ADOMIAN'S METHOD FOR HAMMERSTEIN INTEGRAL EQUATIONS ARISING FROM CHEMICAL REACTOR THEORY

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ABSTRACT: An ordinary differential equation with a parameter in the boundary conditions describes the steady state in an adiabatic tubular chemical reactor. In this paper, the problem is considered as a Hammerstein integral equation and solutions are obtained using Adomian's decomposition method.

KEYWORDS: Chemical Reactor Theory, Adomian's method, Hammerstein Integral Equations.

1 INTRODUCTION

We consider the mathematical model for an adiabatic tubular chemical reactor which processes an irreversible exothermic chemical reaction. For steady state solutions, the model can be reduced to the ordinary differential equation

$$u'' - \lambda u' + F(\lambda, \mu, \beta, u) = 0 \tag{1}$$

with boundary conditions

$$u'(0) = \lambda u(0) \quad u'(1) = 0 \tag{2}$$

where

$$F(\lambda, \mu, \beta, u) = \lambda\mu(\beta - u)\exp(u)$$

(see [1], [2]). The unknown u represents the steady state temperature of the reaction, and the parameters λ, μ and β represent the Peclet Number, the Damkohler Number and the dimensionless adiabatic temperature rise respectively. This problem has been studied by numerous authors (e.g. [1], [3], [4]) who have demonstrated numerically the existence of solutions (sometimes multiple solutions), for particular parameter ranges.

In order to develop results concerning the solution of (1)-(2), the problem can be converted, using Green's Function technique, into a Hammerstein integral equation

$$u(x) = \int_0^1 k(x, y) f(y, u(y)) dy \qquad 0 \le x \le 1 \tag{3}$$

where $k(x,y)$ is defined by

$$k(x,y) = \begin{cases} e^{\lambda(x-y)} & \text{if } 0 \le x < y \\ 1 & \text{if } y \le x \le 1 \end{cases}$$

and

$$f(y,u) = \mu(\beta - u)\exp(u);$$

(see [2]).

We consider (3) as an integral equation in the space $C[0,1]$ of continuous functions on the closed interval $[0,1]$ with norm defined by

$$\|u\| = \sup_{x\in[0,1]} |u(x)|.$$

Throughout, we assume λ and μ are positive, and β is nonnegative. The following existence and uniqueness theorem can be achieved using the Contraction Mapping Principle.

Theorem 1.1: For any $M > 0$, the Hammerstein integral equation (3) has a unique solution in $B(M) = \{u \in C[0,1] : \ \|u\| \le M\}$ provided

$$\mu < \min\{\frac{M}{\|K\|(\beta+M)e^M}, \frac{1}{\|K\|(|\beta-1|+M)e^M}\}$$

Proof: The given restriction of μ ensures that the Hammerstein integral equation (3) defines a contraction mapping on $B(M)$. The result follows from the application of the Contraction Mapping Principle and is given in [2].

This Hammerstein integral equation cannot be solved exactly. The purpose of this paper is to consider the application of Adomian's decomposition method which has been shown to be particularly well suited for the solution of Hammerstein integral equations (see [5]). An advantage of this method is that it produces an analytic approximation to the solution, i.e. a function defined on $[0,1]$, rather than approximate numerical values at a discrete set of points.

It is our experience that clear descriptions of Adomian's method are not readily available in the literature. Thus in Section 2, a brief formulation of the method is presented. The method was originally developed for stochastic equations [6], but our application and hence our description is restricted to deterministic equations. In Section 3, the method is applied to the Hammerstein integral equation (3) in two cases: (i) $\beta \neq 0$ and (ii) $\beta = 0$. In the latter case we verify that the method gives the expected unique trivial solution. Finally, in Section 4, the results for case (i) with particular values of the parameters are compared with numerical results for two more classical methods of solution.

2 FORMULATION OF ADOMIAN'S METHOD

Adomian's decomposition method is used for solving operator equations of the form

$$u = v + Nu \tag{4}$$

where $N : X \longrightarrow X$ is a nonlinear mapping from a Banach space X into itself and $v \in X$ is known. Since the method does not resort to linearization or assumptions of weak nonlinearity, the nonlinearities which can be handled are quite general and the solutions generated may be more realistic than those achieved by simplifying the model of the physical problem to achieve conditions required for other techniques [7].

Adomian's method assumes that the solution u can be expanded as an infinite series

$$u = \sum_{n=0}^{\infty} u_n \qquad u_n \in X \quad \forall n \tag{5}$$

and that the image Nu has an expansion

$$Nu = \sum_{n=0}^{\infty} A_n \qquad A_n \in X \quad \forall n. \tag{6}$$

Substituting (5) and (6) into (4) gives

$$\sum_{n=0}^{\infty} u_n = \sum_{n=0}^{\infty} A_n + v \tag{7}$$

which is satisfied formally if we set

$$\begin{aligned} u_0 &= v \\ u_{n+1} &= A_n \qquad \forall \;\; n = 0, 1, 2, \ldots . \end{aligned} \tag{8}$$

Thus, we need to determine the so called Adomian polynomials A_n, $n = 0, 1, 2, \ldots$. (We should point out that, as we shall see, they need not be polynomials.)

To determine the A_n's, a scalar parameter λ is introduced to set

$$u(\lambda) = \sum_{n=0}^{\infty} \lambda^n u_n \quad \in X \tag{9}$$

and

$$Nu(\lambda) = \sum_{n=0}^{\infty} \lambda^n A_n \quad \in X \tag{10}$$

so that (5) and (6) are special case of (9) and (10) respectively with $\lambda = 1$ and $u = u(1)$. That is $u(\lambda)$ and $Nu(\lambda)$ are assumed to be analytic vector valued function of λ both with radius of convergence greater than 1.

Now, (9) and (10) are Maclaurin expansions in X and as in [7] and [8], we can deduce that the coefficients A_n, $n = 0, 1, 2, \ldots$ are given by

$$A_n = \frac{1}{n!}\frac{d^n}{d\lambda^n} Nu(\lambda)|_{\lambda=0}. \tag{11}$$

Thus,

$$\begin{aligned} A_0 &= Nu(\lambda)|_{\lambda=0} = Nu_0 \\ A_1 &= \frac{d}{d\lambda} Nu(\lambda)|_{\lambda=0} = (DN)(u_0)u_1 \\ A_2 &= (DN)(u_0)u_2 + \frac{1}{2!}(D^2N)(u_0)u_1^2 \end{aligned} \tag{12}$$

and so on, where $D^rN(u_0)$ denotes the rth Fréchet derivative of N at $u_0 \in X$.

We should note that while A_n is a polynomial in $u_1, \ldots, u_n$, its dependence on u_0 is decided by the form of N and its derivatives. However, generally, A_n depends only on $u_0, u_1, \ldots, u_n$, so that (8) allows successive calculation of u_n, $n = 0, 1, 2, \ldots$. At any stage, the solution can be approximated by the partial sum $S_n = \sum_{i=0}^{n-1} u_i$. Various papers claim general proofs of the convergence of the Adomian's series to a solution of the nonlinear equation; see for example [5], [8], [9]. However, these are unconvincing and we have been unable to find a clear general proof of convergence of Adomian's method.

3 APPLICATION TO THE HAMMERSTEIN INTEGRAL EQUATION

Consider the general Hammerstein integral equation

$$u(x) = v(x) + \int_0^1 k(x, y) f(y, u(y)) dy \tag{13}$$

where k is continuous on $[0, 1] \times [0, 1]$ and f is continuous on $[0, 1] \times \mathbf{R}$.

This equation is in a form suitable for the application of Adomian's method, as derived in Section 2, with the nonlinear term $N : C[0, 1] \longrightarrow C[0, 1]$ defined by

$$Nu(x) = \int_0^1 k(x, y) f(y, u(y)) dy.$$

The Fréchet derivatives are given by

$$(DN)(u_0)u(x) = \int_0^1 k(x, y) f_2(y, u_0(y)) u(y) dy$$

(see [10]) where f_2 denotes the partial derivative of f with respect to its second variable, and in general

$$(D^nN)(u_0)(u_1, u_2, \ldots, u_n)(x) = \int_0^1 k(x, y) f_{(2^n)}(y, u_0(y)) u_1(y) u_2(y) \ldots u_n(y) dy,$$

where $f_{(2^n)}$ denotes the $n-$th partial derivative of f with respect to its second variable.

Now using (8) and (12), we can evaluate, successively

$$\begin{aligned} u_0 &= v \\ u_1 &= A_0 \\ &\vdots \\ u_n &= A_{n-1}. \end{aligned}$$

We apply this to the Hammerstein integral equation (3) in two cases.

Case 1 : $\beta \neq 0$

In this case our Hammerstein integral equation (3) modeling the chemical reaction, contains all three positive parameters λ, μ, β.

We consider (3) as an equation in $C[0,1]$ with $v \in C[0,1]$ and $N : C[0,1] \longrightarrow C[0,1]$ defined by

$$v(x) = 0, \qquad x \in [0,1]$$

and

$$Nu(x) = \mu \int_0^1 k(x,y)(\beta - u(y)) \exp u(y) dy.$$

The Fréchet derivatives at $u_0 \in C[0,1]$ are given by

$$(D^n N)(u_0)(u_1, \ldots, u_n)(x) = \mu \int_0^1 k(x,y)(\beta - n - u_0(y)) \exp[u_0(y)] u_1(y) \ldots u_n(y) dy.$$

Thus, from (8) and (12), we obtain

$$u_0(x) = v(x) = 0$$

$$u_1(x) = A_0(x) = \mu\beta \left[x - \frac{1}{\lambda}(e^{\lambda(x-1)} - 1) \right]$$

$$u_2(x) = A_1(x) = \mu^2\beta(\beta - 1) \left[e^{\lambda(x-1)} [\frac{x}{\lambda} - \frac{2}{\lambda} - \frac{3}{\lambda^2}] + \frac{x^2}{2} + \frac{2x}{\lambda} + \frac{(2 + e^{-\lambda})}{\lambda^2} \right].$$

Subsequent calculations to evaluate u_3, u_4, etc, to obtain numerical results in Section 5 have been done using the Computer Algebra Package, Maple.

What we do not have is a proof of whether the resulting series converges to a solution or not; but it seems that the convergence may depend on the parameters μ, β and λ. Even the most recent work of Adomian [7] does not address the issue of convergence. This clearly leaves scope for further work in this area.

Case 2 : $\beta = 0$

With $\beta = 0$ the nonlinear term in (3) becomes

$$f(y, u) = -\mu u \exp(u)$$

and thus $N : C[0,1] \longrightarrow C[0,1]$ is defined by

$$(Nu)(x) = -\int_0^1 k(x,y)\mu u(x)\exp(u(x))dy.$$

The Fréchet derivatives are given by the general formula

$$(D^n N)(u_0)(u_1,\ldots,u_n)(x) = -\mu \int_0^1 k(x,y)(n+u_0(y))\exp[u_0(y)]u_1(y)\ldots u_n(y)dy.$$

Following the procedure of Adomian's method, we have

$$u_0(x) = 0 \qquad \forall \quad x \in [0,1]$$

$$u_1(x) = A_0(x) = 0 \qquad \forall \quad x \in [0,1]$$

since $\quad u_0(y) = 0 \quad \forall \quad y \in [0,1]$.

Then, similarly,

$$u_2(x) = A_1(x) = 0 \qquad \forall \quad x \in [0,1]$$

since $\quad u_1(y) = 0 \quad \forall \quad y \in [0,1]$.

It is clear that, in this case

$$u_n = A_{n-1} = 0 \quad \in C[0,1] \qquad \forall \quad n$$

and Adomian's method give the obvious trivial solution $u = 0$. The method has worked, but does not produce any interesting results.

4 COMPARISON OF NUMERICAL RESULTS

To validate the application of Adomian's method to the Hammerstein integral equation (3), we compare the solution developed in Section 3 with numerical results from some classical techniques. The Contraction Mapping Principle used to prove the existence and uniqueness of the solution of the Hammerstein integral equation (3) gives an iterative procedure that is known to converge to this solution. However, the required integrations cannot be done analytically. Therefore, in applying the Contraction Mapping Principle, the integrations are evaluated numerically using the Trapezoidal rule.

For the following numerical results, the Computer Algebra Package, Maple is used. We note that we truncate the numerical results after the sixth decimal point. We use particular values of the parameters, $\lambda = 10$, $\beta = 3$, $\mu = 0.02$ (for $M = 2$, $\mu = 0.02$

satisfies Theorem 1.1). For such values for the parameters, a unique solution in $B(2) \in C[0,1]$ is guaranteed by the Contraction Mapping Principle. In evaluating the solution by applying the Contraction Mapping Principle, we use the Trapezoidal rule with a strip width $h = 0.025$.

For further comparison a shooting method has been applied to the original boundary value problem (1)-(2). We use the boundary condition at zero and assume the value of the solution at zero; then this initial value problem is solved using Maple and the value of $u'(1)$ is monitored. We seek the best initial value $u(0)$ to get $u'(1) = 0$. We find that $u(0) = 0.0060483735$ gives $u'(1) = -0.88 \times 10^{-6} \approx 0$.

On the other hand, for Adomian's method where the integration can be done analytically as above, there is a rapid convergence (the third and fourth iterations are almost identical). The following table gives a comparison of the results from the Contraction Mapping Principle, the shooting method and Adomian's method.

x	Contraction Principle	Shooting method	Adomian's method
0	0.006079	0.006048	0.006048
0.2	0.018224	0.018192	0.018192
0.4	0.030456	0.030424	0.030424
0.6	0.042701	0.042669	0.042669
0.8	0.054401	0.054371	0.054371
1	0.061459	0.061458	0.061458

As shown in the table, Adomian's method results agree with those of the shooting method up to the sixth decimal place. The results from the Contraction Mapping principle agree to at least three decimal place; but, these will involve errors due to the numerical integrating procedure used.

5 CONCLUSION

Adomian's method is relatively straightforward to apply at least with the assistance of a powerful Computer Algebra Package and, in simple cases, produces a series that can converge rapidly to known solution [7].

As shown in the previous section, for particular parameter values in our Hammerstein integral equation (3), Adomian's method appears to show rapid convergence to the unique solution obtained using the Contraction Mapping Principle. The accuracy of Adomian's method has been further confirmed by comparison with a numerical solution of the original boundary value problem obtained using a shooting method. This result confirms the view expressed by Some [5] who compared various numerical methods for solving Hammerstein integral equations and concluded that Adomian's method was fast and efficient.

However, we do not offer a proof of the convergence of Adomian's method in this application. Although a number of authors claim such results, no convincing proof of the convergence of the method is known to us. Convergence must depend on the nature of the nonlinearity. Clearly, one necessary condition is that the nonlinear mapping is Fréchet differentiable, but there may be stricter requirements. It is essential that such question be answered if Adomian's method is to be regarded as a robust algorithm for the numerical solution of nonlinear equations.

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