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APPROXIMATE ANALYTICAL SOLUTION OF NON-LINEAR INITIAL VALUE PROBLEM FOR AN AUTOCATALYSIS IN A CONTINUOUS STIRRED TANK REACTOR: HOMOTOPY ANALYSIS METHOD

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ABSTRACT

In this paper, a non-isothermal version of Gray and Scott autocatalytic reactions has been modeled using mass and energy balances. The approximate analytical solution of non-isothermal continuous stirred tank reactor in which two parallel autocatalytic reactions is derived by using the Homotopy analysis method (HAM). Our analytical results are compared with the numerical simulation and a satisfactory agreement is noted. The Homotopy analysis method is less computational and is applicable for solving other non-linear boundary value problem, because it contains the convergence control parameter h.

Keywords: *Gray-Scott model; Autocatalytic process; System of non-linear differential equations; Homotopy analysis method; Numerical simulation.*

INTRODUCTION

A chaotic system is a nonlinear deterministic system that shows a complex behavior. In general, for a certain set of parameter values, a nonlinear system can exhibit oscillations or even chaotic behavior. Chemical system can have complex dynamics due to their nonlinear nature. There are extensive theoretical and experimental studies indicating presence of complex chaotic behavior in chemical reactions and chemical reactors. Gray & Scott have investigated the behavior of an isothermal Continuous Stirred Tank Reactor (CSTR) with autocatalytic reaction [1]. They observed limit cycles and instabilities in such a system [2]. Lynch *et al.* showed that chaotic oscillations are possible in a non-isothermal CSTR in which two, exothermic, first order, irreversible reactions are taking place in parallel [3]. Mankin & Hudson showed that chaos can occur in a forced exothermic chemical reactor [4]. They also showed existence of chaos in two coupled non-isothermal CSTRs [5]. A tutorial review article on the research works regarding this topic up to 1988 is given by Doherty & Ottino [6]. An interesting variety of steady state behaviors are also observed in a non-isothermal CSTR [7]. Pellegrini & Biardi showed that using a PI controller in a CSTR can lead to chaos [8]. Perez *et. al* by changing parameters of the PI controller and cooling water flow rate in a CSTR could generate self oscillation and chaotic dynamics [9]. Peng *et al*. observed chaotic behavior in a closed three-variable autocatalator [10]. Lynch showed that dynamics of a parallel cubic autocatalator can lead to chaos as the input concentration ratio to the reactor increases [11]. It was also shown that chaos occurs in a mixed cubic and quadratic autocatalytic reaction [12]. Lynch proved that existence of chaotic behavior does not depend on presence of a reaction step involving cubic autocatalysis, and showed that chaotic behavior is preserved when the cubic step is replaced by successive bimolecular steps involving an intermediate [13]. An extended review regarding chaos and its applications in the process system engineering has been made by Lee & Chang [14]. Chaotic behavior is irregular, complex and generally undesirable. Therefore, within the research area of nonlinear dynamics, control of chaos has received increasing attention. Chaos control has been of broad interest since early 1990s. In 1990, Ott *et al.* showed that a chaotic attractor can be converted to one of a large number of possible attracting periodic motions by making only small time dependent perturbations in system parameters [15]. This method is applied to a prototype model for isothermal chemical chaos to stabilize unstable limit cycles out of chaotic behavior [16]. Bandyopadhyay *et al*. have successfully applied this approach to stabilize the dynamics of a chaotic non-isothermal CSTR [17].

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Another method was proposed by Pyragas in which a chaotic system can be stabilized by using proportional delayed feedback [18]. Chaotic dynamics of a set of coupled non-isothermal CSTRs is stabilized using this technique by Chen *et al.* [19]. This method has also been applied to the Belousov- Zhabotinsky (BZ) reaction to stabilize unstable periodic orbits embedded in the chaotic reactors [20]. Another approach for controlling a chaotic process is designing a model based controller. A controller based on internal model control has been designed by Bandyopdhyay *et al.* for a chaotic CSTR [21].

In this paper, it has been shown that a non-isothermal CSTR, in which two parallel autocatalytic reactions take place, may have chaotic behavior. The concentration control has been performed for this reactor through an optimal state feedback with integral action. Since implementation of the proposed controller requires system states, a nonlinear observer has been used for state estimation. The local asymptotic stability of the proposed control scheme including observer dynamics has been shown and its effectiveness has been demonstrated through simulation.

2. MATHEMATICAL FORMULATION OF THE PROBLEM

In this section we study the autocatalytic process in a continuous stirred tank reactor originally considered by Gray and Scott [1-2] and subsequently investigated by Lynch (1992). The system is capable of producing self-sustained oscillations based on cubic autocatalysis with catalyst decay and process mechanistically as follows.

$A + 2B \rightarrow 3B, r_A = ec_A c_B^{\,2}$

$B \rightarrow C, r_C = k_2 c_B$

$D + 2B \rightarrow 3B, r_D = k_3 c_D c_B^{\,2}$

Where $A, B, C \text{ and } D$ are the participating chemical species, k_1, k_2 and k_3 are the rate constants for the chemical reactions. This process is represented by the following set of ordinary differential equations.

$$\frac{dX}{dt} = 1 - X - aXZ^2 \tag{1}$$

$$\frac{dY}{dt} = 1 - Y - bYZ^2 \tag{2}$$

$$\frac{dZ}{dt} = 1 - (1+c)Z + daXZ^2 + ebYZ^2 \tag{3}$$

The initial conditions are

$$X(0) = 0, Y(0) = 0 \text{ and } Z(0) = 0. \tag{4}$$

Where X, Y and Z denote the dimensionless concentrations of species A, B and D While a, b and c denote the Damkohler numbers for A, B and D respectively. The ratio of feel concentrations of A to that of B is denoted by d and the same ratio of D to B by e. The process is chaotic, with a well-defined attractor for specific ranges of the two parameters, d and e. For the settings $a = 18000; b = 400; c = 80; d = 1.5;\ f = 4.2$.

3. SOLUTION OF THE INITIAL VALUE PROBLEM BY USING HOMOTOPY ANALYSIS METHOD (HAM)

Homotopy analysis method (HAM) is a non perturbative analytical method for obtaining series solutions to non-linear equations and has been successfully applied to numerous problems in science and engineering [22-33]. In comparison with other perturbative and non-perturbative analytical methods, HAM offers the ability to adjust and control the convergence of a solution via the so-called convergence-control parameter. Because of this, HAM has proved to be the most effective method for obtaining analytical solutions to highly nonlinear differential equations. Previous applications of HAM have mainly focused on non-linear differential equations in which the non-linearity is a polynomial in terms of the unknown function and its derivatives.

Liao [22-30] proposed a powerful analytical method for non-linear problems, namely the Homotopy analysis method. This method provides an analytical solution in terms of an infinite power series. However, there is a practical need to evaluate this solution and to obtain numerical values from the infinite power series. In order to investigate the accuracy of the Homotopy analysis method (HAM) solution with a finite number of terms, the system of differential equations were solved. The Homotopy analysis method is a good technique comparing to another perturbation method.

Homotopy perturbation method is a special case of Homotopy analysis method. Different from all reported perturbation and non-perturbative techniques, the Homotopy analysis method itself provides us with a convenient way to control and adjust the convergence region and rate of approximation series, when necessary. Briefly speaking, the Homotopy analysis method has the following advantages: It is valid even if a given non-linear problem does not contain any small/large parameter at all; it can be employed to efficiently approximate a non-linear problem by choosing different sets of base functions. The Homotopy analysis method contains the auxiliary parameter h, which provides us with a simple way to adjust and control the convergence region of solution series. Using this method, the approximate analytical solution of the eqns. (1)-(4) (see Appendix B) are as follows:

$$X = (1-e^{-t}) - h\left[\frac{a}{k^2}\left(1-\frac{3}{1-k}+\frac{3}{1-2k}-\frac{1}{1-3k}\right)e^{-t} - \frac{a}{k^2}\left(1-\frac{3e^{-kt}}{1-k}+\frac{3e^{-2kt}}{1-2k}-\frac{e^{-3kt}}{1-3k}\right)\right] \quad (5)$$

$$Y = (1-e^{-t}) - h\left[\frac{b}{k^2}\left(1-\frac{3}{1-k}+\frac{3}{1-2k}-\frac{1}{1-3k}\right)e^{-t} - \frac{b}{k^2}\left(1-\frac{3e^{-kt}}{1-k}+\frac{3e^{-2kt}}{1-2k}-\frac{e^{-3kt}}{1-3k}\right)\right] \quad (6)$$

$$Z = \frac{1}{k}(e^{-kt}-1) - h\left[\left(\frac{ad+be}{k^2}\left(1-\frac{3}{1-k}+\frac{3}{1-2k}-\frac{1}{1-3k}\right)e^{-kt} + \frac{ad+be}{k^2}\left(1-\frac{3e^{-kt}}{1-k}+\frac{3e^{-2kt}}{1-2k}-\frac{e^{-3kt}}{1-3k}\right)\right)\right] \quad (7)$$

4. NUMERICAL SIMULATION

In order to find the accuracy of our analytical method, the non-linear differential eqns. (1), (2) and (3) are also solved by numerical methods. The function bvp4c in Matlab/Scilab software which is a function of solving non-linear initial value problems for ordinary differential equations are used to solve these equations numerically. Our analytical results are compared with the numerical simulation and it gives a satisfactory agreement (See figures (1-5)). The Matlab/Scilab program is also given in Appendix D.

5. RESULTS AND DISCUSSIONS

Figure (1-5) represents the dimensional concentrations X, Y and Z versus the dimensional time t. From Fig.1, it is clear that when t increases the dimensionless concentrations also increases for some fixed values of a, b, c, d, e and $t = 0 - 0.001$. From Fig. 2, it is clear that when t increases the dimensionless concentrations also increases in some fixed values of a, b, c, d, e and $t = 0 - 0.005$. From Fig.3, it is clear that when t increases the dimensionless concentrations also increases in some fixed values of a, b, c, d, e and $t = 0 - 0.001$. From Fig.4, it is clear that when t increases the dimensionless concentrations also increases for some fixed values of a, b, c, d, e and $t = 0 - 0.005$. From Fig.5, it is clear that when t increases the dimensionless concentrations also increases in some fixed values of a, b, c, d, e and $t = 0 - 0.01$. All the above results are confirmed in Fig.(6-8).

6. CONCLUSION

The non-linear initial value problem for autocatalytic stirred tank reactor has been solved analytically and numerically. The approximate analytical expressions of the concentrations of the three species of autocatalytic stirred tank reactor have been solved analytically by using the Homotopy analysis method (HAM). The primary result of this work is simple and approximate expressions of the concentrations for all values of the dimensionless parameters a, b, c, d and e. This analytical result will be useful to analyse the behaviour of the concentrations of all the species. This method is an extremely simple and it is also a promising method to solve other non-linear equations.

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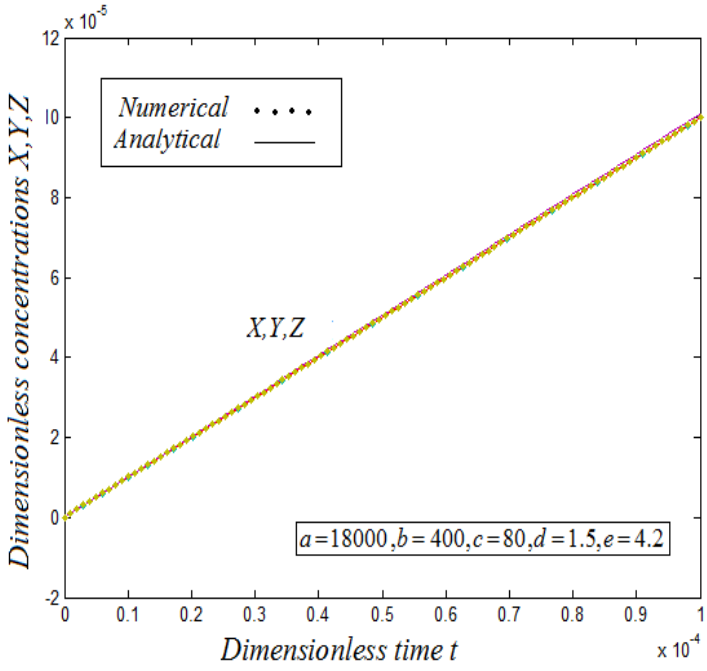

Fig.1: Dimensionless concentrations X, Y and Z versus the dimensionless time profile. The temperature profile were computed using the eqns.((1)-(3)) for some fixed values of the dimensionless parameters a, b, c, d, e when $h = -1$ for X and Y $h = -0.00563$ for Z and $t = 0.0001$.

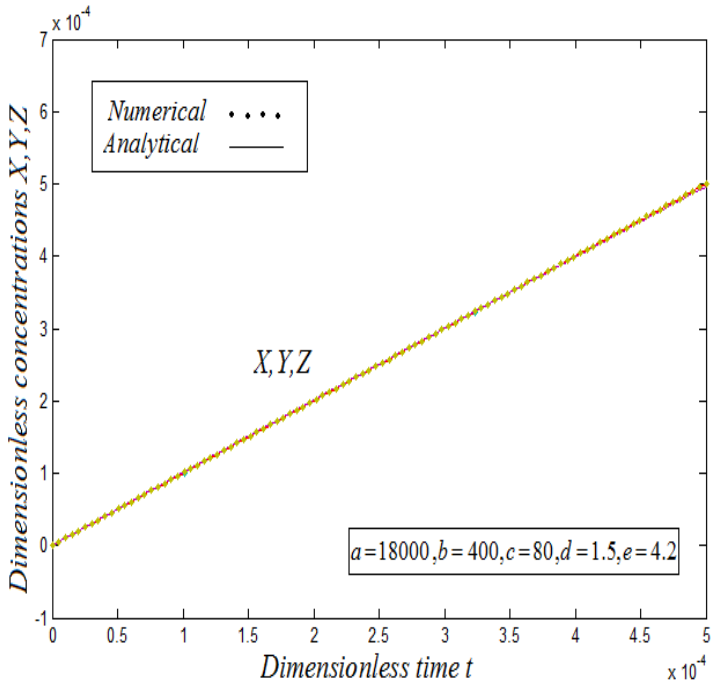

Fig.2: Dimensionless concentrations X, Y and Z versus the dimensionless time profile. The temperature profile were computed using the eqns. ((1)-(3)) for some fixed values of the dimensionless parameters a, b, c, d, e when $h = -1$ for X and Y $h = -0.00563$ for $t = 0.0005$.

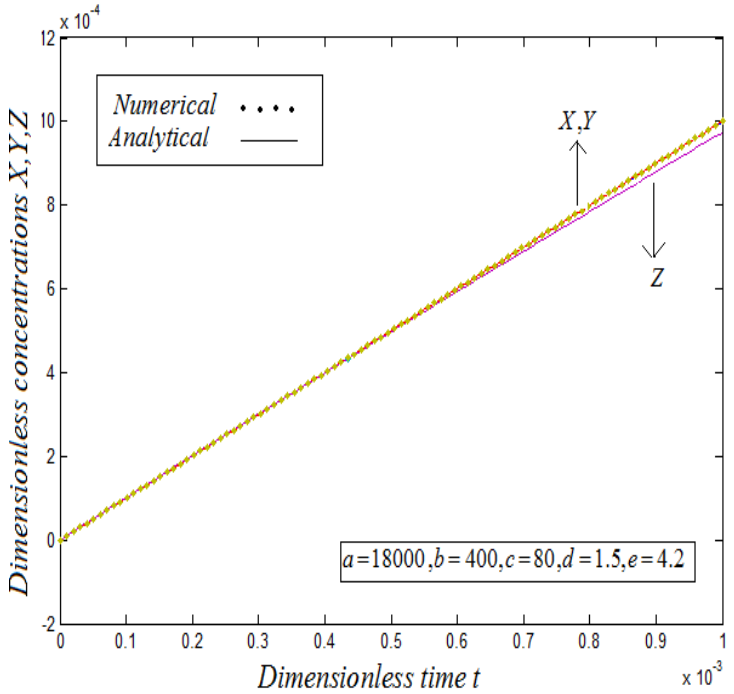

Fig.3: Dimensionless concentrations X, Y and Z versus the dimensionless time profile. The temperature profile were computed using the eqns. ((1)-(3)) for some fixed values of the dimensionless parameters a, b, c, d, e when $h = -1$ for X and Y and $h = -0.00563$ for Z and $t = 0.001$.

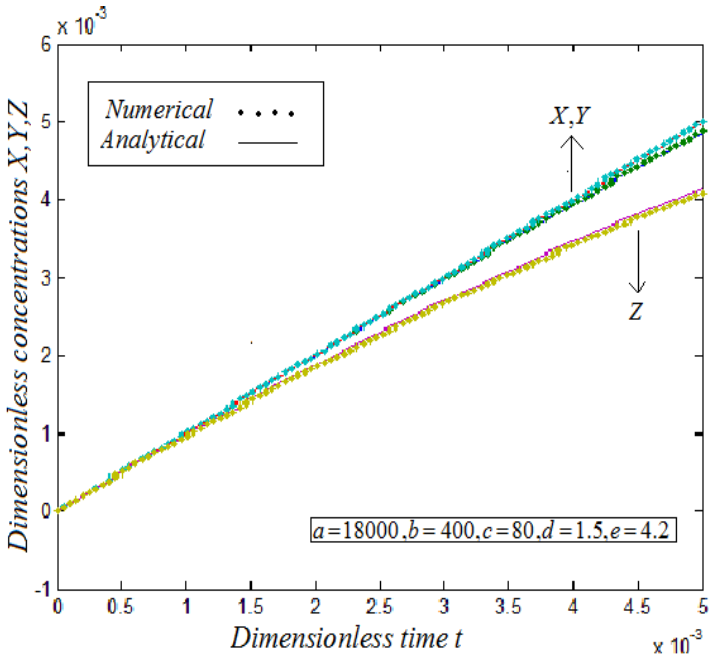

Fig.4: Dimensionless concentrations X, Y and Z versus the dimensionless time profile. The temperature profile were computed using the eqns. ((1)-(3)) for some fixed values of the dimensionless parameters a, b, c, d, e when $h = -1$ for X and Y and $h = -0.00563$ for Z and $t = 0.005$.

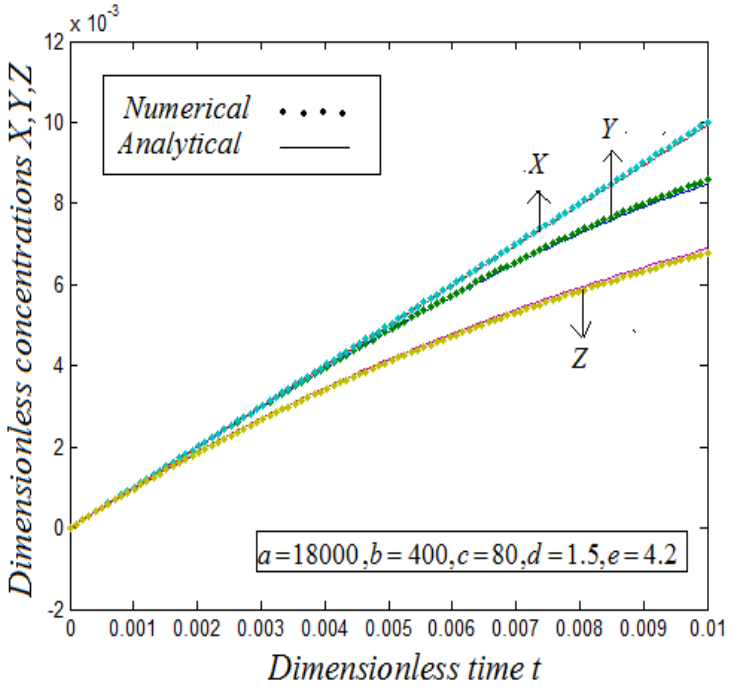

Fig.5: Dimensionless concentrations X, Y and Z versus the dimensionless time profile. The temperature profile were computed using the eqns. ((1)-(3)) for some fixed values of the dimensionless parameters a, b, c, d, e when $h = -1$ X and Y and $h = -0.00563$ for Z $t = 0.01$.

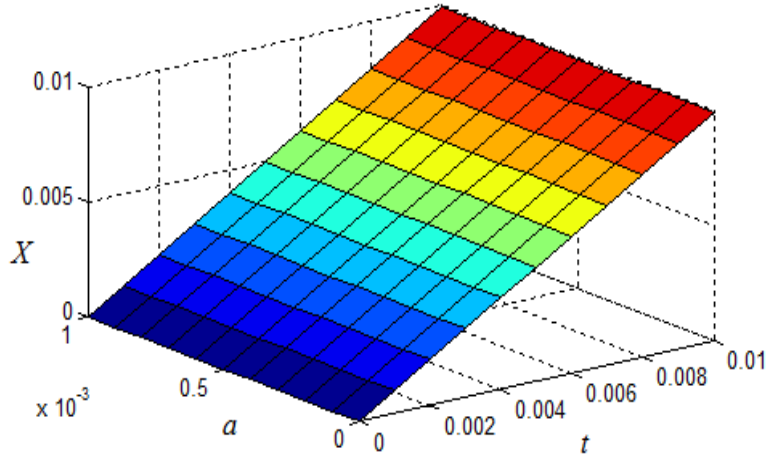

Fig.6: Plot of normalized three dimensional concentration X versus dimensionless time t for various values of a. The curve was computed using the eqn. (5).

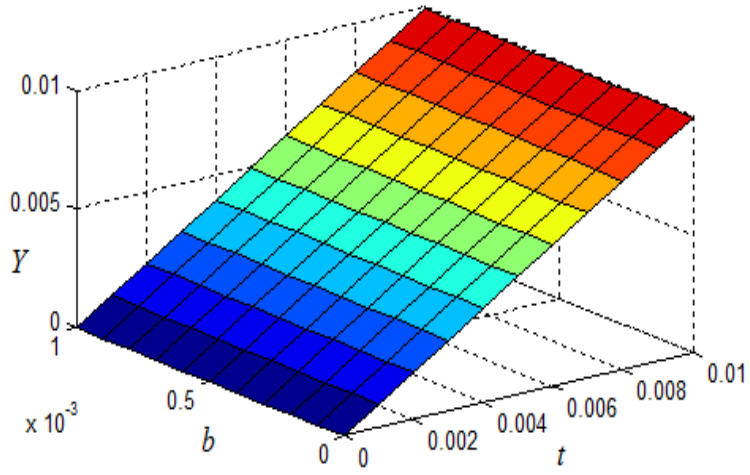

Fig.7: Plot of normalized three dimensional concentrations Y versus dimensionless time t for various values of b. The curve was computed using the eqn. (6).

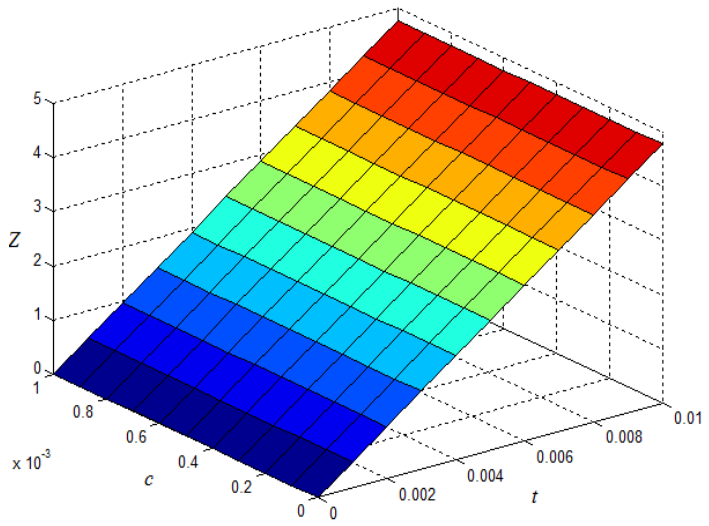

Fig.8: Plot of normalized three dimensional concentration Z versus the dimensionless time t for various values of c. The curve was computed using the eqn.(7).

APPENDIX: A

Basic concept of Homotopy analysis method

Consider the following differential equation [22-33]:

$$N[u(t)] = 0 \tag{A.1}$$

Where N is a nonlinear operator, t denotes an independent variable, $u(t)$ is an unknown function. For simplicity, we ignore all boundary or initial conditions, which can be treated in the similar way. By means of generalizing the conventional Homotopy method, Liao [22] constructed the so-called zero-order deformation equation as:

$$(1-p)L[\varphi(t;p) - u_0(t)] = phH(t)N[\varphi(t;p)] \tag{A.2}$$

where $p \in [0,1]$ is the embedding parameter, $h \neq 0$ is a nonzero auxiliary parameter, $H(t) \neq 0$ is an auxiliary function, L an auxiliary linear operator, $u_0(t)$ is an initial guess of $u(t)$, $\varphi(t:p)$ is an unknown function. It is important, that one has great freedom to choose auxiliary unknowns in HAM. Obviously, when $p = 0$ and $p = 1$, it holds:

$$\varphi(t;0) = u_0(t) \text{ and } \varphi(t;1) = u(t) \tag{A.3}$$

respectively. Thus, as p increases from 0 to 1, the solution $\varphi(t;p)$ varies from the initial guess $u_0(t)$ to the solution $u(t)$. Expanding $\varphi(t;p)$ in Taylor series with respect to p, we have:

$$\varphi(t;p) = u_0(t) + \sum_{m=1}^{+\infty} u_m(t)\, p^m \tag{A.4}$$

where

$$u_m(t) = \frac{1}{m!}\frac{\partial^m \varphi(t;p)}{\partial p^m}\Big|_{p=0} \tag{A.5}$$

If the auxiliary linear operator, the initial guess, the auxiliary parameter h, and the auxiliary function are so properly chosen, the series eqn.(A.4) converges at $p = 1$ then we have:

$$u(t) = u_0(t) + \sum_{m=1}^{+\infty} u_m(t)\,. \tag{A.6}$$

Differentiating the eqn. (A.2) for *m* times with respect to the embedding parameter p, and then setting $p = 0$ and finally dividing them by m!, we will have the so-called $m-th$ order deformation equation as:

$$L[u_m - \chi_m u_{m-1}] = hH(t)\Re_m(\vec{u}_{m-1}) \tag{A.7}$$

where

$$\Re_m(\vec{u}_{m-1}) = \frac{1}{(m-1)!}\frac{\partial^{m-1} N[\varphi(t;p)]}{\partial p^{m-1}} \tag{A.8}$$

and

$$\chi_m = \begin{cases} 0, & m \leq 1, \\ 1, & m > 1. \end{cases} \tag{A.9}$$

Applying L^{-1} on both side of the eqn. (A7), we get

$$u_m(t) = \chi_m u_{m-1}(t) + hL^{-1}[H(t)\Re_m(\vec{u}_{m-1})] \tag{A.10}$$

In this way, it is easily to obtain u_m for $m \geq 1$, at M^{th} order, we have

$$u(t) = \sum_{m=0}^{M} u_m(t) \tag{A.11}$$

When $M \to +\infty$, we get an accurate approximation of the original equation (A.1). For the convergence of the above method we refer the reader to Liao [22]. If equation (A.1) admits unique solution, then this method will produce the unique solution.

APPENDIX: B

Solution of the non-linear initial value problem (eqns. (1)-(4)) by using Homotopy analysis method.

In this Appendix, we indicate how the eqns. (5)-(7) are derived in this paper.

$$\frac{dX}{dt} = 1 - X - aZ^2 \tag{B.1}$$

$$\frac{dY}{dt} = 1 - Y - bYZ^2 \tag{B.2}$$

$$\frac{dZ}{dt} = 1 - (1+c)Z + daZ^2 + ebYZ^2 \tag{B.3}$$

We construct the Homotopy as follows:

$$(1-p)\left[\frac{dX}{dt} + X\right] = hp\left[\frac{dX}{dt} - 1 + X + aXZ^2\right] \tag{B.4}$$

$$(1-p)\left[\frac{dY}{dt} - 1 + Y\right] = hp\left[\frac{dY}{dt} - 1 + Y + bYZ^2\right] \tag{B.5}$$

$$(1-p)\left[\frac{dZ}{dt} - 1 + (1+c)Z\right] = hp\left[\frac{dZ}{dt} - 1 + (1+c)Z - adXZ^2 - ebYZ^2\right] \tag{B.6}$$

The approximate solution of the eqns. (B.2) is,

$$X = X_0 + pX_1 + p^2X_2 + \ldots\ldots\ldots \tag{B.7}$$

Similarly the approximate solutions of the eqns. (B.3) and (B.4) are as follows:

$$Y = Y_0 + pY_1 + p^2Y_2 + \ldots\ldots\ldots \tag{B.8}$$

$$Z = Z_0 + pZ_1 + p^2Z_2 + \ldots\ldots\ldots \tag{B.9}$$

The initial approximations are given by

$$X(0) = 0, Y(0) = 0 \text{ and } Z(0) = 0 \tag{B.10}$$

Substituting the eqns. (B.7), (B.8) and (B.9) in to the eqns. (B.4), (B.5) and (B.6) respectively we get

$$(1-p)\left[\frac{d(X_0 + pX_1 + p^2X_2 + \ldots\ldots)}{dt} + \left(X_0 + pX_1 + p^2X_2 + \ldots\ldots\ldots\right)\right]$$
$$= hp\left[\begin{array}{l}\dfrac{d}{dt}\left(X_0 + pX_1 + p^2X_2 + \ldots\ldots\ldots\right) - 1 + \left(X_0 + pX_1 + p^2X_2 + \ldots\ldots\ldots\right) \\ +aZ^2\left(X_0 + pX_1 + p^2X_2 + \ldots\ldots\ldots\right)\end{array}\right] \tag{B.11}$$

$$(1-p)\left[\frac{d(Y_0 + pY_1 + p^2Y_2 + \ldots\ldots)}{dt} - 1 + Y\right]$$
$$= hp\left[\begin{array}{l}\dfrac{d(Y_0 + pY_1 + p^2Y_2 + \ldots\ldots)}{dt} - 1 + (Y_0 + pY_1 + p^2Y_2 + \ldots\ldots) \\ +bZ^2(Y_0 + pY_1 + p^2Y_2 + \ldots\ldots)\end{array}\right] \tag{B.12}$$

$$(1-p)\left[\frac{d(Z_0+pZ_1+p^2Z_2+.....)}{dt}-1+(1+c)Z\right]$$
$$=hp\left[\begin{array}{l}\frac{d(Z_0+pZ_1+p^2Z_2+.....)}{dt}-1+(1+c)(Z_0+pZ_1+p^2Z_2+.....)\\+adX(Z_0+pZ_1+p^2Z_2+.....)^2+ebY(Z_0+pZ_1+p^2Z_2+.....)^2\end{array}\right] \quad (B.13)$$

Comparing the coefficients of like powers of p in the eqns. (B.11) – (B.13) we get

$$p^0:\frac{dX_0}{dt}-1+X_0=0 \quad (B.14)$$
$$p^1:\frac{dX_1}{dt}-(h+1)\frac{dX_0}{dt}-hX_0az^2=0 \quad (B.15)$$
$$p^0:\frac{dY_0}{dt}-1+Y_0=0 \quad (B.16)$$
$$p^1:\frac{dY_1}{dt}-(h+1)\frac{dY_0}{dt}-hY_0bz^2=0 \quad (B.17)$$
$$p^0:\frac{d^2Z_0}{dt^2}-1+(1+c)Z=0 \quad (B.18)$$
$$p^1:\frac{dZ_1}{dt}-(h+1)\frac{dZ_0}{dt}-hadZ^2-hebZ^2=0 \quad (B.19)$$

Solving the eqns. (B.15)-(B.20) and using the initial approximations the eqns. (B.10) and (B.11) we can obtain the following results.

$$X_0=(1-e^{-t}) \quad (B.21)$$
$$X_1=-h\left[\frac{a}{k^2}\left(1-\frac{3}{1-k}+\frac{3}{1-2k}-\frac{1}{1-3k}\right)e^{-t}-\frac{a}{k^2}\left(1-\frac{3e^{-kt}}{1-k}+\frac{3e^{-2kt}}{1-2k}-\frac{e^{-3kt}}{1-3k}\right)\right] \quad (B.22)$$
$$Y_0=1-e^{-t} \quad (B.23)$$
$$Y_1=-h\left[\frac{b}{k^2}\left(1-\frac{3}{1-k}+\frac{3}{1-2k}-\frac{1}{1-3k}\right)e^{-t}-\frac{b}{k^2}\left(1-\frac{3e^{-kt}}{1-k}+\frac{3e^{-2kt}}{1-2k}-\frac{e^{-3kt}}{1-3k}\right)\right] \quad (B.24)$$
$$Z_0=\frac{1}{k}(e^{-kt}-1) \quad (B.25)$$
$$Z_1=-h\left[\frac{ad+be}{k^2}\left(1-\frac{3}{1-k}+\frac{3}{1-2k}-\frac{1}{1-3k}\right)e^{-kt}+\frac{ad+be}{k^2}\left(1-\frac{3e^{-kt}}{1-k}+\frac{3e^{-2kt}}{1-2k}-\frac{e^{-3kt}}{1-3k}\right)\right] \quad (B.26)$$

According to the HAM, we can conclude that

$$X=\lim_{p\to 1}X(t)=X_0+X_1 \quad (B.27)$$
$$Y=\lim_{p\to 1}Y(t)=Y_0+Y_1 \quad (B.28)$$
$$Z=\lim_{p\to 1}Z(t)=Z_0+Z_1 \quad (B.29)$$

After putting (B.21), (B.22) in (B.27), (B.23), (B.24) in (B.28), (B.25), (B.26) in (B.29) we obtain the solution in the text (the eqns. (5)-(7)).

APPENDIX: D

Matlab/Scilab Program to find the numerical solution of non-linear equations (1)-(4)

```
function
options= odeset('RelTol',1e-6,'Stats','on');
%initial conditions
x0 = [0; 0; 0];
tspan = [0,0.0001];
tic
[t,x] = ode45(@TestFunction,tspan,x0,options);
toc
figure
hold on
plot(t, x(:,1))
plot(t, x(:,2))
plot(t,x(:,3))
legend('x1','x2','x3')
ylabel('x')
xlabel('t')
return
function [dx_dt]= TestFunction(t,x)
a=18000;b=400;c=80;d=1.5;e=4.2;
dx_dt(1)=1-x(1)-a*x(1)*x(3)^2;
dx_dt(2)=1-x(2)-b*x(2)*x(3)^2;
dx_dt(3)=1-(1+c)*x(3)+d*a*x(1)*x(3)^2+e*b*x(2)*x(3)^2;
dx_dt = dx_dt';
return
```

APPENDIX : E
Nomenclature

Symbol	Meaning
t	Dimensionless time
A	Participating chemical species
B	Participating chemical species
C	Participating chemical species
D	Participating chemical species
a	Damkohler number for the spice A
b	Damkohler number for the spice B
c	Damkohler number for the spice C
d	Dimensionless parameter
e	Dimensionless parameter
X	Dimensionless concentrations
Y	Dimensionless concentrations
Z	Dimensionless concentrations
k_1	Rate constants for the chemical reactions
k_2	Rate constants for the chemical reactions
k_3	Rate constants for the chemical reactions

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