Solution of a Singular BVP of Reaction-diffusion in a Biocatalyst by OHAM

Mohammad Danish, Shashi Kumar and Surendra Kumar

***Abstract*— This research work presents the application of a newly developed efficient method namely, optimal homotopy analysis method (OHAM) to solve the nonlinear singular boundary value problems (SBVPs) which frequently arise in chemical and biochemical engineering. For demonstration, the reaction-diffusion process occurring in a spherical porous biocatalyst has been successfully solved with the Michaelis-Menten form of kinetics. The obtained results show a close agreement when compared with the numerical solutions and are found to be equally good or superior to those obtained by available approximate method. The OHAM is a versatile method and can be applied to solve any type of singular or nonsingular BVPs. Besides, its computer implementation in symbolic soft computing tools is also convenient.**

***Index Terms*— reaction-diffusion process, effectiveness factor, bio-catalyst, homotopy analysis method**

I. Introduction

NONLINEAR singular boundary value problems (SBVPs) are widely encountered in various engineering disciplines [1-5]. Due to the singularity and nonlinearity, these equations pose difficulties in obtaining their solutions and different analytical and numerical techniques are employed or devised to solve these problems [1-14]. Recently, an approximate method namely, homotopy analysis method (HAM) has been developed to solve different types of nonlinear problems. Many problems of engineering and allied disciplines have been successfully solved by it [7, 9]. In this work, we present the application of an efficient variant of HAM i.e., OHAM [10] to solve one such problem. For demonstration, the reaction-diffusion process inside a biocatalyst has been solved with the Michaelis-Menten kinetics [13, 14]. The resulting problem is a SBVP [6-8, 11, 12]. It should, however, be noted that other forms of kinetics can also be treated in a similar way. This problem relates to the design of a biocatalytic reactor and is of interest to chemical/biochemical engineers.

Manuscript received January 21, 2011.
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II. Homotopy Analysis Method

HAM is basically a powerful approximate analytical tool for solving various types of nonlinear equations [9]. The primary aim of HAM is to decompose the original difficult nonlinear equation into a family of infinite and easily solvable linear equations. The solutions of thus derived linear equations are then combined to yield the HAM series solution. The main advantages of this method are that it does not require the presence of small/large parameter unlike the perturbation method or delta decomposition method and can be applied to any type of nonlinearity [9]. Further, working of HAM reduces to those of other methods for a certain choice of auxiliary quantities defined later [9, 15]. Besides, it can easily be implemented in various symbolic soft computing tools e.g. Mathematica, Maple etc. A brief description of the HAM is presented below and the other details of this method can be found in the original work of Liao [9].

A. Selection of the Auxiliary Quantities and Construction of the Zero Order Deformation Equation

The first step in HAM is to choose the auxiliary quantities (parameters/functions/operators) corresponding to the given nonlinear equation, and to form the related zero order deformation equation [9]. The application of HAM is shown by considering a nonlinear BVP in the following operator form.

$$N[y(x)] = 0 \quad \text{with } B\left[y(x), \frac{dy(x)}{dx} \right] = 0 \tag{1}$$

Where N represents the nonlinear operator form of the differential equation and B is the associated boundary operator. The following zero order deformation equation corresponding to Eq. (1) is constructed [9]:

$$(1-\lambda)L[\psi(x,\lambda) - y_0(x)] \quad = \quad \lambda h H(x) N[\psi(x,\lambda)] \tag{2}$$

Where, $\lambda \in [0,1]$ is a hypothetical embedding parameter and $h \neq 0$ is an auxiliary parameter (also called convergence control parameter). $H(x) \neq 0$ is an auxiliary function and is added so as to ensure that in the later operations, the rule of coefficient of ergodicity is not violated [9]. L is an auxiliary linear operator with the conditions that the order of this operator is same as that of the highest order operator in Eq. (1) and $L[0] = 0$. $y_0(x)$ is the initial guess and $\psi(x,\lambda)$ is the unknown function. There are certain advantages of incorporating these auxiliary quantities: (i) applicability and effectiveness of HAM are enhanced while treating different types of nonlinear equations and (ii) for a particular set of these auxiliary quantities, the working of HAM reduces to those

ISBN: 978-988-18210-6-5
ISSN: 2078-0958 (Print); ISSN: 2078-0966 (Online)

of other approximate methods namely, Adomian decomposition method and δ-decomposition method [9, 15].

B. Formulation of the Higher Order Equation

It is clear from the Eq. (2) that as the parameter λ varies from 0 to 1, the unknown function $\psi(x,\lambda)$ varies from initial guess $y_0(x)$ to the solution $y(x)$ of the original equation, i.e. $\lim_{\lambda\to 0}\psi(x,\lambda)\to y_0(x)$ and $\lim_{\lambda\to 1}\psi(x,\lambda)\to y(x)$. By using Taylor's theorem the unknown function $\psi(x,\lambda)$ is expanded around $\lambda=0$ and the following series is obtained.

$$\psi(x,\lambda)=\psi(x,0)+\sum_{m=1}^{\infty}\frac{1}{m!}\frac{\partial^m\psi(x,\lambda)}{\partial\lambda^m}\bigg|_{\lambda=0}\lambda^m$$

$$=y_0(x)+\sum_{m=1}^{\infty}y_m(x)\lambda^m \tag{3a}$$

$$\text{Where, } y_m(x)=\frac{1}{m!}\frac{\partial^m\psi(x,\lambda)}{\partial\lambda^m}\bigg|_{\lambda=0} \tag{3b}$$

The m^{th} order deformation equation is constructed by substituting Eq. (3a) in Eq. (2) and by differentiating m times the resultant with respect to λ, and evaluating it at λ=0. m^{th} order deformation equation thus obtained provides the estimate of the m^{th} term of the HAM solution ($y_m(x)$). Following m^{th} order deformation equation is obtained.

$$L[y_m(x)-\chi_m y_{m-1}(x)] = hH(x)R_m[\vec{y}_{m-1},x] \tag{4a}$$

Where, the vector $\vec{y}_{m-1}$ denotes the set of functions $\vec{y}_{m-1}=\{y_0(x),y_1(x),...,y_{m-1}(x)\}$,

$$R_m[\vec{y}_{m-1},x] = \frac{1}{(m-1)!}\frac{\partial^{m-1}N[\vec{y}_{m-1}(x,\lambda)]}{\partial\lambda^{m-1}}\bigg|_{\lambda=0} \tag{4b}$$

$$\text{with } \chi_m = \begin{cases}0, & m\le 1\\ 1, & m\ge 2\end{cases} \tag{4c}$$

A slight rearrangement of the Eq. (4a) yields the following recursive scheme.

$$y_m(x) = \chi_m y_{m-1}(x)+hL^{-1}[H(x)R_m[\vec{y}_{m-1},x]] \tag{5}$$

Where, L^{-1} is the inverse of the linear operator L; for example, if $L=d/dx$ then one has $L^{-1}=\int_0^x[.]dx$ and so on.

C. Final Solution

Finally, with the help of Eqs. (3a) and (5), the approximate HAM solution is obtained for a pre-specified number of terms (n_T), i.e.

$$\psi(x,1) = y(x) \approx y_{HAM}(x) = y_0(x)+\sum_{m=1}^{n_T-1}y_m(x) \tag{6}$$

It has been shown by Liao [9] that if the auxiliary linear operator, auxiliary parameter, auxiliary function and initial guess are chosen properly then the above HAM series will converge to one of the solutions of Eq. (1). Generally, $H(x)$, L and $y_0(x)$ are chosen a priori to apply this scheme. However, in classical HAM, the value of h is basically selected from the valid region of the so-called h-curve [9]. In most of the problems, the valid region in the h-curve is flat and many values of h can be chosen. To avoid this uncertainty, we have adopted the OHAM which is described in the following section.

III. Optimal Homotopy Analysis Method

The main steps in the presented OHAM [10] are same as those of HAM, but in the OHAM, h is chosen by minimizing the sum of square of residual error of the HAM solution. The residual error can be found by substituting the HAM solution in the original Eq. (1), as shown below:

$$\text{Residual error at } x = N[y_{HAM}(x,h)] = N\left[\sum_{m=0}^{n_T-1}y_m(x,h)\right]$$

The sum of square of residual error is given by the following equation.

$$\Re=\int_0^1\left(N\left[\sum_{m=0}^{n_T-1}y_m(x,h)\right]\right)^2dx \tag{7}$$

For minimization of $\Re$, $\frac{\partial\Re}{\partial h}=0$, and the equation below can be employed for finding the optimal value of h.

$$\frac{\partial\Re}{\partial h}=\frac{\partial}{\partial h}\int_0^1\left(N\left[\sum_{m=0}^{n_T-1}y_m(x,h)\right]\right)^2dx=0 \tag{8a}$$

Since, the analytical integration in the above equation may be quite tedious, hence, the following simple but efficient approximation can be employed.

$$\frac{\partial\Re}{\partial h}\approx\frac{\partial}{\partial h}\sum_{i=1}\left(N\left[\sum_{m=0}^{n_T-1}y_m(x_i,h)\right]\right)^2=0 \tag{8b}$$

Where, Δx is the equispaced interval in the region of interest. Once, the value of h is available, the OHAM solution can easily be constructed by using Eq. (6).

IV. Solution of Reaction-Diffusion Process in a Biocatalyst

Consider an inert permeable spherical solid particle. Bacterial immobilization has been done inside the porous particle by usual methods, and this porous particle with bacteria immobilized inside it is termed as biocatalyst. This biocatalyst is immersed in a pool of liquid containing the substrate. It is assumed that the resistance due to film surrounding the biocatalyst is negligibly small under the operating conditions in the bioreactor. Thus, the substrate (A) diffuses inside biocatalyst and the biochemical reaction occurs therein simultaneously. The component mass balance for the substrate over a thin spherical shell inside the biocatalyst yields the following model equation with the associated BCs (boundary conditions).

$$D_e\left(\frac{d^2C_A}{dr^2}+\frac{2}{r}\frac{dC_A}{dr}\right)=\frac{r_mC_A}{K_m+C_A} \tag{9a}$$

$$\text{BC I: } C_A=C_{AS} \text{ at } r=R \text{ (catalyst surface)} \tag{9b}$$

$$\text{BC II: } \frac{dC_A}{dr}=0 \text{ at } r=0 \text{ (center of the catalyst)} \tag{9c}$$

In above model equation, it is assumed that the biochemical reaction follows Michaelis-Menten kinetics. The derivation of Eqs. (9) may be found in an excellent text book by Fogler [12]. Introducing the following dimensionless variables [13],

ISBN: 978-988-18210-6-5
ISSN: 2078-0958 (Print); ISSN: 2078-0966 (Online)

$$y = \frac{C_A}{C_{AS}}, x = \frac{r}{R}, \phi = \sqrt{\frac{(-r_{AS})R^2}{D_e C_{AS}}} = \sqrt{\frac{R^2 r_m}{D_e K_m (1+\beta)}},$$

$$\beta = \frac{C_{AS}}{K_m}$$

where ϕ denotes the Thiele modulus and ϕ^2 signifies the ratio of the intrinsic chemical reaction rate in the absence of mass transfer limitation to the rate of diffusion through the catalyst, i.e.

$$\phi^2 = \frac{\textit{reaction rate at the catalyst surface}}{\textit{diffusion rate through the catalyst pores}}$$

the Eqs. (9a) - (9c) are reduced into the following dimensionless forms:

$$\frac{d^2y}{dx^2} + \frac{2}{x}\frac{dy}{dx} - \phi^2 \frac{(1+\beta)y}{(1+\beta y)} = 0 \qquad (10a)$$

BC I: $y = 1$ at $x = 1$ (catalyst surface) (10b)

BC II: $\frac{dy}{dx} = 0$ at $x = 0$ (center of the catalyst) (10c)

Many researchers have investigated the above reaction diffusion problem in various contexts and a lot of literature is available. Different numerical schemes e.g. finite difference methods and orthogonal collocation methods have been applied to solve this problem and a good account of work can be found in various books [3-5, 11]. Recently, Adomian decomposition method and HAM have been applied to solve the same problem but in a slab geometry [6, 7]. Asymptotic matching approach has been applied in [13] however, again for a slab catalyst. For spherical catalyst, the restarted Adomian decomposition method has been used in [8].

Following quantities are defined for finding the OHAM solution of Eqs. (10).

$$N[y] = \frac{d^2y}{dx^2} + \frac{2}{x}\frac{dy}{dx} - \phi^2 \frac{(1+\beta)y}{(1+\beta y)}, \quad L^{-1} = \int_0^x \frac{1}{x^2}\int x^2[.]\,dx\,dx,$$

$$H(x) = 1,\ y_0(x) = C_2$$

And the following m[th] order deformation equation is constructed:

$$y_m(x) = \chi_m y_{m-1}(x) + h\int_0^x \frac{1}{x^2}\int x^2 R_m[\vec{y}_{m-1}, x]\,dx\,dx \qquad (11)$$

With the help of the above defined quantities and by iteratively employing Eq. (11), following four terms (n_T =4) OHAM solution is found.

$$y_{OHAM} = C_2 - \frac{C_2 h(3+3h+h^2)(1+\beta)\phi^2}{6+6C_2\beta}x^2 + \frac{C_2 h^2(3+2h)(1+\beta)^2\phi^4}{120(1+C_2\beta)^3}x^4 + \frac{C_2 h^3(-3+10C_2\beta)(1+\beta)^3\phi^6}{15120(1+C_2\beta)^5}x^6 \qquad (12)$$

C_2 and h can respectively be found from BC I and Eq. (8b); BC II is satisfied automatically.

As an example, one finds $C_2 = 0.20511$ and $h = -0.77673$ for ϕ=3, β=1 for n_T= 4 and the following OHAM solution is found by substituting these values in Eq. (12).

$$y_{OHAM} = 0.205106 + 0.504909x^2 + 0.276144x^4 + 0.0138409x^6 \qquad (13)$$

The following expression is obtained for the same values of parameters (ϕ=3, β=1) by using the relation of Li et al. [14].

$$y_{Li} = 0.106107 + 0.287786\,x^2 + 0.606107\,x^3 \qquad (14)$$

For several values of ϕ and β (ϕ=3, β=1; ϕ=3, β=10), the dimensionless concentration profiles computed by using OHAM have been shown in Figs. 1 & 2. These figures also show the numerically obtained profiles and those obtained by the approximate relation of Li et al. [14]. From these figures, following observations may be made:

- The OHAM solutions match closely with the numerically obtained solutions and are either equally good or are better than those obtained by Li et al [14].
- The accuracy of OHAM solutions increases with the increase in number of terms.

Further, Figs. 3 & 4 show the residual error profiles of the OHAM solution and the one obtained by the relation of Li et al. [14]. Here also, one observes that the residual error profiles decrease with the increase in number of terms.

Beside concentration profile, there exists another important quantity namely, effectiveness factor (η), that is relevant in the design of biochemical reactors.

Effectiveness factor is defined by the following relation:

$$\eta = \frac{\textit{actual reaction rate within catalyst pores}}{\textit{reaction rate at the surface conditions}}$$

For a spherical catalyst, the above definition can mathematically be expressed in dimensionless form as follows [13]:

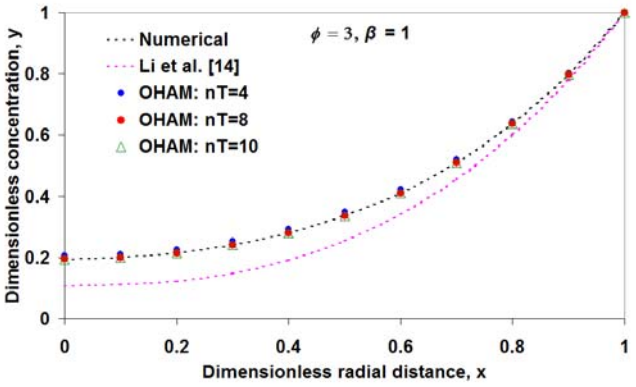

Fig. 1. Comparison of dimensionless concentration profiles obtained by different methods (ϕ =3, β =1)

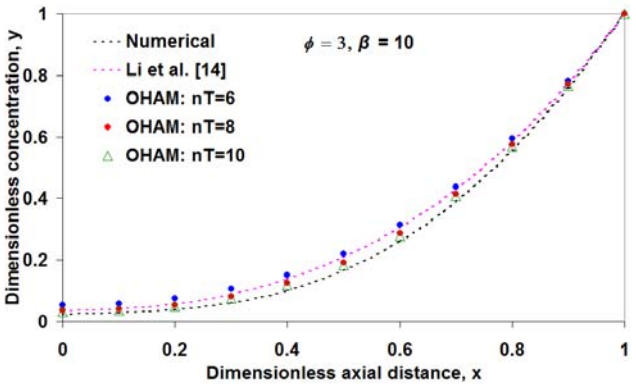

Fig. 2. Comparison of dimensionless concentration profiles obtained by different methods (ϕ =3, β =10)

ISBN: 978-988-18210-6-5
ISSN: 2078-0958 (Print); ISSN: 2078-0966 (Online)

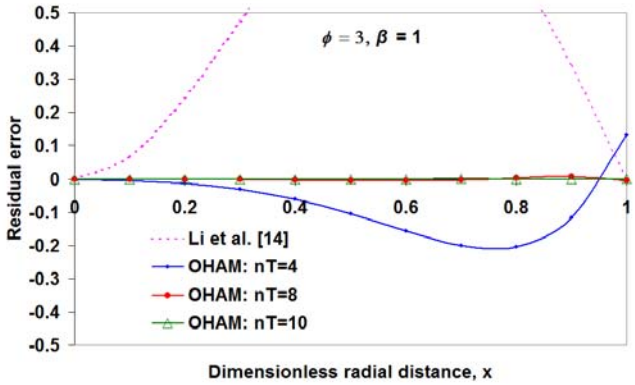

Fig. 3. Comparison of residual error profiles obtained by OHAM for various values of n_T with those obtained by relation of Li et al. [14]

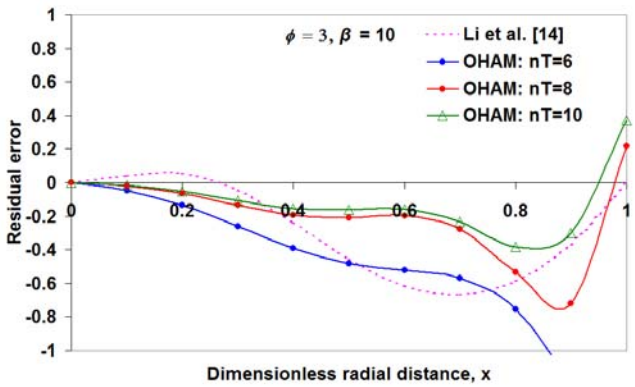

Fig. 4. Comparison of residual error profiles obtained by OHAM for various values of n_T with those obtained by relation of Li et al. [14]

$$\eta = \frac{3}{\phi^2}\frac{dy}{dx}\bigg|_{x=1} \tag{15}$$

Using Eq. (15) and four terms OHAM solution [Eq. (12)], one finds the following expression for η.

$$\eta_{OHAM} = \frac{1}{840(1+C_2\beta)^5} C_2 h(1+\beta)\Big(-840(3+3h+h^2)(1+C_2\beta)^4 + h^2(1+\beta)^2(-3+10C_2\beta)\phi^4 + 84h(3+2h)(1+\beta)(\phi+C_2\beta\phi)^2) + 84h(3+2h)(1+\beta)(\phi+C_2\beta\phi)^2\Big) \tag{16}$$

For different values of ϕ and β, the Table 1 shows the values of η obtained by using numerical method, OHAM and the relations provided by Li et al. [14]. It is clear that the OHAM predictions are close to those of numerical method. Besides, the error in the prediction of η decreases as one increases the terms in OHAM. One should be careful while comparing the results with those of Li et al. [14], since, dimensionless quantities defined in Li et al. [14] are different. It should also be noted that the approximate relation given by Li et al. [14] is specific to this particular equation as well as to the Michaelis-Menten form of kinetics whereas, OHAM presented in this paper is quite general and can be applied to other forms of equations [9].

TABLE I
COMPARISON OF EFFECTIVENESS FACTOR OBTAINED BY DIFFERENT METHODS

ϕ	β	η				
		Numerical solution	Li et al. [14]	OHAM (present work)		
				n_T = 6	n_T = 8	n_T = 10
3	1	0.7439	0.7980	0.7445	0.7441	0.7439
3	10	0.8679	0.8216	0.76534	0.8253	0.8474

V. Conclusions

The efficacy of OHAM has been demonstrated by solving a singular boundary value problem of chemical/bio-chemical engineering namely, reaction-diffusion process inside a porous biocatalyst in which occurring biochemical reaction follows Michaelis-Menten kinetics. The results thus obtained match well with the numerical solutions and prove its effectiveness.

OHAM is quite advantageous as it is applicable to any type of nonlinearity and can easily be programmed in symbolic languages as available in standard mathematical soft computing tools e.g. Mathematica.

Acknowledgment

M. Danish is thankful to his parent institution A.M.U., Aligarh-202002, U.P., India for kindly granting study leave to pursue his doctoral work at I.I.T. Roorkee, Roorkee-247667, Uttarakhand, India.

Nomenclature

C_2	[-]	constant
C_A	[mol.m^{-3}]	concentration of species A inside the catalyst pores
C_{AS}	[mol.m^{-3}]	concentration of species A at the catalyst surface
D_e	[m^2.s^{-1}]	diffusion coefficient of species A inside the catalyst pores
K_m	[mol.m^{-3}]	parameter in Michaelis-Menten kinetics
n_T	[-]	total number of terms in HAM/OHAM solution
r	[m]	coordinate in the radial direction
r_m	[mol.m^{-3}.s^{-1}]	parameter in Michaelis-Menten kinetics
R	[m]	radius of the catalyst pellet
$\Re$	[-]	sum of square of residual error
x	[-]	dimensionless radial distance
$y(x)$	[-]	dimensionless concentration

Greek letters

λ	[-]	hypothetical embedding parameter in HAM/OHAM, $\lambda \in [0,1]$
ϕ	[-]	Thiele Modulus

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ISBN: 978-988-18210-6-5
ISSN: 2078-0958 (Print); ISSN: 2078-0966 (Online)

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ISBN: 978-988-18210-6-5
ISSN: 2078-0958 (Print); ISSN: 2078-0966 (Online)