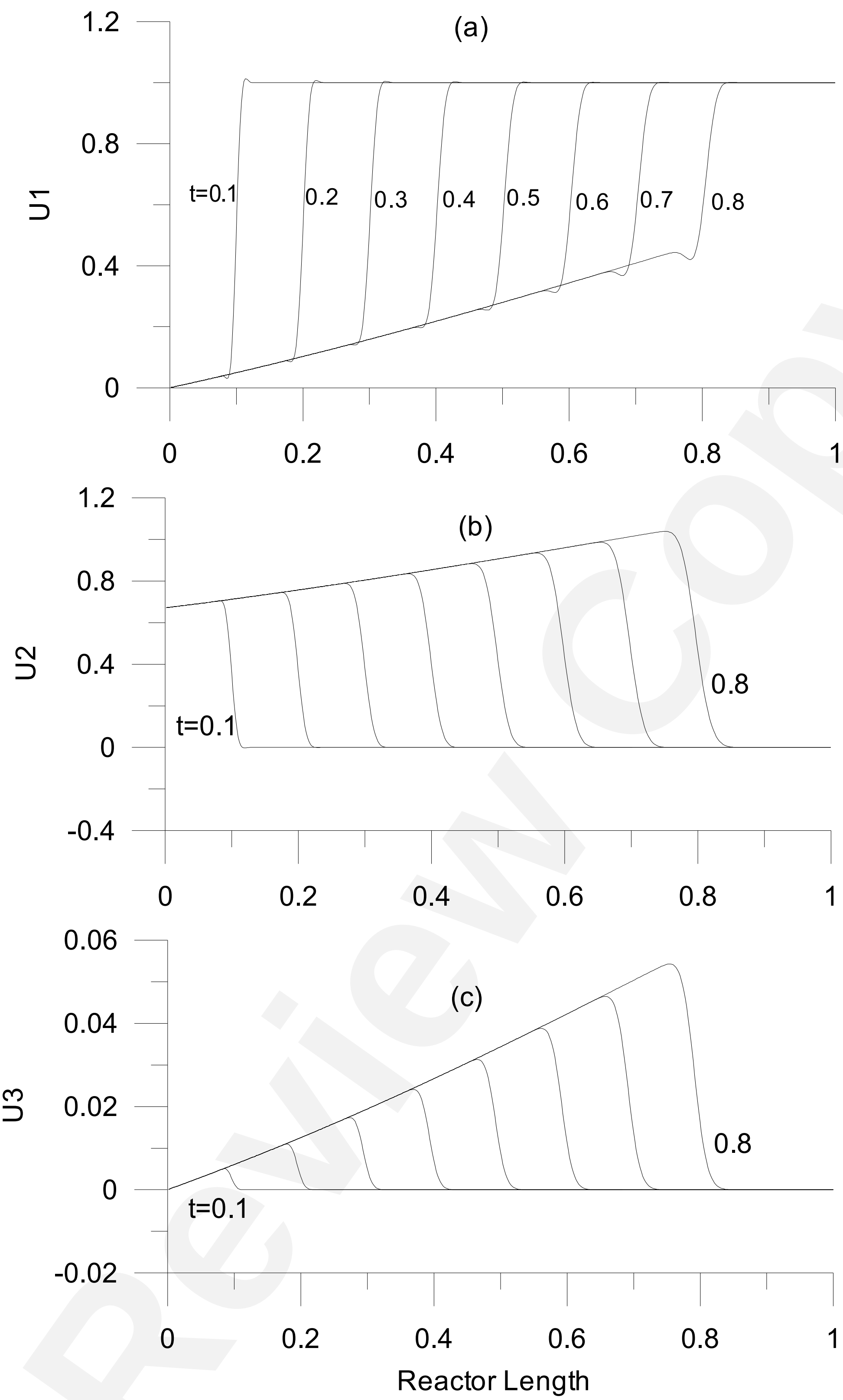

Figure (1): Transient concentration profiles for species A (a), B (b) and C (c) at different short times for *Pe*=10000 using QUICK method with 500 grids.

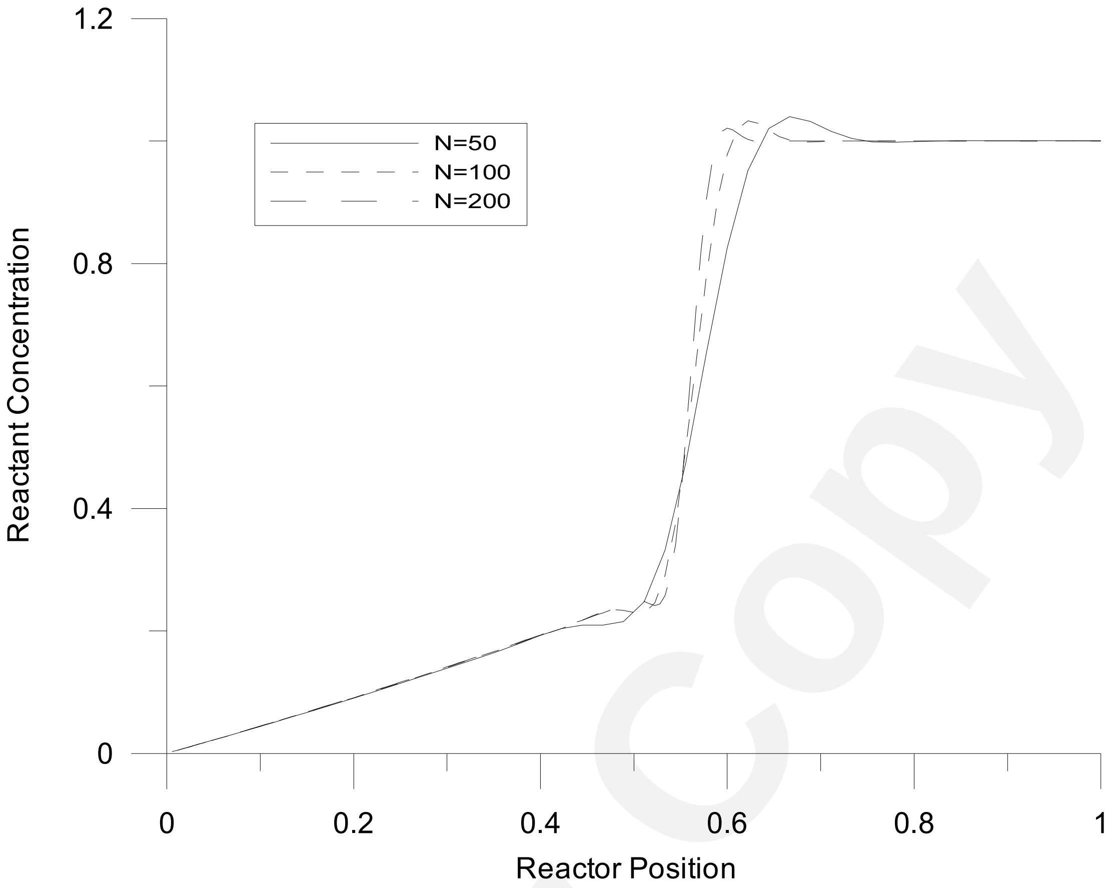

Figure (2): Transient concentration profile for species A at t=0.5 obtained using QUICK method with different grids number.

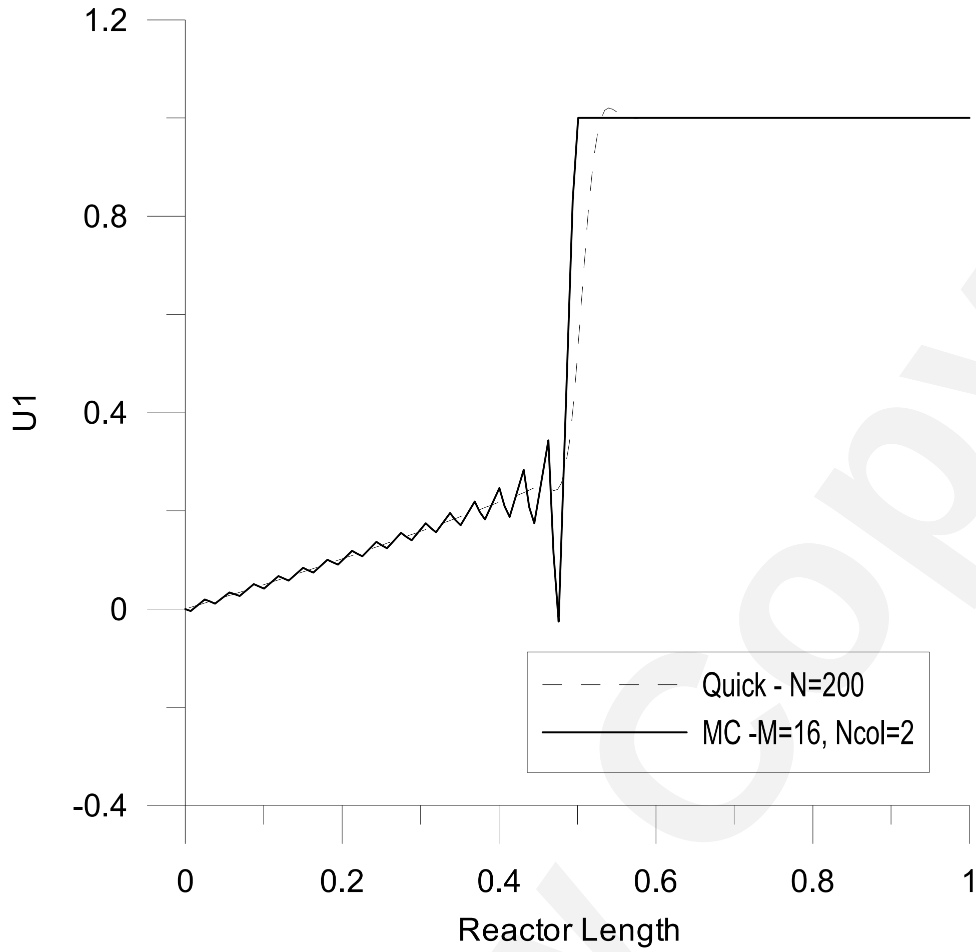

Figure (3): Dynamic concentration profile for species A at t=0.5 using moving collocation method (M=16, N=2) and QUICK method.

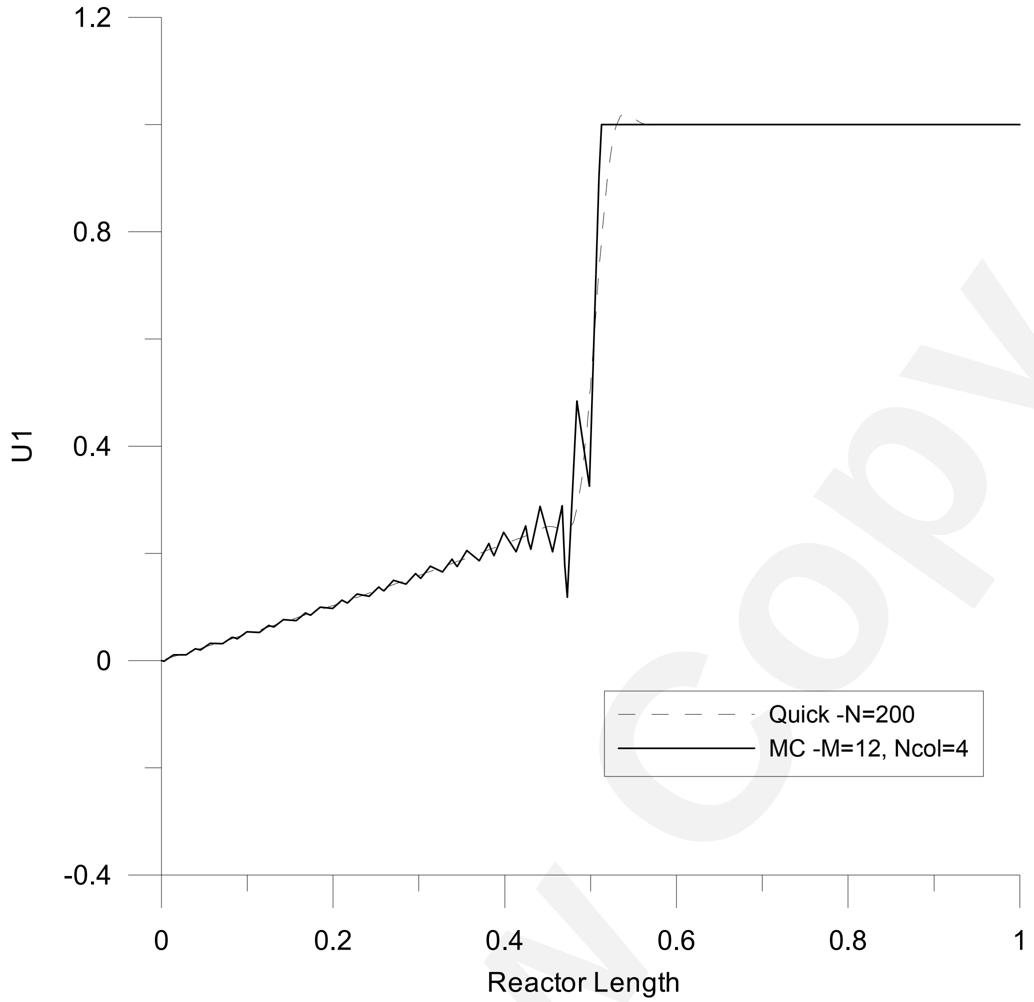

Figure (4): Dynamic concentration profile for species A at t=0.5 using moving collocation method (M=12, Ncol=4) and QUICK method (N=200).

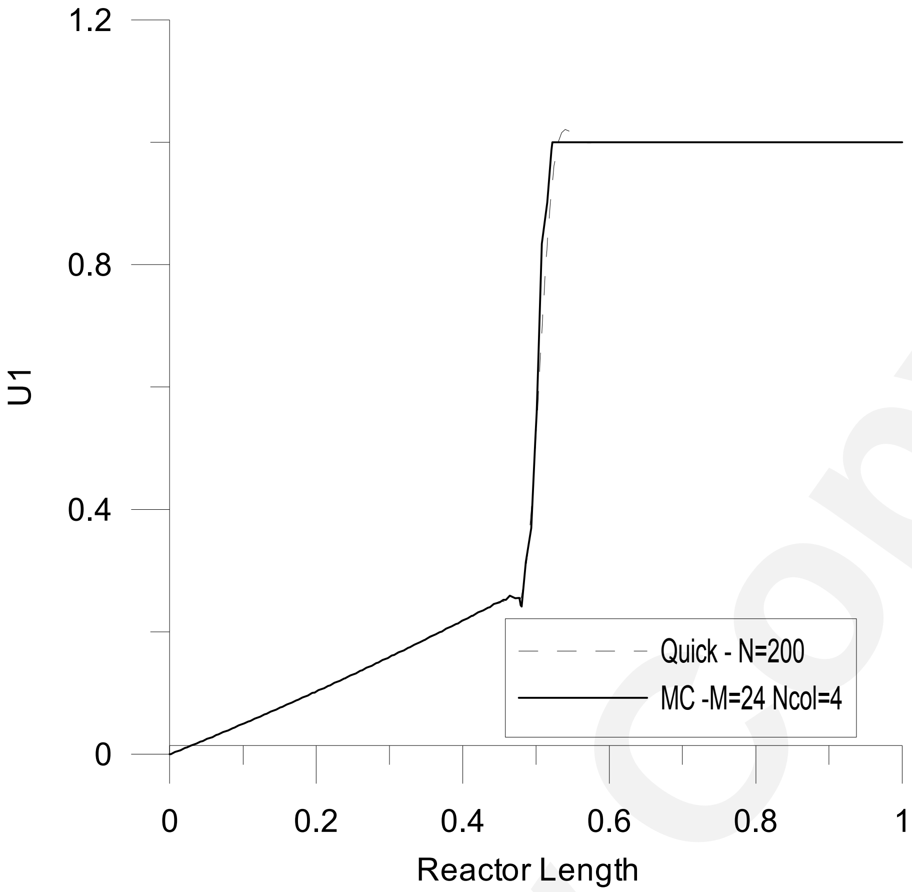

Figure (5): Dynamic concentration profile for species A at t=0.5 using moving collocation method (M=24, Ncol=4) and QUICK method (N=200).

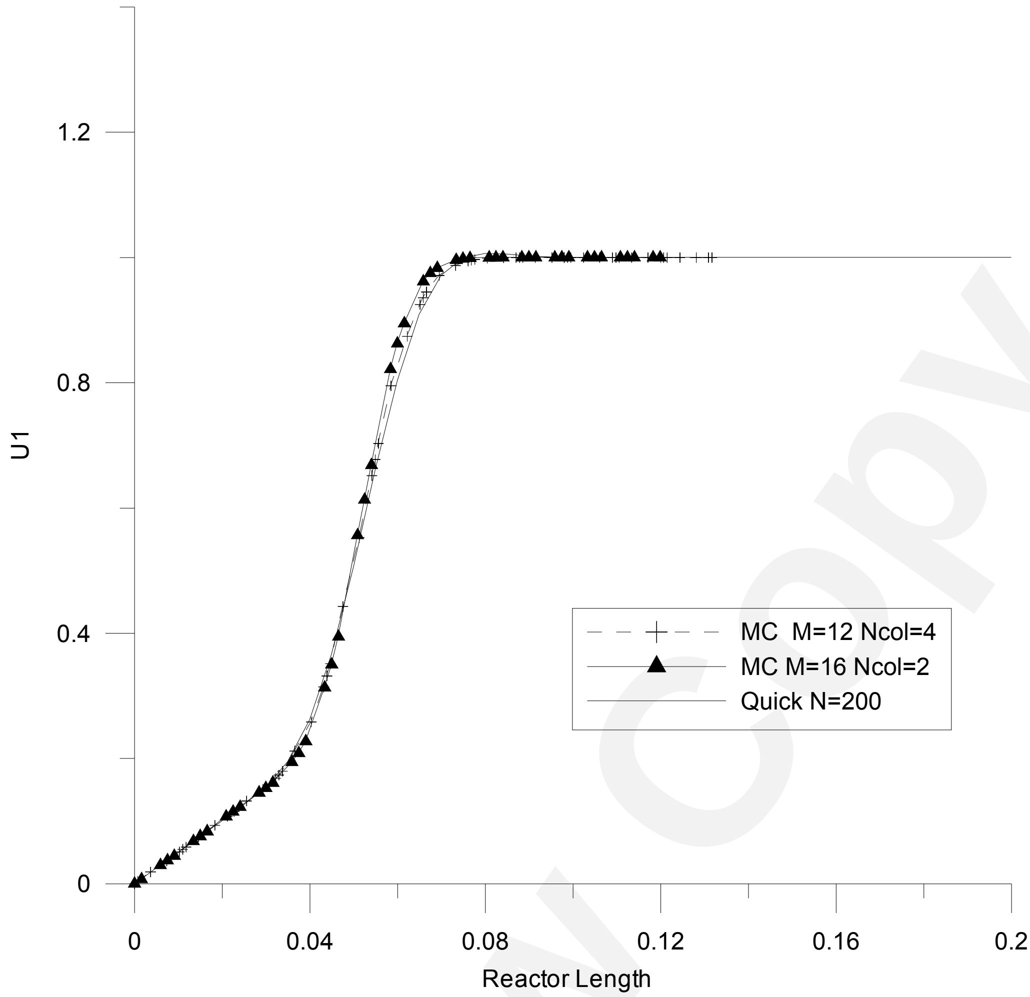

Figure (6): Dynamic concentration profile for species A at t=0.5 using moving collocation method and QUICK method for V=0.1.