J. King Saud Univ., Vol. 11, *Eng. Sci.* (2), pp. 175-190, (A.H. 1419/1999)

CHEMICAL ENGINEERING

Studies on the Method of Orthogonal Collocation II. An Efficient Numerical Method for the Solution of the Transient Heat Conduction Problem

Mostafa Ali Soliman and A.A. Ibrahim
Department of Chemical Engineering, College of Engineering, King Saud University, P.O. Box 800, Riyadh 11421, Saudi Arabia

(Received 10 December 1997 ; accepted for publication, 11 May 1998)

Abstract. An efficient numerical method for the solution of the transient heat conduction problem is developed using the orthogonal collocation method. The method is based on dividing the domain of temperature change into two zones; a zone for which the temperature profile is steep and a zone with no temperature change. As time increases the inactive zone disappears and a modified collocation method is used.

Introduction

The problem of transient heat conduction in a body has attracted the attention of many investigators. Finlayson [1] presents some of the methods used for its numerical solution including finite difference, finite element and orthogonal collocation. Villadsen and Michelsen [2] pointed to the need for applying special methods for short time since the steepness of profile at this period necessitates the use of a large number of collocation points which in turn increases the stiffness of the differential equations making them more difficult to solve. Soliman and Ibrahim [3] applied a one point collocation to the problem. Thus an approximate solution is obtained. We used in this work the concept of dividing the domain for short time into an active zone and an inactive (dead zone). In this paper we extend this approach to multi-point orthogonal collocation method. In addition the method is applied successfully to transient diffusion problems with chemical reactions. Only one dimensional conduction is considered.

Method Development

The transient heat conduction problem is represented by

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial r^2} + \frac{a}{r}\frac{\partial u}{\partial r} \tag{1}$$

with the initial condition

$$\text{at} \qquad t = 0, u = 0 \qquad \text{for} \qquad r \in [0, 1] \tag{2}$$

and the boundary conditions

$$\frac{\partial u}{\partial r} = 0 \qquad \text{at } r = 0, \qquad t \geq 0 \tag{3}$$

$$\frac{\partial u}{\partial r} = Bi(1 - u_s) \qquad \text{at } r=0, \qquad t > 0 \tag{4}$$

where u is the dimensionless temperature, u_s is the surface temperature, r is the dimensionless distance, and a takes the values of 0,1,2 for a slab, cylinder and sphere respectively.

Two collocation methods have been suggested by Villadsen and Michelsen [2]. One of them gives collocation points which depend on Biot number Bi. This is difficult to apply in multi-point collocation. The other method relates the heat flux at the surface to the average temperature. Either method suffers from inaccuracy at short time because of the steepness of the temperature profile. In this paper we use the second method for long time and develop a method suitable for short time.

For long time, we notice that

$$\left.\frac{\partial u}{\partial r}\right|_{r=1} = \frac{\partial \int_0^1 r^a \, u \, dr}{\partial t} = Bi(1 - u_s) \tag{5}$$

Using Radau quadrature, we could write the average temperature as

$$\bar{u} = \int_0^1 r^a \, u \, dr = \sum_{i=1}^{N} w_i \, u_i + w_{N+1} \, u_s \tag{6}$$

where N is the number of collocation points, and w_i's are the quadrature weights obtained from programs presented in reference[2]. Thus equation (5) can be written as

$$\frac{du_s}{dt} = \frac{Bi(1-u_s) - \sum_{i=1}^{N} w_i \frac{du_i}{dt}}{w_{N+1}} \tag{7}$$

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

$$\frac{du_i}{dt} = \sum_{j=1}^{N}(B_{ij} + \frac{a}{r_i}A_{ij})u_j + (B_{i,N+1} + \frac{a}{r_i}A_{i,N+1})u_s \qquad i = 1,2,\ldots,N \tag{8}$$

where A's and B's are the weights for 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

$$\int_0^1 (1-x)^{\alpha} x^{\beta} P_n^{\alpha,\beta}(x) P_m^{\alpha,\beta}(x)\, dx = 0 \qquad n \neq m \tag{9}$$

with $\alpha = 1, \beta = (a-1)/2$ and $x = r^2$ (10)

For short time, we divide the domain into a zone of temperature change and a zone of no temperature change. We use the following coordinate transformation

$$z^2 = \frac{(r-\lambda(t))^2}{(1-\lambda(t))^2} \qquad \text{for} \qquad \lambda \le r \le 1 \tag{11}$$

and the temperature is given by

$$u = 0 \qquad \text{for} \quad 0 \le r \le \lambda \tag{12}$$

Also let

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

such that

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

substituting equations (11 and 13) in equations (1 and 5) we obtain

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

$$-\frac{v}{u_s(1-\lambda)}\frac{d[u_s(1-\lambda)]}{dt} \tag{15}$$

and

$$\frac{\partial (1-\lambda) u_s \int_0^1 (z(1-\lambda)+\lambda)^a \, v dz}{dt} = Bi\,(1-u_s) \tag{16}$$

In addition to these equations, we need an equation which determines the boundary of the active zone. From reference [4], the following condition is used,

$$v(o)\,\frac{\partial^2 v}{\partial z^2}\Big|_{z=0} = 0 \tag{17}$$

The solution of equations (11-17) has been attempted with little success because

(a) the equations are very stiff since they have (1-λ) in the denominator. This takes a value of zero at zero time.

(b) The usual collocation points obtained from equations (9) and (10) may not be the best for equation (15) since the nature of the equation changed due to the transformation (11). To avoid these difficulties the following averaging approach is developed.

We develop the method for the case of a slab (a=0) and then extend the method to other shapes.

First we apply the collocation method at points $z = z_i$ for equation (15) to obtain

$$\frac{dv_i}{dt} = \frac{1}{(1-\lambda)^2}\left[\sum_{j=1}^{N} B_{ij} v_j + B_{i,N+1} - \left(\sum_{j=1}^{N} A_{ij} V_j + A_{i,N+1}\right)\frac{(1-z_i)}{2}\frac{d(1-\lambda)^2}{dt} + \frac{v_i}{2}\frac{d(1-\lambda)^2}{dt}\right] - \frac{v_i}{u_s(1-\lambda)}\frac{d(u_s(1-\lambda))}{dt} \quad (18)$$

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

Then we require that the numerical integration of equation (15) is zero, i.e.

$$\sum_{i=1}^{N} w_i \frac{dv_i}{dt} = 0 \quad (19)$$

This would mean that although the individual vi's change with time, their average is constant. Next we make the following approximations:

$$\sum_{i=1}^{N} B_{ij} v_j + B_{i,N+1} = \phi^2 v_i, \qquad i = 1, 2, \ldots, N \quad (20)$$

$$\sum_{i=1}^{N} w_i \left(\sum_{j=1}^{N} A_{ij} V_j + A_{i,N+1}\right)\frac{(1-z_i)}{2} = \delta^2 v_i \quad (21)$$

where ϕ^2, δ^2 are parameters to be determined.
Substituting equations (18, 20 and 21) into equation (19) we obtain

$$\frac{d(1-\lambda)^2}{dt} = \frac{\left[\phi^2 - \frac{(1-\lambda)}{u_s}\frac{d(u_s(1-\lambda))}{dt}\right]}{(\delta^2 \quad 0.5)} \quad (22)$$

This is the equation needed to be solved for λ expressing the movement of the active zone. Together with equation (16), these are the only equations needed to be solved in the active zone.

Now to obtain ϕ^2 and vi's we need to solve the system of equations (20) subject to equation (17).

To obtain δ^2, we need to carry out the following asymptotic analysis. From a Laplace transform analysis of the governing equations (1 - 5) we obtain, as $t \to 0$, and $Bi > 0$,

$$\overline{u} = u_s (1-\lambda) \int_0^1 v \, dz \to Bi\, t \tag{23}$$

$$u_s \to \frac{2Bi\sqrt{t}}{\sqrt{\pi}} \tag{24}$$

We also notice that equation (20) is the discretized form for the equation describing diffusion with a first order reaction for which as $\phi \to \infty$, we have

$$\int_0^1 v \, dz \to \frac{1}{\phi} \tag{25}$$

From (23 - 25), we obtain

$$(1-\lambda) \to \frac{\sqrt{\pi t}\,\phi}{2} \tag{26}$$

For the case of $Bi \to \infty$ and $t \to 0$, we will have

$$(1-\lambda) \to \frac{2\sqrt{t}}{\sqrt{\pi}}\phi \tag{27}$$

Also as $t \to 0$, we have

$$\frac{(1-\lambda)}{u_s}\frac{d(u_s(1-\lambda))}{dt} \to \frac{d(1-\lambda)^2}{dt} \tag{28}$$

and as

$$u_s = 1 (Bi \to \infty) \quad \frac{(1-\lambda) d(u_s (1-\lambda))}{u_s \, dt} = \frac{1}{2}\frac{d(1-\lambda)^2}{dt} \tag{29}$$

Thus equation (22) becomes as $t \to 0$;

$$\frac{d(1-\lambda)^2}{dt} = -\frac{\phi^2}{(\delta^2 + 0.5)} \ (Bi \to 0) \tag{30}$$

and

$$\frac{d(1-\lambda)^2}{dt} - \frac{\phi^2}{\delta^2} \ (Bi \to \infty) \tag{31}$$

Now we choose

$$\frac{d(1-\lambda)^2}{dt} = \frac{\phi^2}{(\delta^2 + \frac{0.5}{1+Bi})} \ (\text{for } t \to 0) \tag{32}$$

and

$$\delta^2 = \frac{\left(\frac{4}{\pi} - 0.5\right) + Bi\frac{\pi}{4}}{(1+Bi)} \tag{33}$$

Note that the asymptotic values of $(1-\lambda)$ $(26, Bi \to 0)$ and $(27, Bi \to \infty)$ are satisfied in equations (32,33).

Now we can state the procedure for solving equations (1-4) for the case of a slab (a = 0) as follows:

(1) Solve the non-linear equations (20, 17) for ϕ^2, and vi. Calculate δ^2 from equation (33).

(2) Obtain $E_1 = \int_0^1 v\,dz$

(3) Solve equations (16, 22 (or 32 for $t \cong 0$))for u_s, $(1 - \lambda)$ until $\lambda = 0$.
Calculate $\bar{u} = u_s(1-\lambda)E_1$.

(4) Solve the differential equations (7, 8) and obtain $\bar{v}_i = \frac{u_i}{u_s}$ and

$E_2 = \int_0^1 \bar{v}\,dz$ until $E_2 = E_1$. Notice that $\bar{v}_i \neq v_i$. We continue the solution of step (3) using equations (7 and 8) and using the values $\bar{v}_i$ and calculate $\bar{u} = \int_0^1 u\,dr - u_s\int_0^1 \bar{v}\,dr$.

In effect we are using equations (7 and 8) for long time and correlating $\bar{u}$ for short time using equations(16 and 22).

Let us now extend the method to any shape and include a non-linear source term which could represent a diffusion problem with chemical reaction. In other words we would like to solve the equation.

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial r^2}+\frac{a}{r}\frac{\partial u}{\partial r}-R(u) \tag{34}$$

Without going into the derivation which is similar to what we have done, we need to solve the following equations for short time

$$\frac{d\bar{u}}{dt}=\frac{d}{dt}\left[(1-\lambda)u_s\int_0^1[z(1-\lambda)+\lambda]^a\, \upsilon dz\right]$$

$$=Bi(1-u_s)-(1-\lambda)\int_0^1 R(u_s\nu)[z(1-\lambda)+\lambda]^a\, \nu dz \ldots \tag{35}$$

$$\frac{d(1-\lambda)^2}{dt}=\frac{\left[\phi^2+0-\frac{(1-\lambda)}{u_s}\frac{d(u_s(1-\lambda))}{dt}\right]}{(\delta^2-0.5)} \tag{36}$$

where

$$\theta=\sum_{i=1}^{N} w_i\left[\frac{a(1-\lambda)(\sum_{J=1}^{N}(A_{ij}\,\nu_j)+A_{i,N+1})}{[(1-\lambda)z_i+\lambda)]}-\frac{(1-\lambda)^2 R(u_s\,\nu_i)}{u_s}\right]/\sum_{i=1}^{N} w_i\nu_i \ldots \tag{37}$$

with equation (32) as the limit of equation (37) as $t\to 0$.

Note that to evaluate the integrals in equation (35), we need to interpolate for values of v_i at the collocation points of $\alpha=1$, $\beta=0, 1/2$ so that we can evaluate integrals containing z_i (using weights for $\alpha=1, \beta=0$) and z_i^2 (using weight for $\alpha=1$, $\beta=1/2$).

For long time we solve the differential equations,

$$\frac{du_i}{dt} = \sum_{j=1}^{N} (B_{ij} + \frac{a}{r_i} A_{ij}) u_j + (B_{i,N+1} + \frac{a}{r_i} A_{i,N+1}) u_s - R(u_i) \tag{38}$$

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

and

$$\frac{du_s}{dt} = \frac{[Bi(1-u_s) - \sum w_i (\frac{du_i}{dt} + R(u_i))]}{w_{N+1}} - R(u_s) \tag{39}$$

The steps to be taken to switch from short time to long time equations are the same as for a slab.

Numerical Results

In this section we compare three methods for the solution of transient heat conduction and diffusion problems. The first method (M1) is the standard collocation method based on the discretization of the flux in equation (14). The second method (M2) is the collocation method using equations (7 and 8) or (38 or 39) in the whole time interval. The third method (M3) is the one developed in this paper based on patching together a short time and long time solution.

The following three examples are solved to illustrate the performance of the different methods. In all examples the exact solution is obtained by sixteen points standard collocation method.

Example 1: Transient Heat Conduction in a Slab

Three different values for Biot number (Bi = 1000, 10, 1) are tested. Different numbers of collocation points are tried, but in the Figures we only report the cases of N = 1, and N = 2. For the case of Bi = 1000, M1, M2, (Fig. 1) gives almost identical profiles because the surface temperature is accurately determined by either method. In fact M2 requires the solution of stiff equations (large Bi) and thus M1 is preferred in this case. M3 gives better results. For one point collocation method, M3 is much better than M1, M2. For the case of Bi = 10, Fig. 2, M2 becomes more accurate than M1 for the same number of collocation points and approaches the accuracy of M3. For the case of Bi = 1, Fig. 3, the performance of M2 becomes very close to that of M3 whereas M1 is not accurate for a low number of collocation points. The reasons are that for low Biot number the profile is not very steep at initial time and the surface temperature is not accurately determined by M1.

Example 2: Transient Diffusion with a First Order Reaction

In this case R(u) in equation (34) is given by

$$R(u) = 100\, u$$

In Fig. 4 the results are given for the case of Bi = 10. The present method (M3) performs much better than M2 and M1, even with one collocation point. The profile is steep for all time and thus for M3 the short time solution is used for all time for N = 1, 2.

Example 3: Transient Diffusion with a Second Order Reaction

In this case, R(u) is given by

$$R(u) = 100\ u^2$$

In Fig. 5 the results are given for the case of Bi = 10. M3 is the best for one point collocation. For two points collocation the performance of M2 is close to that of M3. For one point collocation the short time solution is used for M3 whereas for two collocation points the short time solution is used up to $t \cong 0.14$.

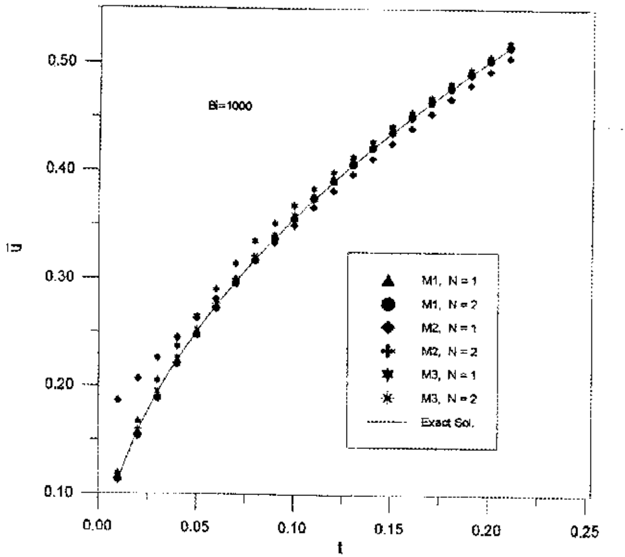

Fig. 1. Comparison of average temperature for different methods and number of collocation points(Example 1).

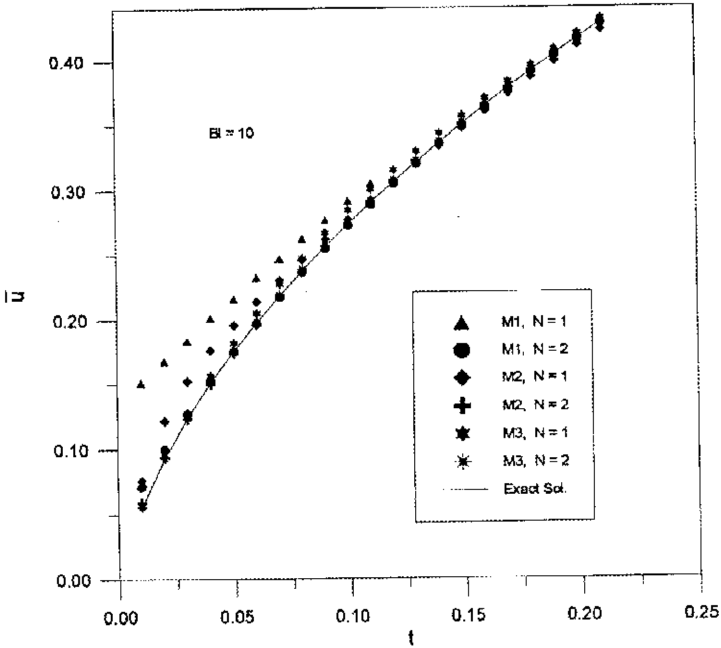

Fig. 2. Comprison of average temperature for different methods and number of collocation points (Example 1).

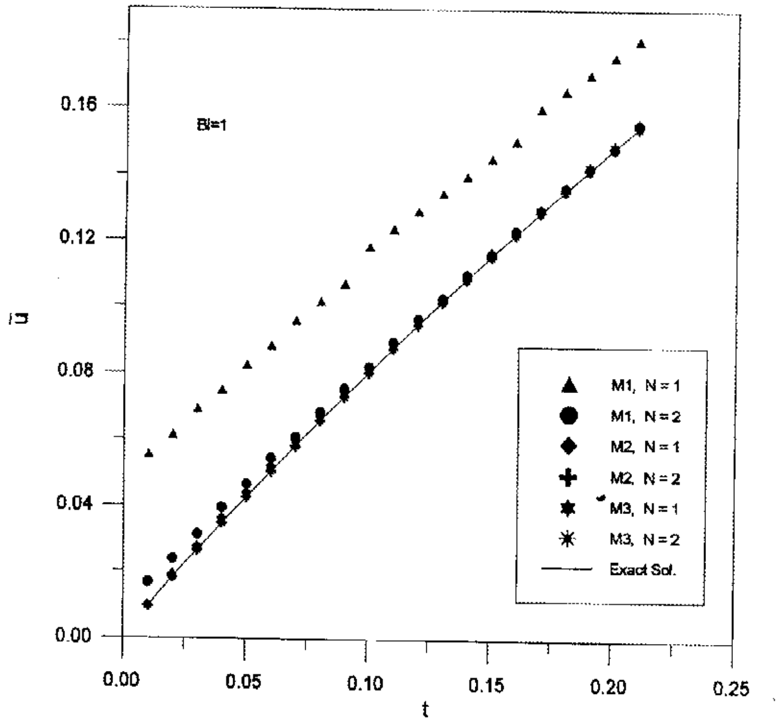

Fig. 3. Comprison of average temperature for different methods and number of collocation points (Example 1).

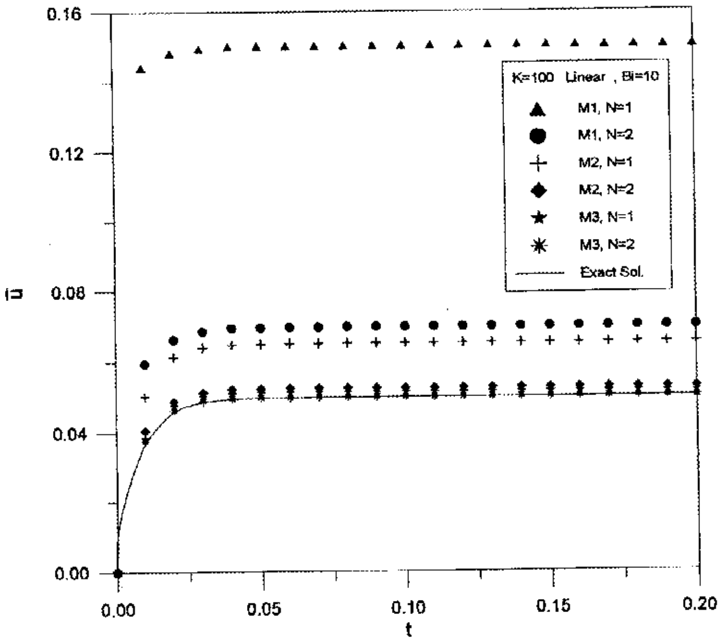

Fig. 4. Comprison of average temperature for different methods and number of collocation points (Example 2).

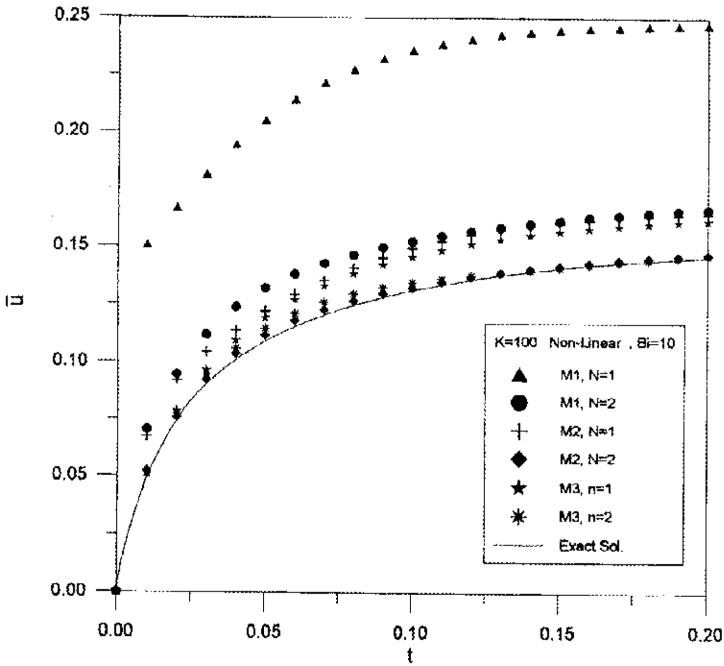

Fig. 5. Comprison of average temperature for different methods and number of collocation points (Example 3).

Conclusions

A collocation method is developed in this paper for transient heat conduction and diffusion problems. The method takes into consideration the steepness of the profile at short time. Numerical results indicate that the method gives accurate results with a low number of collocation points.

Notation

a	Shape factor in eq. (1)
Bi	Biot number
N	Number of collocation points
r	Dimensionless distance
t	Dimensionless time
u	Dimensionless temperature
u_s	Surface temperature
$\bar{u}$	Average temperature
w	Quadrature weights

Greek letters

λ	Dimensionless distance of the inactive zone

Acknowledgment. The authors gratefully acknowledge the Research Center at College of Engineering, King Saud university, Riyadh, Saudi Arabia for its support of the project.

References

[1] Finlayson, B. *Nonlinear Analysis in Chemical Engineering*. New York: McGraw-Hill, 1980.

[2] Villadsen, J. and M.L. Michelson. *Solution of Differential Equation Models by Polynomial Approximation*. Englewood Cliffs, New Jersey: Prentice Hall, 1978.

[3] Soliman, M.A. and A.A. Ibrahim. "Studies on the Method of Orthogonal Collocation, I. A One Point Collocation Method for the Transient Heat Conduction Problem." *J. King Saud Univ., Eng. Sci.*, (in Press).

[4] Soliman, M.A. "Collocation with Low Order Polynomials for Fast Reactions in Catalyst Particles." *Chem. Eng. Sci.*, 44 (1989), 1459.

دراسات على طريقة التنظيم المتعامد
٢ – طريقة عددية ذات كفاءة لحل مسألة التوصيل الحراري الانتقالي

مصطفى علي سليمان و أحمد عيديد إبراهيم
قسم الهندسة الكيميائية ،كلية الهندسة ، جامعة الملك سعود ، ص.ب ٨٠٠ ،
الرياض ١١٤٢١ ، المملكة العربية السعودية

(استلم في ١٠/١٢/١٩٩٧م ؛ وقبل للنشر في ١١/٥/١٩٩٨م)

ملخص البحث. طُورت طريقة عددية ذات كفاءة لحل مسألة التوصيل الحراري الانتقالي باستخدام طريقة التنظيم المتعامد . وتعتمد هذه الطريقة على تقسيم مجال درجة الحرارة إلى قسمين : قسم تنحدر فيه درجة الحرارة سريعاً وقسم لا يحدث فيه تغيّر في درجة الحرارة ، وبمرور الوقت يختفي القسم ذو درجة الحرارة الثابتة وتستخدم طريقة معدّلة للتنظيم المتعامد على كل المجال .