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Studies on the Method of Orthogonal Collocation VI: A Moving Collocation Method for the Solution of the Transient Heat Conduction Problem

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Abstract. A new moving collocation method is introduced for solving the problem of time-dependent heat conduction with source term in one dimension. The method is based on dividing the solution domain into active and inactive zones. The numerical results show that the proposed method is able to simulate the sharp profile at short time with very few collocation points as opposed to the global collocation method.

Notation

- a Shape factor
- Bi Biot number
- N Number of collocation points
- r Dimensionless distance
- t Dimensionless time
- u Dimensionless temperature or concentration
- u_s Surface temperature or concentration
- w Quadrature weights
- λ Dimensionless distance of the inactive zone

Introduction

For the numerical solution of time-dependent partial differential equations, which involve large solution variations, a variety of numerical methods have been presented to gain significant improvement in accuracy over traditional fixed grid sizes. The problems of transient heat conduction and material diffusion are examples of such problem. The conduction problem has attracted the attention of many investigators. Finlayson [1]

presents some of the numerical methods used for solving the transient conduction or diffusion problems including finite difference, finite element and orthogonal collocation. The collocation method has several important advantages over the other discretization methods. It provides a high order of convergence, gives a continuous approximate solutions, and easily handles general boundary conditions while still being simple to program.

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 [2] 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 in part II of this series by Soliman and Ibrahim [3]. 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. Yoshida *et al.* [4] used a similar approach to solid gas reactions in which a moving front naturally exists.

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 steepness profile observed for transient heat conduction and diffusion problems. However, the present method does not require the knowledge of the asymptotic solution, which is not easy to obtain for a general problem.

Moving Collocation Method Formulation

Consider the one-dimensional transient heat conduction problem with source term represented in the form:

$$\frac{\partial u}{\partial t} = \frac{1}{r^a} \frac{\partial}{\partial r} \left(r^a \frac{\partial u}{\partial r} \right) - f(u)$$
(1)

supplemented with the boundary conditions:

$$\frac{\partial u}{\partial r} = 0$$
 at $r = 0$, $t \ge 0$ (2)

$$\frac{\partial u}{\partial r} = Bi(1 - u_s) \qquad \text{at } r = 1, \quad t > 0 \tag{3}$$

and the initial conditions:

at
$$t = 0, u = 0$$
 for $r \in [0, 1]$ (4)

where u is the dimensionless temperature, u_s is the surface temperature, r is the dimensionless distance, Bi is the Biot number, a, the shape factor, takes the value of 0, 1, 2 for a slab, cylinder and sphere respectively and f(u) is the non-linear source term.

A number of collocation methods have been developed to solve the conduction problem for short times. Villadsen and Michelsen [2] have proposed two methods. In the first, they relate the needed number of collocation points to the Biot number while the second method relates the heat flux at the surface to the average temperature. Both method suffer from inaccuracy at short time because of the steepness of the temperature profile. In this work we use the second method of Villadsen and Michelsen [2] for long time and develop a new adaptive method for short time.

Long Time Formulation

For long time, the temperature gradient at the external surface is given as follows:

$$\frac{\partial u}{\partial r}\Big|_{r=1} = \frac{\partial \int r^a u dr}{\partial t} + \int r^a f(u) dr = Bi(1-u_s)$$
(5)

Using Radau quadrature, we can write the average temperature as:

$$\overline{u} = \int_{0}^{1} r^{a} u dr = \sum_{i=1}^{N} w_{i} u_{i} + w_{N+1} u_{s}$$
(6)

and the non-linear source term as:

$$\int_{0}^{1} r^{a} f dr = \sum_{i=1}^{N} w_{i} f_{i} + w_{N+1} f_{s}$$
(7)

where N is the number of collocation points and wi's are the quadrature weights.

Now we can express the long time equations (5) in the form:

$$\frac{du_s}{dt} = \frac{Bi(1-u_s) - \sum_{i=1}^{N} w_i \frac{du_i}{dt} - \sum_{i=1}^{N} w_i f_i - w_{N+1} f(u_s)}{w_{N+1}}$$
(8)

The time derivatives of the temperature at the collocation points are obtained by applying the collocation method to the original equation (Eq. 1) to obtain

$$\frac{du_i}{dt} = \sum_{j=1}^N (B_{ij} + \frac{a}{r_i} A_{ij}) u_j + (B_{i,N+1} + \frac{a}{r_i} A_{i,N+1}) u_s - f(u_i) \qquad i = 1, 2, \dots, N$$
(9)

where A's and B's are the weights of the discretized first and second derivatives, respectively.

The collocation points are chosen as the zeros of Jacobi orthogonal polynomials $P_n^{\alpha,\beta}(x)$ satisfying the orthogonality conditions:

$$\int_{0}^{1} (1-x)^{\alpha} x^{\beta} P_{n}^{\alpha,\beta}(x) P_{m}^{\alpha,\beta}(x) d = \mathfrak{A} \qquad n \neq m$$
(10)

with

$$\alpha = 1, \beta = (a - 1)/2$$
 and $x = r^2$

Short Time Formulation

For short time, we divide the domain into two zones; a zone of temperature change and a zone of no temperature change. In order to define the intermediate boundary zone we make use of the following transformation:

$$z^{2} = \frac{\left[r - \lambda(t)\right]^{2}}{\left[1 - \lambda(t)\right]^{2}} \qquad \text{for} \quad \lambda \le r \le 1$$
(11)

The zero temperature zone is given by:

$$u = 0$$
 for $0 \le r \le \lambda$ (12)

Consider the following definition for the temperature:

$$u = u_s v \tag{13}$$

such that the surface boundary condition becomes:

$$v\Big|_{z=1} = 1 \tag{14}$$

Substituting Eqs. (11 and 13) in Eqs. (1 and 5) we have:

$$\frac{\partial v}{\partial t} = \frac{1}{(1-\lambda)^2} \left[\frac{\partial^2 v}{\partial^2 z} + \frac{a(1-\lambda)}{z(1-\lambda)+\lambda} \frac{\partial v}{\partial z} - \left(\frac{1-z}{2} \frac{\partial v}{\partial z} - \frac{v}{2}\right) \frac{d(1-\lambda)^2}{dt} - \frac{(1-\lambda)^2 f(u)}{u_s} \right] - \frac{v}{u_s(1-\lambda)} \frac{d[u_s(1-\lambda)]}{dt}$$
(15)

and

$$\frac{d}{dt}\left[(1-\lambda)u_s\int_0^1(z(1-\lambda)+\lambda)^a v dz\right] + (1-\lambda)\int_0^1(z(1-\lambda)+\lambda)^a f(u_s v) dz = Bi(1-u_s)$$
(16)

In addition to these equations, we need an extra equation to determine the boundary of the active zone. In this work, we consider the following condition:

$$z = 0$$
 $(r = \lambda)$ $v(0)\frac{\partial^2 v}{\partial z^2} = 0$ (17)

The initial conditions needed to solve Eq. (15) is obtained as its limit as λ goes to 1. This leads to the equation:

$$\frac{d^2v}{dz^2} = \frac{A(1-z)}{2} \frac{dv}{dz}$$
(18)

subject to the same boundary conditions (2, 14, 17);

where A is the initial condition for the moving front $\frac{d(1-\lambda)^2}{dt}$.

The time derivatives of the temperature at the collocation points for short times are obtained by applying the collocation method to Eq. 15 to obtain:

$$\frac{dv_{i}}{dt} = \frac{1}{(1-\lambda)^{2}} \left[\frac{\sum_{j=1}^{N} B_{ij}v_{j} + B_{i,N+1} + \left(\frac{a(1-\lambda)}{z(1-\lambda)+\lambda} - \frac{1-z}{2}\frac{d(1-\lambda)^{2}}{dt}\right) \left(\sum_{j=1}^{N} A_{ij}v_{j} + A_{i,N+1}\right) \right] \\ - \frac{v_{i}}{2}\frac{d(1-\lambda)^{2}}{dt} - \frac{(1-\lambda)^{2}f(u_{i})}{u_{s}} \\ - \frac{v_{i}}{u_{s}(1-\lambda)}\frac{d[u_{s}(1-\lambda)]}{dt} \\ i = 1, 2, \dots, N$$
(19)

Numerical Algorithm

The algorithm for the solution of Eqs. (1-4) can be summarized as follows:

- 1. Solve the system of N+1 algebraic equations obtained by substituting λ =1 in Eq. (19) and Eq. (17). This serves as initial conditions.
- 2. Solve the N+1 differential Eqs. (16, 19) together with the algebraic Eq. (17) using initial temperature profile obtained in step (1) for v_i , u_s , and λ until $\lambda = 0$. DASSL code [5] for the solution of differential algebraic equations can be used for this purpose.
- 3. When λ becomes zero, switch to the solution of the N+1 differential Eqs. (8-9) for v_i , and u_s .

Numerical Results

The developed method is applied to the case of a slab (a=0) with and without source terms. The proposed moving collocation (MC) method is compared with the global collocation method (GC) for three cases; transient heat conduction, transient diffusion with linear source term (first order chemical reaction), and transient diffusion with non-linear source term (second order chemical reaction). The performance of the proposed method is examined by plotting the short time profile for time=0.001 and by plotting the average temperature for the time period (0 to 0.2).

Case 1: Transient heat conduction

For this case the source term is set to zero. The exact solution can be obtained analytically using the separation of variable method. The exact solution of the heat conduction problem in a slab is:

$$u(t,r) = 1 - 4\sum_{m=1}^{\infty} \frac{\sin(\alpha_m)}{2\alpha_m + \sin(2\alpha_m)} \exp(-\alpha_m^2 t) \cos(\alpha_m r)$$

where α 's are the roots of the equation:

$$\tan(\alpha) = \frac{Bi}{\alpha}$$

The roots can be found numerically or graphically. For the case of Bi=100, the first five roots are:

 $\alpha_1 = 1.5552$, $\alpha_2 = 4.6658$, $\alpha_3 = 7.7764$, $\alpha_4 = 10.8871$, $\alpha_5 = 13.9981$

We consider the high Biot number case since for low Biot numbers, the temperature profiles are not very steep at initial time. For the case Bi=100, Figs. 1 and 2 show the

temperature profile along the slab length at t=0.001. It can be seen that for one collocation point the moving method is much better than the global collocation method as shown in Fig. 1. Fig. 2 shows that when using four collocation points, the moving collocation method becomes more accurate and approaches the exact solution while the global method exhibits oscillatory behavior in the no temperature change zone. In Fig. 3, the average temperature profiles for both methods are plotted. The moving method with one point is more accurate than the global method with one collocation point.

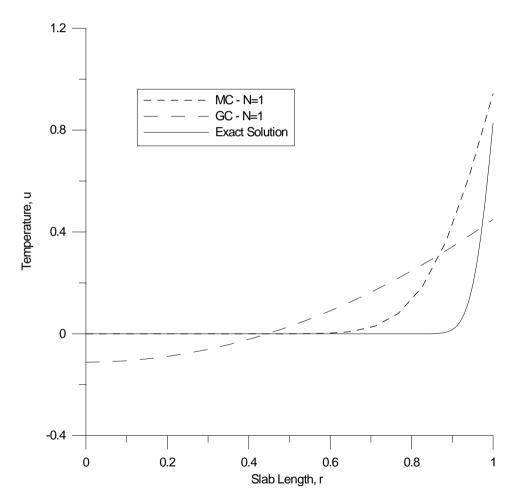


Fig. 1. Comparison of temperature profiles along the slab at t=0.001.

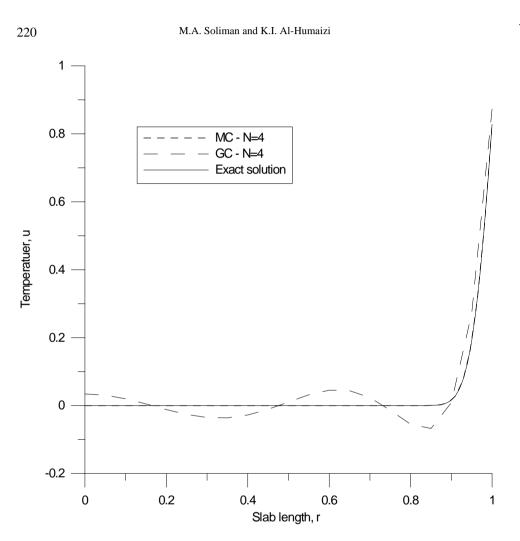


Fig. 2. Comparison of temperature profiles along the slab at t=0.001. Collocation methods with 4 points.

Case 2: Transient diffusion with a first-order chemical reaction

The source term for this case is represented by:

$$f = ku$$

with k=100 and Bi=100. Fig. 4 shows that the performance of moving collocation method for one collocation point is much better than that of the global method for short time solution t=0.01. For the case of four collocation points, both methods predictions are very close to the exact solution. Fig. 5 shows the superiority of the moving method over the traditions method for longer time period.

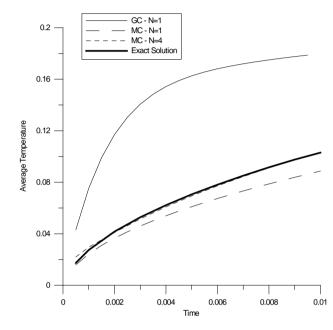


Fig. 3. Comparison of average temperature for different methods.

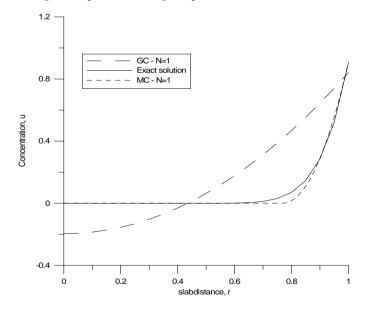


Fig. 4. Comparison of temperature profiles along the slab at t=0.01.

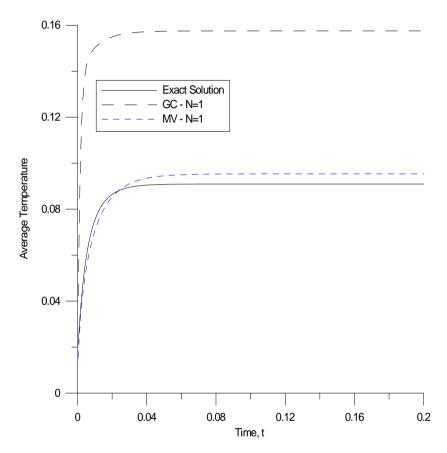


Fig. 5. Comparison of average temperature for diffierent methods for the diffusion problem with 1st order reaction.

Case 3: Transient diffusion with second-order chemical reaction

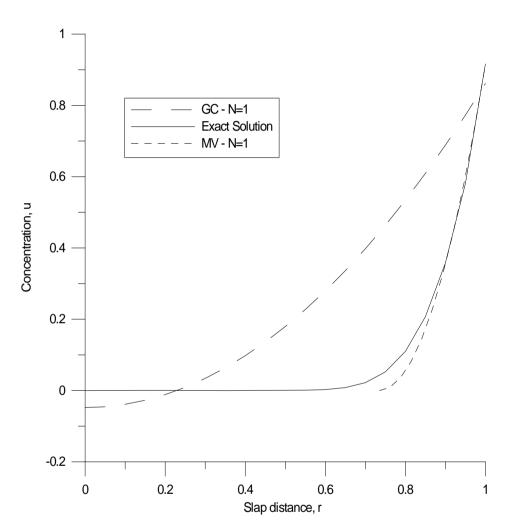
The source term for this case is represented by:

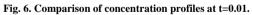
$$f = ku^2$$

with *k*=100 and Bi=100.

In Fig. 6, we plot the transient temperature profiles along the slab at t=0.01. Similar to the previous cases, the moving collocation method gives very close solution to the exact solution with one collocation point in the active zone. Figure 7 shows that the moving collocation predicts the average concentration much better than the global method.

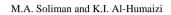
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Conclusion

A moving collocation method is developed in this paper for transient heat conduction and mass diffusion problems. The numerical results show that accurate solutions can be obtained with very few collocation points as opposed to the global collocation method, which requires more collocation points to be able to simulate sharp profiles which occurs at short time.



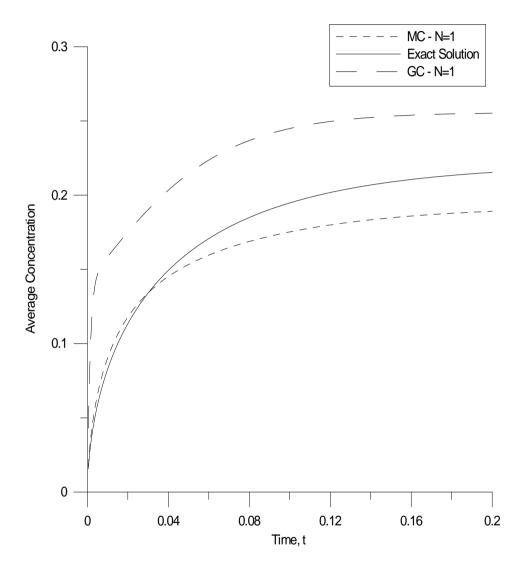


Fig. 7. Average concentration profile for the diffusion case with 2nd order reaction.

References

 Finlayson, B. Non-linear Analysis in Chemical Engineering. New York: McGraw-Hill, 1980.
 Villadsen, J. and Michelsen, M.I. Solution of Differential Equation Models by Polynomial Approximation. New Jersey: Prentice Hall, 1978.

- Soliman, M.A. and Ibrahim, A.A. "Studies on the Method of Orthogonal Collocation II: An Efficient Numerical Method for the Solution of the Transient Heat Conduction Problem." *J. King Saud Univ.*, 11, [3] Eng. Sci., No. 2 (1999), 175-190.
- Eng. Sci., NO. 2 (1999), 175-190.
 Yoshida, K., Kunii, D. and Shimizu, F. "Application of Collocation Techniques for Moving Boundary Problems in Solid-gas Reactions." J. Chem Eng. Japan, 8 (1975), 417-419.
 Petzold, L.R.. A Description of DASSL: A Differential/Algebraic System Solver. Livermore, CA: SAND82-8637, Sandia Labs, 1982. [4]
- [5]

دراسات على طريقة التنظيم المتعامد: طريقة التنظيم المتعامد المتحركة لحل مسألة التوصيل الحراري الانتقالي

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(قدم للنشر في ٢٨/٢٨ /٢٠٠٤م ؛ قبل للنشر في ٢٨/٢٩م)

ملخص البحث. يركز هذا البحث على تطوير طريقة عددية حديثة مبنية على طريقة التنظيم المتعامد لحل مسألة التوصيل الحراري أو الانتشار المادي المتغير مع الوقت في اتجاه واحد مع وجود مصدر داخلي للحرارة أو المادة. تعتمد هذه الطريقة على تقسيم الحل في الوقت الابتدائي إلى قسمين متحركين مع الوقت: قسم متغير وقسم جامد حيث يتم تركيز نقاط التنظيم المتعامد في القسم المتغير. أظهرت النتائج العددية أن الطريقة المقترحة قادرة على وصف الحل الانتقالي السريع بعدد قليل من نقاط التعامد مقارنة مع الطريقة التقليدية.